Domain Decomposition Methods for Uncertainty Quantification

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in partial fulfillment of the requirements for the degree

Doctor of Philosophy

by

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Abstract

In conjunction with modern high performance computing platforms, domain decomposition methods permit computational simulations of physical and engineering systems using extremely high resolution numerical models. Such numerical models substantially reduce discretization error. In realistic simulations of numerous physical and engineering systems, it is however necessary to quantify confidence in numerical simulations for their acceptability as reliable alternatives to field experiments. The spectral stochastic finite element method is a popular computational tool for uncertainty quantification in many engineering systems of practical interest. For large-scale engineering systems, the spectral stochastic finite element method becomes computationally challenging as the size of the resulting algebraic linear system grows rapidly with the spatial mesh resolution and the order of the stochastic dimension. To address this issue, domain decomposition methods are described for uncertainty quantification of large-scale engineering systems. The mathematical framework is based on non-overlapping domain decomposition in the geometric space and functional expansion along the stochastic dimension. For numerical illustrations, two-dimensional and three-dimensional flow through porous media and elasticity problems with spatially varying non-Gaussian material properties are considered. The parallel performance of the algorithms are investigated with respect to the mesh size, subdomain size, fixed problem size per subdomain, level of uncertainty and the order of stochastic dimen-

sion. For a fixed mesh resolution, the probabilistic domain decomposition techniques cannot reduce the total solution time beyond a certain number of processors due to hardware related issues such as latency and bandwidth of the communication network. To fully exploit the massively parallel computers, parallelization is exploited in temporal dimension for uncertain dynamical systems. In particular, a probabilistic version of a parallel time integration scheme is developed to simulate the trajectories of a noisy non-linear dynamical system described by stochastic differential equations. The numerical experiments are performed on a Linux cluster using MPI and PETSc parallel libraries.

Dedicated to the living memory of my beloved Mother.

“Finding a good preconditioner to solve a given sparse linear system is often viewed as a combination of art and science.”

Yousef Saad, *Iterative methods for sparse linear systems*, 2003.

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List of Acronyms

PDEs Partial Differential Equations

SPDEs Stochastic Partial Differential Equations

SSFEM Spectral Stochastic Finite Element Method

MC Monte Carlo

PCGM Preconditioned Conjugate Gradient Method

MINRES Minimal Residual Method

KLE Karhunen-Loeve Expansion

PCE Polynomial Chaos Expansion

gPCE generalized Polynomial Chaos Expansion

DDM Domain Decomposition Method

L Lumped preconditioner

WL Wighted Lumped preconditioner

NN Neumann-Neumann preconditioner

NNC Neumann-Neumann with a Coarse problem

PP-DDM Primal-Primal Domain Decomposition Method

DP-DDM Dual-Primal Domain Decomposition Method

BDDM Balancing Domain Decomposition Method

BDDC Balancing Domain Decomposition by Constraints

FETI Finite Element Tearing and Interconnecting

FETI-DP Dual-Primal Finite Element Tearing and Interconnecting

PETSc Portable, Extensible Toolkit for Scientific Computation

MPI Message Passing Interface

SRBM Stochastic Reduced Basis Method

Chapter 1

Introduction

1.1 Background

High resolution numerical models can offer a cost-effective alternative to expensive physical experiments [1–3]. Aided by high performance computing platforms, parallel numerical algorithms such as domain decomposition methods permit numerical simulations with substantial model resolution and thereby significantly reduce the discretization error [4–7]. In modeling numerous practical engineering systems, the random heterogeneity of the model parameters can adversely affect the numerical prediction [1, 3, 8–10]. For realistic simulation, it is therefore necessary to quantify uncertainty in the numerical simulations to assess the confidence in the computer predictions [3, 9–11].

Uncertainty quantification involves investigating the discrepancy between a physical phenomenon and its computational simulations [12]. Uncertainty quantification methods aim to characterize such discrepancies in order to provide a confidence bound on the numer-

ical predictions [3, 13–17]. To this end, the probability theory offers a rich mathematical framework to represent uncertainty in terms of random variables and stochastic processes, provided sufficient information is available to statistically characterize the physical properties of the random medium [1, 9, 11]. Within the probabilistic framework, uncertainty propagation may be construed to be identifying the dependency of the solution process on the random variables and stochastic processes used to characterize uncertainty in the system parameters [3].

The probabilistic methods for uncertainty quantification in engineering can be broadly classified into sampling and non-sampling based approaches [2, 3, 9, 17, 18]. The choice of a specific methodology for the analysis and the selection of a particular numerical solution strategy depends on the nature of uncertainty and complexity of the problem [1, 2, 9].

Monte Carlo (MC) simulation is a robust and straightforward method for uncertainty propagation through the system [3, 17, 19]. MC method involves repeatedly generating independent realizations of the uncertain system parameters based on their prescribed probability distributions [3, 8]. For each of these realizations, the deterministic model is used in a black box fashion to generate the corresponding output. Statistical analysis on the ensemble of solution process (constructed from the realizations) is conducted to extract the desired statistical properties of the solution process. The rate of convergence of the MC method is independent of the number of the uncertain system parameters [3, 17]. The slow convergence rate of MC method however, is the main limitation of this sampling technique [3, 17]. MC method is an embarrassingly parallel algorithm. In practice however,

MC simulation may become impractical for high resolution models where a single deterministic computation requires high computational effort [20, 21].

Alternative to MC sampling technique is the perturbation method. In the perturbation method, the solution process and the stochastic operator are expanded about their respective mean values using Taylor series [9, 11, 17, 22]. Taylor series expansion in the perturbation method is limited to small coefficient of variation [9, 23]. The perturbation method is often used to evaluate the first two moments of the solution process as for higher order moments the resulting expansion becomes difficult to handle in general [9, 23]. For high level of uncertainty, more terms in Taylor series are required. While increasing the order of the expansion, *secular terms* (terms growing without bound) appear in the higher-order expansion [11]. These terms lead to divergence of the series expansion [11].

Another non-sampling method is the Neumann series expansion. In this approach, the inversion of the stochastic stiffness matrix is approximated using Neumann series [8, 11, 22]. The advantage of the Neumann series expansion approach is that only a deterministic matrix needs to be inverted once [9, 20]. Similar to the perturbation method, the Neumann expansion is often limited to problems with a small magnitude of uncertainty [8, 17, 20].

Due to the high computational cost of MC simulation and the limitations of the perturbation and Neumann series expansion approaches, significant attention has been focused on the Spectral Stochastic Finite Element Method (SSFEM) [2, 11, 24]. The SSFEM has been applied successfully to a wide variety of problems including structural mechanics [25–28],

computational fluid dynamics [3, 16, 29, 30], transport in porous medium [25, 31], fluid-structure interactions [32], chemistry [33, 34] biomedical engineering [35] and acoustic scattering [36].

In the context of SSFEM, randomness in the system is treated as an additional dimension to the problem [37] with an associated Hilbert space of real-valued second order random variables [3, 19, 38]. The solution process is represented by a functional expansion along the new dimension and the coefficients of the expansion are determined either through Galerkin (intrusive) or pseudo-spectral (non-intrusive) projection [30].

In the intrusive approach [1, 2, 11, 24, 39, 40], Galerkin projection onto the space spanned by orthogonal polynomial basis transforms the original stochastic problem into a coupled set of deterministic problems [41]. The solution of this coupled deterministic system provides the expansion coefficients of the solution process. In the non-intrusive approach [15, 42], the expansion coefficients of the solution process are obtained through orthogonal projection on a selected set of prescribed basis functions. The inner product in the orthogonal projection (defined as a statistical average) is evaluated numerically using random sampling, quadrature rule or sparse grid techniques [3, 13, 30, 42].

Stochastic collocation method is another non-intrusive technique [8, 43]. In the context of the stochastic collocation method, the solution process is approximated by Lagrange interpolation polynomials. The basis of the polynomials is constructed using a set of prescribed structured collocation points (defined by a tensor product or sparse grid) and the coefficients of the polynomial are the solution at the collocation points [13, 43, 44].

The implementations of the non-intrusive (collocation and pseudo-spectral) methods involve repeatedly solving deterministic problems corresponding to the collocation points or realizations of the random variables used to represent the system parameters [3, 44, 45]. The advantage of the non-intrusive approach lies in its ability to reuse existing deterministic legacy codes. To achieve the same level of accuracy, the non-intrusive methods may require solutions of considerably larger number of equations than the size of the linear systems arising from Galerkin projection in the intrusive approach [44, 45]. In the Galerkin projection approach, the error due to the finite representation is minimum leading to optimal accuracy [13, 17]. On the contrary, there is no explicit control of the error in the collocation methods except at the collocation points where the error is zero. Therefore the accuracy of the solution depends on the selection of the collocation points [3, 17, 30, 46].

The stochastic reduced basis methods (SRBMs) [47–49] is an efficient tool to reduce the computational complexity of the intrusive SSFEM approach. In the SRBMs, the solution process is represented as a linear combination of a set of basis vectors from the preconditioned stochastic Krylov subspace [47–49]. Galerkin projection scheme is employed to obtain a reduced order deterministic set of equations for the expansion coefficients [47–49]. The order of the resulting set of equations in the SRBMs is much less than that in the standard intrusive SSFEM. In contrast to the standard intrusive SSFEM approach in which the basis functions of the solution process are Hermite polynomials, the stochastic basis vectors are problem dependent in the SRBMs [28]. At much lower computational complexity, the accuracy of the first two statistical moments of the solution processes obtained from the

SRBMs is comparable to those from the standard intrusive SSFEM [47–49]. The SRBMs rely on the preconditioned stochastic Krylov subspace to construct a reduced order expansion for the solution process. Efficient and scalable preconditioners therefore, could be beneficial in further reducing the computational complexity of the SRBMs for large-scale problems with many random variables.

1.2 Statement of the Problem

The computational cost of the SSFEM primarily depends on the size of the finite element mesh, the dimension and order of the orthogonal polynomial used in the expansion of the random system parameters and the solution process [37, 38]. The Galerkin projection in the SSFEM leads to a set of deterministic linear systems with a block matrix structure, coupling all the coefficients of the solution process [3, 37, 50]. The size of the resulting linear systems grows rapidly with the spatial mesh resolution and the order of the stochastic dimension [37, 38]. The solution of these systems of linear equations poses significant computational challenge and therefore efficient solvers are required [3, 14, 51]. To this end, the development of robust and efficient numerical solution strategies is of paramount importance for the applicability of the SSFEM for large-scale practical (industrially relevant) problems [28]. These numerical algorithms must be parallel and scalable in order to fully take advantage of the advances of high performance computing platforms.

Iterative numerical methods based on Krylov subspace, carefully designed for the SSFEM problem, may provide a suitable solution technique [3, 50]. The reuse of the existing iterative solvers developed for deterministic problem can be a feasible strategy [3]. However, the reliability and robustness of the iterative methods mainly depend on the preconditioning techniques [52]. Thus preconditioners, suitably customized for the SSFEM problem are needed to improve the performance of the ensuing linear solver [3, 51].

Previous work in the literature has been devoted to formulating robust and efficient iterative solution techniques to tackle the resulting linear systems arising in the context of the stochastic Galerkin projection based SSFEM, namely the intrusive SSFEM. However, the solution of the coupled set of deterministic systems in the SSFEM remains to be a major computational challenge for uncertainty quantification of large-scale systems. In general, the previous attempts to solve the linear systems for the SSFEM can be categorized into preconditioned iterative solvers [27, 37, 50, 53, 54] and multigrid methods [51, 55, 56].

For a symmetric positive definite system, the iterative solvers reported in the literature are Preconditioned Conjugate Gradient Method (PCGM) [27, 37, 50, 54] and block Gauss-Jacobi method [53]. The global stochastic stiffness matrix, arising from stochastic Galerkin projection is block-diagonally dominant (for small magnitude of fluctuations around the mean material properties), this fact motivates the use of block-Jacobi preconditioner to accelerate the rate of convergence of the iterative solvers [3, 37, 50]. Each diagonal block of the preconditioning matrix is constructed based on a factorization of the mean matrix. This type of preconditioner is termed as a *mean-based preconditioner*. Different

deterministic techniques are proposed in the literature to factorize each building blocks of the preconditioning matrix in a black-box fashion. Indeed, Incomplete LU factorization [37, 53, 57], sparse inverse [50], algebraic multigrid [21, 57], domain decomposition method [27] and the existing deterministic parallel solver [54, 58] are used to solve each diagonal blocks of the block-Jacobi preconditioning matrix. Although the block-Jacobi preconditioner demonstrates an improvement of the convergence rate of the iterative solver compared to the traditional Jacobi preconditioner, the performance of the block-Jacobi preconditioner is sensitive to the level of uncertainty in the system parameters [50, 53, 57]. In addition, the convergence rate of the preconditioner may deteriorate when the system parameters are non-Gaussian in nature that leads to large contribution from the off-diagonal blocks to the SSFEM stiffness matrix [37, 57].

Multigrid methods are the second type of iterative solvers used in the literature to tackle the linear system of stochastic Galerkin projection [51, 55, 56]. The multigrid solver demonstrates a convergence rate that is independent of the size of the spatial discretization and the order of the stochastic dimension. However, the performance of the multigrid solver is substantially dependent on the level of the coefficient of variation of the system parameters [51]. Furthermore, some of the multigrid parameters may need to be carefully selected to gain the optimal convergence rate [51].

Domain decomposition methods have become major computational tools for parallel computing of large-scale numerical models of partial differential equations (PDEs) [4, 6, 7, 52, 59]. Domain decomposition algorithms can achieve the highest level of paralleliza-

tion in the context of the numerical solution of PDEs [52, 60–62]. Domain decomposition algorithms are particularly useful in developing efficient preconditioners to accelerate the convergence rate of the iterative solvers [52, 63–67].

To this end, a theoretical framework for domain decomposition method of uncertain systems defined by SPDEs is presented in [68]. The methodology is based on Schur complement based domain decomposition in the physical space and functional decomposition in the stochastic dimension [68]. This approach can take advantage of the well-developed parallel algorithms devised for deterministic systems [68]. A direct substructuring technique is implemented. The serial implementation of the algorithm demonstrates the effectiveness of the methodology in reducing the total execution time [69].

1.3 Research Objective and Scope

The main objective of this study is to develop the next generation uncertainty quantification algorithms which efficiently exploit the modern supercomputers in order to enable high fidelity simulations with new capability to quantify uncertainty in the prediction of computational mechanistic models. The investigation is directed towards devising efficient parallel and scalable computational algorithms to quantify and propagate uncertainty in large-scale engineering systems using high performance computing platforms.

The SSFEM is a popular computational tool for uncertainty quantification in numerous engineering problems of practical interest. For large-scale engineering systems, the

application of SSFEM becomes computationally challenging as the size of the resulting algebraic linear system grows rapidly with the spatial mesh resolution and the order of the stochastic dimension. To address this issue, a non-overlapping domain decomposition approach (namely a *substructuring* method) of SPDEs is introduced in [68] in the framework of SSFEM. A dense direct solver is used to tackle the *extended* Schur complement system (the interface problem).

For large-scale problems, the solution of the extended Schur complement system using direct solvers becomes impractical due to overwhelming memory requirements and poor scalability to large number of processors [52]. In order to tackle the interface problem of the stochastic system using iterative substructuring technique, a parallel PCGM equipped with a parallel extended lumped preconditioner is adopted [70]. The iterative algorithm circumvents the need to construct both the local and global extended Schur complement matrices explicitly. Despite being superior to the direct solver (in terms of memory requirement and floating point operations), the PCGM based iterative solver equipped with the lumped preconditioner exhibits performance degradation as the number of subdomains increases and therefore scalable preconditioner is needed to enhance the performance of the algorithm [70].

As already demonstrated for the deterministic PDEs, the Neumann-Neumann preconditioner achieves a convergence rate that is independent of the spatial mesh size and exhibits a good scalability for a moderate number of subdomains [4, 5, 7, 71, 72]. The Neumann-Neumann preconditioner approximates the inverse of the global Schur complement matrix

by a weighted sum of the inverse of the local Schur complement matrices. This approximation is rational since the global Schur complement matrix is the sum of the local Schur complement matrices [73]. The Neumann-Neumann method paves the way for constructing two-level preconditioners. These facts motivate the development of Neumann-Neumann preconditioner in the context of stochastic PDEs [74, 75].

The PCGM equipped with the one-level Neumann-Neumann preconditioner exhibits a convergence rate that is almost insensitive to the level of uncertainty in the system parameters [74, 75]. As no mechanism for global information exchange exists in the one-level Neumann-Neumann preconditioner, its performance deteriorates for relatively large number of subdomains. For scalability, the global communication is required to propagate information across the subdomains [4–7].

To this end, a two-level domain decomposition method is reported to tackle the large-scale linear system within the framework of the intrusive SSFEM [76, 77]. The implementation of the algorithm involves solving a local problem on each subdomain that constructs the local part of the preconditioner [7] and a coarse problem that propagates information globally among the subdomains. This information exchange achieved by the coarse problem makes the preconditioner scalable. This method bears similarity with a version of the Balancing Domain Decomposition by Constraints (BDDC) for deterministic PDEs [66, 78].

A primal-primal iterative substructuring technique is introduced to solve the large-scale linear system arising from the finite element discretization of SPDEs [79, 80]. The mathe-

mathematical framework naturally leads to a coarse problem connecting the subdomains globally and provides a mechanism to propagate information across the subdomains. The global spread of information in the primal-primal preconditioner leads to a scalable performance. In an abstract sense, the primal-primal preconditioner may be viewed as another extension of BDDC for SPDEs.

For deterministic PDEs, BDDC and dual-primal finite element tearing and interconnect FETI-DP [64, 81] are perhaps the most popular non-overlapping domain decomposition techniques for the iterative solution of large-scale deterministic linear systems [82]. It has already been demonstrated that the condition number and thus the parallel performance of BDDC and FETI-DP are quite similar [65, 67, 78, 83–85]. It is therefore natural to ask whether the similarity of BDDC and FETI-DP extends to stochastic systems

To address this question, we formulate a probabilistic version of the FETI-DP iterative substructuring technique for the intrusive SSFEM [79, 80, 86]. In the probabilistic setting, the operator of the dual interface system in the dual-primal approach contains a coarse problem. The introduction of the coarse problem [65] leads to a scalable performance of the dual-primal iterative substructuring method for uncertainty quantification of large-scale computational models.

The parallel performances of the aforementioned algorithms are studied for two- and three-dimensional stochastic PDEs with spatially varying non-Gaussian random coefficients. For efficient memory usage and minimum floating point operations, the numerical

implementation of the algorithms exploit the multi-level sparsity structure of the coefficient matrix of the stochastic system, namely (a) the sparsity structure due to the finite element discretization and (b) the block sparsity structure arising from the orthogonal representation and projection of the stochastic processes. PETSc [87] and MPI [88] parallel libraries are used for efficient parallel implementation of the algorithms. The graph partitioning tool METIS [89] is used for optimal decomposition of the finite element mesh.

For a fixed mesh resolution, domain decomposition algorithms cannot reduce the total execution time beyond a critical number of subdomains/processors as the interprocessor communication overhead and memory bandwidth requirement predominate over floating point operations. In order to exploit the remaining idle processors in multi-processor computers, the recent research initiatives have been directed towards achieving time domain parallelism (e.g., [90, 91]). To this end, we adapt the so-called *parareal* algorithm for ordinary differential equations (ODEs) to simulate the trajectories (sample paths) of a noisy non-linear dynamical system described by stochastic differential equations (SDEs). To assess the performance of the parallel algorithm, a numerical investigation is conducted to simulate the sample path of a Duffing oscillator driven by combined deterministic and random inputs. The parareal scheme may also be applied for efficient simulation of SPDEs in conjunction with the probabilistic domain decomposition methods developed in this thesis.

1.4 Organization of the Thesis

An introduction to the probabilistic methods for uncertainty quantification, the motivation for the research and the thesis statement are presented in Chapter 1. The SSFEM formulation and a brief literature review on the solution strategies to tackle the associated linear systems of equations are provided in Chapter 2. In Chapter 3, a review of domain decomposition methods for the deterministic systems is provided. In addition, a novel primal-primal iterative substructuring algorithm equipped with a two-level scalable preconditioner is introduced. Iterative substructuring technique for the numerical solution of stochastic systems is described in Chapter 4. The mathematical framework and parallel implementations of one-level domain decomposition preconditioners for the stochastic systems are provided in Chapter 5. In Chapter 6, a two-level domain decomposition method is reported to tackle the large-scale linear system within the framework of the intrusive SSFEM. Chapter 7 provides the mathematical framework of the primal-primal iterative substructuring technique for the solution of the large-scale linear system in the SSFEM. In Chapter 8, we report a probabilistic version of the dual-primal domain decomposition method for the intrusive SSFEM. Numerical illustrations to the mathematical formulation is presented in Chapter 9 for two-dimensional problems. Chapter 10 provides numerical experiments for three-dimensional problems. In Chapter 11, the development of the probabilistic parallel time integration scheme is provided. In Chapter 12, the main conclusions of the thesis and some suggestions for future research direction are summarized. Some relevant mathematical details are reviewed in the Appendices.

Chapter 2

Finite Element Method for Stochastic PDEs

2.1 Introduction

In modeling numerous engineering and physical systems, it is necessary to consider the random heterogeneity of the model parameters for more realistic computer simulation [3, 8, 11, 92]. When sufficient statistical information is available, probability theory offers a rich mathematical framework to represent uncertainty in terms of random variables and stochastic processes(e.g. [8, 11, 68, 92]).

We assume that the input data (containing sufficient statistical information) permit a representation of the model parameters as stochastic processes that span a function space [3, 11, 68–70, 74, 76, 79, 80]. Using Karhunen-Loeve expansion (KLE), a set of basis func-

tions can be identified to characterize this space [3, 11, 68, 69]. The KLE of a stochastic process is based on the spectral decomposition of its covariance function [3, 11, 68, 69]. When the covariance function of a stochastic process, for example the solution process, is not known *a priori*, KLE cannot be used to represent the process [3, 11, 68, 69]. For stochastic processes with *a priori* unknown covariance function, a set of basis functions in the space of second-order random variables can be used to approximate the processes [3, 11, 68, 69]. The solution process is a function of the system parameters and nodal solution variables, therefore it can be represented as some nonlinear functional of the basis of the KLE used to expressed uncertainty in the system parameters [3, 11, 68, 69]. It has been shown that this functional dependence can be expanded in terms of polynomials in Gaussian random variables, namely the Polynomial Chaos Expansion (PCE) [11, 93]. The expansion coefficients of the solution process can be evaluated either through Galerkin (intrusive) or pseudo-spectral (non-intrusive) projection [30].

In the intrusive approach [1, 2, 11, 24, 39, 40], Galerkin projection on the space spanned by the PC basis is performed to minimize the error of the truncated PCE. The resulting coupled set of equations is solved to obtain the expansion coefficients of the solution process. In the non-intrusive approach [15, 42], the orthogonality of the PC basis is employed to evaluate the expansion coefficients of the solution process [3, 13, 30, 42]. The inner product in the orthogonal projection (defined as a statistical average) involves a multidimensional integral. This integral is evaluated numerically using random sampling, quadrature rule or sparse grid approaches [3, 13, 30].

In this chapter, uncertainty representation using random variables and processes is described. In addition, the intrusive and non-intrusive SSFEM formulation is outlined. A brief literature review is provided on the solution strategies to tackle the linear systems of equations arising in the context of the intrusive SSFEM.

2.2 Uncertainty Representation by Stochastic Processes

2.2.1 Karhunen-Loeve Expansion

The KLE of a stochastic process $\alpha(\mathbf{x}, \theta)$ is based on the spectral expansion of its covariance function $C_{\alpha\alpha}(\mathbf{x}_1, \mathbf{x}_2)$ as [3, 11]

$$\alpha(\mathbf{x}, \theta) = \alpha(\mathbf{x}) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \phi_i(\mathbf{x}) \xi_i(\theta), \quad (2.1)$$

where $\alpha(\mathbf{x})$ is the mean function of the stochastic process, $\{\xi_i(\theta)\}$ is a set of uncorrelated random variables, and λ_i are the eigenvalues and $\phi_i(\mathbf{x})$ are the eigenfunctions of the covariance kernel $C_{\alpha\alpha}(\mathbf{x}_1, \mathbf{x}_2)$ [94]. The eigenvalues and eigenfunctions can be obtained as the solution to the following integral equation [3, 11, 17]

$$\int_D C_{\alpha\alpha}(\mathbf{x}_1, \mathbf{x}_2) \phi_i(\mathbf{x}_1) d\mathbf{x}_1 = \lambda_i \phi_i(\mathbf{x}_2). \quad (2.2)$$

When the marginal probability density function (pdf) of the process is Gaussian, the uncorrelated random variables in KLE are Gaussian and hence they are independent random variables [11, 37]. The KLE is an optimal representation of a stochastic process in the

mean-square sense [3, 11]. For a smooth stochastic process, only a finite number of KLE terms is sufficient to represent the process [3, 11, 17].

2.2.2 Polynomial Chaos Expansion

As mentioned previously, the KLE is based on the spectral expansion of the covariance function and therefore, KLE cannot be used to represent a stochastic process with *a priori* unknown covariance function [11, 37, 95]. In this case, the PCE is used to expand a stochastic process as a sum of its projections on an appropriate basis defined on the space of second-order random variables as [11, 24, 95]

$$\alpha(\mathbf{x}, \theta) = \sum_{i=0}^{\infty} \alpha_i(\mathbf{x}) \Psi_i(\boldsymbol{\xi}), \quad (2.3)$$

where $\alpha_i(\mathbf{x})$ are the PC coefficients and $\Psi_i(\boldsymbol{\xi})$ is a set of multi-dimensional orthogonal Hermite polynomials (with zero mean) in the sense that their inner product $\langle \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) \rangle$ defined as the statistical average of their product, is equal to zero for $i \neq j$, as

$$\langle \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) \rangle = \int \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad (2.4)$$

$$= \delta_{ij} \langle \Psi_i^2(\boldsymbol{\xi}) \rangle, \quad (2.5)$$

where $p(\cdot)$ is the probability density function of $\boldsymbol{\xi}$ and δ_{ij} is the Kronecker delta.

For numerical implementation, the infinite PCE series in Eq.(2.3) is truncated in both the order p of the polynomial chaoses and the dimension of the stochastic space n , resulting a finite PC representation as

$$\omega(\mathbf{x}, \theta) = \sum_{i=0}^N \omega_i(\mathbf{x}) \Psi_i(\xi_1, \xi_2, \dots, \xi_n), \quad (2.6)$$

where N is the number of the terms used in PCE given as

$$N + 1 = \frac{(n + p)!}{n!p!}. \quad (2.7)$$

The truncated PCE series in Eq.(2.6) converges in the mean square sense [11, 96]. The PCE series can be refined by increasing the size of the stochastic dimension (adding more random variables to the set $\{\xi\}$) to capture higher frequency random fluctuation of the underlying stochastic process [96, 97], or by increasing the order of the polynomials in PC series (adding more random function $\Psi_i(\xi)$) to capture strong nonlinear dependence of the solution process on the underlying random variables [96, 97].

2.3 Spectral Stochastic Finite Element Method

Consider a linear elliptic stochastic PDE defined on a domain Ω with a given data on the boundary $\partial\Omega$. The finite element discretization in the spatial domain leads to the following stochastic linear system [3, 11, 17]

$$\mathbf{A}(\theta)\mathbf{u}(\theta) = \mathbf{f}, \quad (2.8)$$

where $\mathbf{A}(\theta)$ is the stiffness matrix with random coefficients, $\mathbf{u}(\theta)$ is the stochastic process representing the response vector and $\mathbf{f}$ is the applied force.

For general non-Gaussian material properties, the PCE can be used to represent uncertainty in the model parameters as [98]

$$\mathbf{A}(\theta) = \sum_{i=0}^L \Psi_i \mathbf{A}_i. \quad (2.9)$$

The solution process can be expanded using the same PC basis as

$$\mathbf{u}(\theta) = \sum_{j=0}^N \Psi_j \mathbf{u}_j. \quad (2.10)$$

Galerkin projection or pseudo-spectral (*discrete projection*) approach can be used to evaluate the PC coefficients $\mathbf{u}_j$ in Eq.(2.10) as delineated next.

2.3.1 Galerkin (Intrusive) Approach

In the intrusive approach, Galerkin projection onto a PC basis Ψ_i is performed to ensure that the error resulting from a finite representation is orthogonal to the space spanned by $\{\Psi_i\}$ [37]. Substituting Eq.(2.9) and Eq.(2.10) into Eq.(2.8) and performing Galerkin projection, the following coupled deterministic systems of equations is obtained

$$\sum_{j=0}^N \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_i \mathbf{u}_j = \langle \Psi_k \mathbf{f} \rangle, \quad k = 0, 1, \dots, N \quad (2.11)$$

Equivalently, Eq.(2.11) can be rewritten as

$$\mathcal{A}\mathcal{U} = \mathcal{F}, \quad (2.12)$$

where

$$\mathcal{A}_{j,k} = \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_i, \quad \mathcal{U} = (\mathbf{u}_0, \dots, \mathbf{u}_N)^T \quad \text{and} \quad \mathcal{F}_k = \langle \Psi_k \mathbf{f} \rangle. \quad (2.13)$$

Eq.(2.12) can be expressed as

$$\begin{bmatrix} \mathcal{A}_{0,0} & \mathcal{A}_{0,1} & \dots & \mathcal{A}_{0,N} \\ \mathcal{A}_{1,0} & \mathcal{A}_{1,1} & \dots & \mathcal{A}_{1,N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{A}_{N,0} & \mathcal{A}_{N,1} & \dots & \mathcal{A}_{N,N} \end{bmatrix} \begin{bmatrix} \mathbf{u}_0 \\ \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_N \end{bmatrix} = \begin{bmatrix} \mathcal{F}_0 \\ \mathcal{F}_1 \\ \vdots \\ \mathcal{F}_N \end{bmatrix}. \quad (2.14)$$

2.3.2 Pseudo-Spectral (Non-Intrusive) Approach

In the non-intrusive approach, the orthogonality property of the PC basis defined in Eq.(2.4) is employed to obtain the PC coefficients of the solution process. Consequently, projection the solution process $\mathbf{u}(\theta)$ given by Eq.(2.10) onto PC basis Ψ_k , leads to

$$\langle \mathbf{u}(\theta) \Psi_k \rangle = \sum_{j=0}^N \langle \Psi_j \Psi_k \rangle \mathbf{u}_j, \quad k = 0, 1, \dots, N. \quad (2.15)$$

Using Eq.(2.4), PC coefficients of the solution process can be evaluated from Eq.(2.15) as

$$\mathbf{u}_j = \frac{\langle \mathbf{u}(\theta) \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int \mathbf{u}(\xi) \Psi_j(\xi) p(\xi) d\xi. \quad (2.16)$$

The integral in Eq.(2.16) is evaluated numerically using random sampling, quadrature rule or sparse grid technique [3, 13, 30]. This integral can be viewed as the correlation between the response process $\mathbf{u}(\xi)$ and the PC basis $\Psi(\xi)$ [3].

2.3.3 Intrusive Versus Non-Intrusive

The implementation of the non-intrusive method involves repeatedly solving deterministic problems that correspond to prescribed values of the system parameters. This approach

can readily exploit existing deterministic solvers [3, 44, 45]. To achieve the same level of accuracy, however, the non-intrusive method requires solution of much larger number of equations than the size of the linear system arising from Galerkin projection in the intrusive SSFEM [44, 45]. In the non-intrusive approach, the error due to the integration rules can cause significant aliasing [17]. In the Galerkin (intrusive) approach, the error due to finite representation is minimum (orthogonal to the space spanned by PC basis) leading to an optimal accuracy of the solution [17, 45]. For large-scale problems (where a single deterministic run is computationally demanding), Galerkin projection approach may be preferred provided efficient solvers can be developed [17, 45].

2.4 Solution Methods for the SSFEM

The Galerkin projection in the SSFEM leads to a coupled systems of linear equations with a block sparsity structure [3, 37, 50]. The solution of this systems of linear equations constitutes a computationally challenging task and therefore efficient solvers are required [3, 51]. A brief literature review on the solution strategies to tackle the linear systems of the SSFEM is provided in the next section.

2.4.1 Literature Review

Ghanem and Kruger (1996) [37] proposed Preconditioned Conjugate Gradient Method (PCGM) equipped with a block-Jacobi preconditioner to solve the linear system arising in the context of SSFEM. Each building block of the preconditioning matrix is based on an incomplete LU factorization of the stiffness matrix [99] corresponding to the mean material

properties as

$$\mathcal{M}^{-1}\mathcal{AU} = \mathcal{M}^{-1}\mathcal{F}, \quad (2.17)$$

where

$$\mathcal{M}^{-1} = \begin{bmatrix} \mathcal{M}_{1,1}^{-1} & 0 & \dots & 0 \\ 0 & \mathcal{M}_{2,2}^{-1} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mathcal{M}_{N,N}^{-1} \end{bmatrix}, \quad (2.18)$$

and

$$\mathcal{M}_{j,j}^{-1} = \langle \xi_0 \Psi_j \Psi_j \rangle ILU(\mathbf{A}_0). \quad (2.19)$$

Due to the block structure of the preconditioning matrix, the operation on each diagonal block can be performed independently. The block-Jacobi preconditioner demonstrated an improvement in the performance of the PCGM compared to the traditional Jacobi preconditioner. For moderate uncertainty and Gaussian material properties, the performance of the block-Jacobi preconditioner is shown to be nearly independent of the level of randomness in the system parameters. Nevertheless, the number of iterations required by the iterative solver to converge grows as the order of the PCE increases.

Pellisetti and Ghanem (2000) [50] applied PCGM equipped with a block-Jacobi preconditioner to solve the linear system arising from the SSFEM. The block-Jacobi preconditioner has the same structure as in Eq.(2.18). However, each individual block is an approximate inverse of the mean stiffness matrix as

$$\mathcal{M}_{j,j}^{-1} = \langle \xi_0 \Psi_j \Psi_j \rangle \mathbf{A}_0^{-1}. \quad (2.20)$$

The inversion of the mean stiffness matrix is evaluated approximately to preserve a prescribed sparsity structure. For a small problem size and Gaussian material properties, the PCGM solver equipped with the block-Jacobi preconditioner showed good performance compared to the classical CGM solver. However, even for a small value of the coefficient of variation of the system parameters, the convergence rate of the block-Jacobi preconditioner deteriorates as the order of PCE increases. On the other hand, finding a good approximate inverse for the mean stiffness matrix is computationally expensive and the cost increases rapidly as the size of the matrix grows.

Maitre et al. (2003) [51] adapted a geometric multigrid method to solve the linear system arising from the stochastic Galerkin projection. A simple V-cycle algorithm is implemented. The multigrid solver showed a convergence rate that is nearly independent of the mesh size. Furthermore, the convergence rate of the multigrid solver does not degenerate as the number of random variables in KLE increases. On the other hand, the convergence rate of the multigrid method decays slightly as the order of the PCE increases. The performance of the multigrid solver is substantially dependent on the level of the coefficient of variation of the system parameters. The structure of the multilevel iteration cycle and some of the multigrid parameters (such as the number of iterations on each grid) need to be carefully selected to gain the optimal convergence rate.

Keese and Matthies (2005) [54, 58] used a hierarchical parallelization approach on a

distributed memory machine to solve the linear system of SSFEM. A coarse-grained parallelization is implemented by constructing each block of the stochastic stiffness matrix. A fine level parallelization is implemented within each individual block. The fine level of parallelization exploits the available deterministic parallel libraries to compute the matrix-vector multiplication and the preconditioner effect. Instead of computing the inverse of each block in the block-Jacobi preconditioner in Eq.(2.18), a system of the following form is solved

$$\mathbf{A}_0 \mathbf{z} = \mathbf{r}. \quad (2.21)$$

The mean stiffness matrix $\mathbf{A}_0$ is a deterministic and thus any existing deterministic parallel solver can be used to tackle it in a black-box fashion. In this hierarchical parallelization approach, the time required to compute the preconditioner effect is inversely proportional to the number of processors.

Chung et. al. (2005) [53] used a block Gauss-Jacobi iterative method equipped with an incomplete block-Jacobi preconditioner defined in Eq.(2.18) to solve the linear system of SSFEM. An element-by-element strategy is proposed to evaluate the matrix-vector product required by the iterative solver. The element-by-element approach only requires the storage of the element stochastic stiffness matrix which is less expensive in terms of memory requirements than that of the full stochastic stiffness matrix. After each multiplication step, the resulting vector however needs to be assembled which consumes a large computation time. Increasing the number of random variables in KLE and the order of PCE do not significantly affect the performance of the block Gauss-Jacobi solver. As the coefficient of

variation of the system parameters increases, the iteration counts grow.

Chao et. al. (2007) [100] used a recycling Krylov subspace method equipped with a *black-box* additive Schwarz domain decomposition preconditioner to solve the SSFEM linear systems. Double orthogonal basis are used to decouple the probabilistic space resulting a sequence of uncoupled systems of linear equations. The recycling technique is used to reduce the computational cost of solving a sequence of related linear systems with multiple right hand sides. Some difficulties arose in using the recycling Krylov subspace method as the linear stochastic systems are not exactly the same. Therefore, a grouping algorithm is proposed to collect the closely related linear systems in subsets and then tackle them using the recycling Krylov subspace method. The recycling technique efficiently reduces the total execution time. The additive Schwarz preconditioner achieves a scalable performance with respect to mesh size and number of subdomains. The double orthogonal basis is a special case and cannot be applied to the general type of uncertainty.

Elman and Furnival (2007) [55] applied geometric multigrid method to solve the linear system in SSFEM. A two-grid correlation scheme based on the spatial discretization is implemented. The convergence rate of the multigrid solver is shown to be independent of the spatial mesh size and the order of the stochastic dimension.

Rosseel et al. (2008) [56] used algebraic multigrid method to solve the linear system arising in the context of SSFEM. The mean stiffness matrix is used to build the hierarchy of meshes for multigrid method. For a Gaussian and non-Gaussian material properties, the

number of multigrid iterations is shown to be independent of the geometric mesh size. The convergence rate of the multigrid solver is shown to be asymptotically independent of the order of PCE in case of material properties with uniform probability density (pdf) but not in case of Gaussian pdf.

Powell and Elman (2009) [21, 57] provided a theoretical basis for the block-Jacobi preconditioner in Eq.(2.18) and established a bound for the condition number. The theoretical results show that, the condition number is independent of the spatial mesh size, but depends on the COV of the system parameters, and additionally, on the order of PCE if unbounded random variables are used. An incomplete Cholesky factorization of the mean stiffness matrix and a black-box algebraic multigrid method are used to implement the block-Jacobi preconditioner. The performance of the algebraic multigrid scheme is independent of the size of the spatial discretization.

Ghosh et al. (2009) [27] used PCGM equipped with the block-Jacobi preconditioner in Eq.(2.18) to solve the linear system in the context of SSFEM. The FETI-DP domain decomposition method is used to compute the preconditioned residual $\mathbf{z}$ in Eq.(2.21). In particular, the FETI-DP solver is used to tackle the linear systems of the following form

$$\frac{1}{\langle \Psi_j^2 \rangle} \mathbf{A}_0 \mathbf{z} = \mathbf{r}. \quad (2.22)$$

The overall iterative scheme consists of two nested PCGM solvers. An outer solver is used to tackle the full stochastic linear system, while an inner solver is used to tackle each individual block of the preconditioner. A recycling Krylov subspace method is utilized to

speed-up the convergence rate of the inner solver. The multiple right-hand sides version of FETI-DP solver helped in reducing the computational cost of the block-Jacobi preconditioner. The iterative scheme demonstrated good scalability with respect to the size of the problem and number of subdomains. It is again worth emphasizing that the FETI-DP method is only used to solve the blocks of the block-Jacobi preconditioner for the global stochastic system.

Sarkar et al. (2009) [68] presented a theoretical framework for the domain decomposition method of uncertain systems defined by SPDEs. The methodology based on Schur complement based domain decomposition in the physical space and functional decomposition in the stochastic dimension. This approach gives the ability to exploit the deterministic domain decomposition algorithms in the context of stochastic PDEs. For numerical validation of the methodology, a direct substructuring technique is implemented to solve a steady state wave propagation problem in one-dimensional random media. A dense direct solver is used to tackle the stochastic Schur complement system.

Ullmann (2010) [101] introduced a Kronecker product preconditioner to improve the performance of the iterative solver for the linear system in SSFEM. The preconditioner exploits the block sparsity structure of the stochastic stiffness matrix. The Kronecker product preconditioner enhances the performance of the PCGM compared to the mean-based preconditioner [101]. Increasing the level of uncertainty in the system parameters and the order of the stochastic expansion leads to a moderate increase in the iteration counts of the PCGM [101]. Unlike the block-Jacobi preconditioner, the Kronecker product precon-

ditioner is not a block-diagonal matrix and therefore it is not an embarrassingly parallel preconditioner.

2.5 Summary

In the SSFEM, uncertainty in the system is treated as an additional dimension to the problem whereby a suitable basis functions is used to discretize the stochastic dimension [37]. The PCE is used to represent the solution process. Using the PC basis, a Galerkin projection is performed to minimize the error of the truncated PCE that leads to a set of coupled deterministic linear system. The solution of this coupled linear system provides the PC coefficients of the solution process. The solution of this large-scale linear system associated with SSFEM constitutes a computationally challenging task and therefore efficient solvers are required.

In general, an iterative solver is used to tackle the linear system in SSFEM. The fact that the full stochastic linear system consists of block submatrices and is diagonally dominant *motivates* the use of block-Jacobi preconditioner to accelerate the convergence rate of the iterative method. Each building block of the preconditioner is constructed based on a factorization of the mean stiffness matrix. Different deterministic techniques are proposed in the literature to solve each diagonal block of the preconditioner in a black-box fashion such as incomplete LU factorization [37, 53, 57], sparse inverse [50], algebraic multigrid [56, 57], domain decomposition method [27], or use of existing deterministic parallel solver [54, 58]. Due to the block diagonal structure of the block-Jacobi preconditioner

tioner, its application requires repeated solution of a linear system with different right hand side which can be performed concurrently. However, the performance of the block-Jacobi preconditioner appears to be sensitive to the level of uncertainty of the system parameters [50, 53, 57]. Furthermore, the convergence rate of the preconditioner may deteriorate when the system parameters are non-Gaussian in nature [37, 57].

2.6 Discussion

The preconditioning technique is the essential ingredient in enhancing the reliability, robustness and performance of the iterative methods used to tackle the linear system arising in SSFEM. The combination of a scalable parallel preconditioner and the CGM solver makes the iterative method well-suited to tackle the SSFEM linear system using high performance computing platforms. The block-Jacobi preconditioner and its generalization (additive Schwarz domain decomposition method) are one-level preconditioning techniques and thus their performance deteriorate as the number of subdomains increases leading to poor scalability [6, 52, 102]. This performance degradation can be attributed to the fact that the information is exchanged only among the neighboring subdomains in one-level preconditioners. There is no mechanism for global communication in the one-level preconditioners [103]. For large-scale stochastic systems, a two-level preconditioner consisting of local (fine) and global (coarse) components is required to make the convergence rate of the iterative solver (nearly) independent of the number of the subdomains.

Chapter 3

Domain Decomposition Methods for Deterministic PDEs

3.1 Introduction

This chapter closely follows the references [4–7]. Domain decomposition methods are generally used to partition a large computational domain into a number of subdomains whereby a smaller problem on each subdomain can be solved independently and concurrently [4–7, 104, 105]. In multi-physics problems, domain decomposition may arise naturally from partitioning the physical system into subregions based on phenomenological considerations, and the physics on each subregion is modeled using a suitable partial differential equation [6]. In parallel computing, domain decomposition method is defined as the process of dividing a data set into a smaller groups that can be distributed among the processors in a distributed memory architecture computers [6]. From algebraic point of view, domain

decomposition method can be described as a parallel algorithm for solving the large-scale linear system arising from the discretization of partial differential equations [6]. In this context, the large-scale linear system is subdivided into a smaller subsystems whose solutions can be used to produce a scalable preconditioner for the original system [106]. Domain decomposition preconditioners whose computational work grows linearly or log-linearly with the number of subdomains are said to be scalable preconditioners [4, 5, 7]. Most of the current interest in domain decomposition algorithms lies in developing scalable parallel preconditioners [4, 64, 107, 108]. Domain decomposition methods have been applied successfully to a wide variety of problems [109] including structural mechanics [64, 65, 81, 110], computational fluid dynamics [60, 111, 112], acoustic scattering [113] and biomechanics [61].

Domain decomposition methods are broadly categorized into overlapping methods (Schwarz methods) and non-overlapping or substructuring methods (Schur complement methods) [4–7, 72]. In Schwarz methods, the solution domain is decomposed into a number of overlapping subdomains and a smaller problem is solved alternately on each subdomain with an appropriate approximate solution on the artificial boundary [4–7]. The solution on the artificial boundary is updated by propagating the solution of the subdomain problem to the boundary [4–7]. The solution converges when the change in the successive solutions on the artificial boundary is less than a prescribed tolerance value [4–7]. Schwarz methods can be viewed as a generalizations of block Jacobi and block Gauss-Seidel iterative methods [4, 5, 114]. The alternating Schwarz method can be used as a preconditioner for Krylov subspace iterative methods, whereby each application of the pre-

conditioner is one iteration of the alternating Schwarz method with zero initial guess [5, 6]. In Schur complement methods, the solution domain is partitioned into a number of non-overlapping subdomains [4–7, 72, 115]. On each subdomain, for example, the finite element stiffness matrix and the load vector are assembled independently, and the degrees of freedom on each subdomains are split into interior and interface variables. Block Gaussian elimination is performed to reduce the global system to the Schur complement system [4–7, 72]. The solution of the Schur complement system gives the interface variables. The interior variables are obtained by solving the interior problem on each subdomain concurrently [63, 78]. Depending on the solution method used to solve the Schur complement system, non-overlapping domain decomposition techniques are referred to as a direct substructuring or iterative substructuring method [6, 7].

The most popular and widely used Schur complement based iterative substructuring techniques can be divided into the primal and the dual methods [65, 110]. In the primal iterative substructuring methods, the continuity condition along the interfaces boundaries are enforced strongly by global assembly [65, 78, 83]. The primal methods contain Neumann-Neumann [71], Balancing Domain Decomposition (BDD) [116, 117], and Balancing Domain Decomposition by Constraints (BDDC) [107, 108]. In the dual iterative substructuring methods the continuity condition along the interfaces boundaries are enforced weakly by Lagrange multipliers [61, 65, 78, 118]. The Finite Element Tearing and Interconnecting (FETI) [119, 120] and the Dual-Primal Finite Element Tearing and Interconnecting (FETI-DP) [64, 81] belong to this class of domain decomposition method.

In this chapter, we review the overlapping and non-overlapping domain decomposition methods. Specifically, we first describe the alternating Schwarz method and represent it as a preconditioner. Next, we describe the well-known primal, dual and dual-primal iterative substructuring techniques. In addition, we present a novel primal-primal iterative substructuring algorithm equipped with a two-level scalable preconditioner.

3.2 Overlapping Domain Decomposition Methods

The Schwarz method is the earliest domain decomposition method [4, 5, 121] which was published in 1890. In the classical Schwarz method, a Laplace equation defined on an irregular domain is solved iteratively on a union of regular subdomains that forms the irregular original domain such as rectangular and circular subdomains [7] (see Fig.(3.1) and Fig.(3.2)).

The Schwarz alternating method is based on splitting the computational domain into a number of overlapping subdomains. The algorithm starts with a suitable initial guess for the solution and precedes by constructing a sequence of improved approximations [72]. The approximate solutions are obtained by alternately solving a local Dirichlet problem with an inhomogeneous boundary condition on the artificial boundary. When the most recent available solution from the adjacent subdomain is used to approximate the artificial boundary condition, the procedure is known as multiplicative Schwarz method which can be viewed as a generalization of the block Gauss-Seidel iteration method [4–6]. The multiplicative Schwarz method is serial algorithm in nature because it requires the solution of one sub-

domain problem prior to another [5, 7]. On the other hand, when the previous solution is used to approximate the artificial boundary condition, the procedure is known as additive Schwarz method which corresponds to a generalized block Jacobi method [5, 6, 72]. The additive Schwarz method is embarrassingly parallel algorithm because there is no dependency between the concurrent approximate solution of the subdomains problems. However, the convergence rate of the additive Schwarz method is slower than that of the multiplicative Schwarz method [4–7]. In practice, the additive Schwarz method is typically employed as a parallel preconditioner to accelerate the convergence rate of Krylov subspace methods [7].

3.2.1 The Alternating Schwarz Method

Consider a linear second-order elliptic partial differential equation (PDE) defined on a domain Ω with a given Dirichlet boundary condition on $\partial\Omega$ as shown in Fig.(3.1). The finite element discretization of the PDE leads to the following sparse symmetric positive definite linear system

$$\mathbf{A}\mathbf{u} = \mathbf{f}, \quad (3.1)$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$ is the stiffness matrix, $\mathbf{u} \in \mathbb{R}^n$ is the response, and $\mathbf{f} \in \mathbb{R}^n$ is the force vector.

Figure 3.1: A typical domain

Let the spatial domain Ω be partitioned into two overlapping subdomains as shown in Fig.(3.2) and such that

$$\Omega = \Omega_1 \cup \Omega_2, \quad \Omega_1 \cap \Omega_2 \neq \emptyset, \quad \text{and} \quad \Gamma = \Gamma_1 \cup \Gamma_2, \quad (3.2)$$

where Γ represents the artificial boundary between the two overlapped subdomains.

Figure 3.2: A typical domain partitioned into two overlapping subdomains

For a typical subdomain Ω_s , the solution vector $\mathbf{u}^s$ can be split as

$$\mathbf{u}^s = \begin{Bmatrix} \mathbf{u}_I^s \\ \mathbf{u}_\Gamma^s \end{Bmatrix}, \quad (3.3)$$

where $\mathbf{u}_I^s$ is the interior solution vector corresponding to the nodes in the interior of the subdomain Ω_s and $\mathbf{u}_\Gamma^s$ is the interface solution vector corresponding to the nodes on the artificial boundary Γ_s . Consequently, the equilibrium equation for a typical subdomain Ω_s can be expressed in the following block form

$$\begin{bmatrix} \mathbf{A}_I^s & \mathbf{A}_\Gamma^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s \\ \mathbf{u}_\Gamma^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \end{Bmatrix}, \quad (3.4)$$

where $\mathbf{A}_I^s \in \mathbb{R}^{n_I^s \times n_I^s}$ represents the stiffness submatrix associated with the nodes in the interior of the subdomain and $\mathbf{A}_\Gamma^s \in \mathbb{R}^{n_I^s \times n_\Gamma^s}$ denotes the stiffness submatrix corresponding to the interaction among the interior and the artificial boundary nodes.

Let $\mathcal{I}_{I_r \rightarrow \Gamma_s}$ be a discrete operator which interpolates the solution of the interior nodes of subdomain Ω_r to the nodes on the artificial boundary Γ_s of the subdomain Ω_s as

$$\mathbf{u}_\Gamma^s = \mathcal{I}_{I_r \rightarrow \Gamma_s} \mathbf{u}_I^r. \quad (3.5)$$

The alternating Schwarz method starts with an initial guess for the solution in one of the subdomains, let us say the second subdomain Ω_2 , as

$$(\mathbf{u}_I^2)^{k-1} = (\mathbf{u}_I^2)^0, \quad (3.6)$$

where k denotes the iteration count.

Next, the solution from the second subdomain Ω_2 is interpolated to the artificial interface boundary of the first subdomain Γ_1 as

$$(\mathbf{u}_I^1)^k = \mathcal{I}_{I_2 \rightarrow \Gamma_1}(\mathbf{u}_I^2)^{k-1}. \quad (3.7)$$

A local Dirichlet problem with non-homogeneous boundary condition is solved next on the first subdomain Ω_1 as

$$\mathbf{A}_I^1(\mathbf{u}_I^1)^k = \mathbf{f}_I^1 - \mathbf{A}_I^1(\mathbf{u}_I^1)^k. \quad (3.8)$$

The current available solution from the first subdomain Ω_1 is propagated to the artificial interface boundary of the second subdomain Γ_2 as

$$(\mathbf{u}_I^2)^k = \mathcal{I}_{I_1 \rightarrow \Gamma_2}(\mathbf{u}_I^1)^k. \quad (3.9)$$

A second subdomain level Dirichlet problem with non-homogeneous boundary condition is solved next on the second subdomain Ω_2 as

$$\mathbf{A}_I^2(\mathbf{u}_I^2)^k = \mathbf{f}_I^2 - \mathbf{A}_I^2(\mathbf{u}_I^2)^k \quad (3.10)$$

The iteration continues until convergence. Different stopping criteria can be used to determine the convergence of the alternating Schwarz algorithm, such as the difference in the current and the previous interior solution of both the subdomains is less than a tolerance prescribed value ϵ_{I_s} as

$$\frac{\|(\mathbf{u}_I^1)^k - (\mathbf{u}_I^1)^{k-1}\|}{\|(\mathbf{u}_I^1)^{k-1}\|} \leq \epsilon_{I_1} \quad \text{and} \quad \frac{\|(\mathbf{u}_I^2)^k - (\mathbf{u}_I^2)^{k-1}\|}{\|(\mathbf{u}_I^2)^{k-1}\|} \leq \epsilon_{I_2}. \quad (3.11)$$

Clearly, the basic Schwarz alternating algorithm to solve Eq.(3.1) starts with an initial guess for the solution on one subdomain and then iteratively constructs a sequence of improved approximate solutions by alternately solving the subdomains problems [4, 5].

The alternating Schwarz method can be outlined in the following algorithm [4–7]:

Algorithm 1: Alternating Schwarz Procedure	
<hr/>	
input	: initial guess $\{(\mathbf{u}_I^2)^0\}$
1	for $k = 1, 2, \dots$, until convergence :
2	do
3	compute : $(\mathbf{u}_I^1)^k = \mathcal{I}_{I_2 \rightarrow I_1}(\mathbf{u}_I^2)^{k-1}$
4	compute : $(\tilde{\mathbf{f}}_I^1)^k = \mathbf{f}_I^1 - \mathbf{A}_I^1(\mathbf{u}_I^1)^k$
5	solve : $\mathbf{A}_I^1(\mathbf{u}_I^1)^k = (\tilde{\mathbf{f}}_I^1)^k$
6	followed by:
7	compute : $(\mathbf{u}_I^2)^k = \mathcal{I}_{I_1 \rightarrow I_2}(\mathbf{u}_I^1)^k$
8	compute : $(\tilde{\mathbf{f}}_I^2)^k = \mathbf{f}_I^2 - \mathbf{A}_I^2(\mathbf{u}_I^2)^k$
9	solve : $\mathbf{A}_I^2(\mathbf{u}_I^2)^k = (\tilde{\mathbf{f}}_I^2)^k$
	output : $(\mathbf{u}_I^1, \mathbf{u}_I^2)$

Note that the most current available value of the solution in Ω_1 is used to generate the values for the inhomogeneous boundary condition on the artificial interface for the solution in Ω_2 . This dependency of the second problem on the first problem makes the basic Schwarz algorithm serial in natural when applied to the case of two subdomains [6, 72].

However, this coupling is useful to exchange information between the adjacent subdomains, and as a result improves the convergence rate of the Schwarz method.

3.2.2 Schwarz Method as a Two-Steps Algorithm

The alternating Schwarz algorithm can be summarized in the following form [6]

$$\mathbf{A}_I^1(\mathbf{u}_I^1)^k = \mathbf{f}_I^1 - \mathbf{A}_I^1 \mathcal{I}_{I_2 \rightarrow I_1}(\mathbf{u}_I^2)^{k-1}, \quad (3.12)$$

$$\mathbf{A}_I^2(\mathbf{u}_I^2)^k = \mathbf{f}_I^2 - \mathbf{A}_I^2 \mathcal{I}_{I_1 \rightarrow I_2}(\mathbf{u}_I^1)^k. \quad (3.13)$$

Adding and subtracting $\mathbf{A}_I^s(\mathbf{u}_I^s)^{k-1}$, $s = 1, 2$ from Eq.(3.12) and Eq.(3.13), the alternating Schwarz algorithm can be expressed as a two-step algorithm as

$$(\mathbf{u}_I^1)^k = (\mathbf{u}_I^1)^{k-1} + [\mathbf{A}_I^1]^{-1}(\mathbf{f}_I^1 - \mathbf{A}_I^1(\mathbf{u}_I^1)^{k-1} - \mathbf{A}_I^1 \mathcal{I}_{I_2 \rightarrow I_1}(\mathbf{u}_I^2)^{k-1}), \quad (3.14)$$

$$(\mathbf{u}_I^2)^k = (\mathbf{u}_I^2)^{k-1} + [\mathbf{A}_I^2]^{-1}(\mathbf{f}_I^2 - \mathbf{A}_I^2(\mathbf{u}_I^2)^{k-1} - \mathbf{A}_I^2 \mathcal{I}_{I_1 \rightarrow I_2}(\mathbf{u}_I^1)^k). \quad (3.15)$$

In case of matching grids, the interpolation operator becomes an identity matrix and two-steps Schwarz scheme reduces into the following form

$$(\mathbf{u}_I^1)^k = (\mathbf{u}_I^1)^{k-1} + [\mathbf{A}_I^1]^{-1}(\mathbf{f}_I^1 - \mathbf{A}_I^1(\mathbf{u}_I^1)^{k-1} - \mathbf{A}_I^1(\mathbf{u}_I^2)^{k-1}), \quad (3.16)$$

$$(\mathbf{u}_I^2)^k = (\mathbf{u}_I^2)^{k-1} + [\mathbf{A}_I^2]^{-1}(\mathbf{f}_I^2 - \mathbf{A}_I^2(\mathbf{u}_I^2)^{k-1} - \mathbf{A}_I^2(\mathbf{u}_I^1)^k). \quad (3.17)$$

The scheme in Eq.(3.16) and Eq.(3.17) can be viewed as a generalized block Gauss-Seidel scheme to solve the following system [6, 72]

$$\begin{bmatrix} \mathbf{A}_I^1 & \mathbf{A}_I^1 \\ \mathbf{A}_I^2 & \mathbf{A}_I^2 \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^1 \\ \mathbf{u}_I^2 \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^1 \\ \mathbf{f}_I^2 \end{Bmatrix}. \quad (3.18)$$

The residual vectors in the interior of the subdomains Ω_1 and Ω_2 can be obtained from Eq.(3.16) and Eq.(3.17) as

$$(\mathbf{r}^1)^k = \mathbf{f}_I^1 - \mathbf{A}_I^1(\mathbf{u}_I^1)^{k-1} - \mathbf{A}_I^1(\mathbf{u}_I^2)^{k-1}, \quad (3.19)$$

$$(\mathbf{r}^2)^k = \mathbf{f}_I^2 - \mathbf{A}_I^2(\mathbf{u}_I^2)^{k-1} - \mathbf{A}_I^2(\mathbf{u}_I^1)^k. \quad (3.20)$$

In a vector form, the residual vector can be expressed as

$$\mathbf{r} = \begin{Bmatrix} \mathbf{r}^1 \\ \mathbf{r}^2 \end{Bmatrix} = \mathbf{f} - \mathbf{A}\mathbf{u}. \quad (3.21)$$

Thus the alternating Schwarz method can be rewritten in a two-step algorithm as [6]

$$\mathbf{u}^{k+\frac{1}{2}} = \mathbf{u}^k + \begin{bmatrix} [\mathbf{A}_I^1]^{-1} & 0 \\ 0 & 0 \end{bmatrix} (\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.22)$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k+\frac{1}{2}} + \begin{bmatrix} 0 & 0 \\ 0 & [\mathbf{A}_I^2]^{-1} \end{bmatrix} (\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{1}{2}}). \quad (3.23)$$

Note that, this form of the iteration scheme does not explicitly depend on the artificial boundaries.

In case of the additive Schwarz method, the two-step scheme is expressed as

$$\mathbf{u}^{k+\frac{1}{2}} = \mathbf{u}^k + \begin{bmatrix} [\mathbf{A}_I^1]^{-1} & 0 \\ 0 & 0 \end{bmatrix} (\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.24)$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k+\frac{1}{2}} + \begin{bmatrix} 0 & 0 \\ 0 & [\mathbf{A}_I^2]^{-1} \end{bmatrix} (\mathbf{f} - \mathbf{A}\mathbf{u}^k). \quad (3.25)$$

Note that the current approximate solution $\mathbf{u}^k$ is used to calculate the residual vector in the second step.

Equivalently, Eq.(3.24) and Eq.(3.25) can be combined as

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \begin{bmatrix} [\mathbf{A}_I^1]^{-1} & 0 \\ 0 & [\mathbf{A}_I^2]^{-1} \end{bmatrix} (\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.26)$$

which can be viewed as a generalization of block-Jacobi method [4, 6].

3.2.3 Schwarz Method as a Richardson's Iteration

The Schwarz alternating method can be viewed as a Richardson's iterative method as explained next [4, 6].

Let $\mathbf{R}_s$ be a restriction operator such that

$$\mathbf{u}_I^1 = \mathbf{R}_1 \mathbf{u} = \begin{bmatrix} \mathbf{I} & 0 \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^1 \\ \mathbf{u}_I^2 \end{Bmatrix}, \quad (3.27)$$

$$\mathbf{u}_I^2 = \mathbf{R}_2 \mathbf{u} = \begin{bmatrix} 0 & \mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^1 \\ \mathbf{u}_I^2 \end{Bmatrix}. \quad (3.28)$$

Using the definition of the restriction operators, the residual vectors in subdomains Ω_1 and Ω_2 can be expressed respectively as [6]

$$\mathbf{r}_1 = \mathbf{R}_1(\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.29)$$

$$\mathbf{r}_2 = \mathbf{R}_2(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{1}{2}}). \quad (3.30)$$

The stiffness matrix of the subdomains Ω_1 and Ω_2 , can be obtained as

$$\mathbf{A}_I^1 = \mathbf{R}_1 \mathbf{A} \mathbf{R}_1^T, \quad (3.31)$$

$$\mathbf{A}_I^2 = \mathbf{R}_2 \mathbf{A} \mathbf{R}_2^T. \quad (3.32)$$

Consequently, the multiplicative Schwarz method (see Eq.(3.22) and Eq.(3.23)) can be rewritten as [5, 6]

$$\mathbf{u}^{k+\frac{1}{2}} = \mathbf{u}^k + \mathbf{R}_1^T (\mathbf{R}_1 \mathbf{A} \mathbf{R}_1^T)^{-1} \mathbf{R}_1 (\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.33)$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k+\frac{1}{2}} + \mathbf{R}_2^T (\mathbf{R}_2 \mathbf{A} \mathbf{R}_2^T)^{-1} \mathbf{R}_2 (\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{1}{2}}). \quad (3.34)$$

Let $\mathbf{B}_s$ be a matrix that restricts the residual to subdomain Ω_s , solves the problem on that subdomain to generate a correction and then extends the correction back to the entire domain as [6]

$$\mathbf{B}_s = \mathbf{R}_s^T (\mathbf{R}_s \mathbf{A} \mathbf{R}_s^T)^{-1} \mathbf{R}_s. \quad (3.35)$$

In terms of $\mathbf{B}_s$ matrix, the two-step multiplicative Schwarz algorithm can be expressed as

$$\mathbf{u}^{k+\frac{1}{2}} = \mathbf{u}^k + \mathbf{B}_1(\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.36)$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k+\frac{1}{2}} + \mathbf{B}_2(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{1}{2}}). \quad (3.37)$$

Substituting Eq.(3.36) into Eq.(3.37), leads to

$$\mathbf{u}^{k+1} = \mathbf{u}^k + (\mathbf{B}_1 + \mathbf{B}_2 - \mathbf{B}_2 \mathbf{A} \mathbf{B}_1)(\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.38)$$

which is a one-step Richardson iterative procedure [6].

Note that the coupling term $\mathbf{B}_2 \mathbf{A} \mathbf{B}_1$ in Eq.(3.38) prevents the parallel implementation of the multiplicative Schwarz scheme. When this term is dropped, the scheme becomes the embarrassingly parallel additive Schwarz method as [5, 6]

$$\mathbf{u}^{k+1} = \mathbf{u}^k + (\mathbf{B}_1 + \mathbf{B}_2)(\mathbf{f} - \mathbf{A}\mathbf{u}^k) \quad (3.39)$$

Although the additive Schwarz method is embarrassingly parallel procedure, it has a convergence rate that is slower than that of the multiplicative Schwarz. The difference of the convergence properties of the additive and multiplicative Schwarz methods is analogous to that of Jacobi and Gauss-Seidel methods [5, 6].

3.2.4 Schwarz Method as a Preconditioner

The Schwarz method can be used as a preconditioner to accelerate the convergence rate of Krylov subspace iterative methods as explained next [5, 6].

Eq.(3.38) can be rearranged as

$$\mathbf{u}^{k+1} - \mathbf{u}^k = (\mathbf{B}_1 + \mathbf{B}_2 - \mathbf{B}_2\mathbf{A}\mathbf{B}_1)(\mathbf{f} - \mathbf{A}\mathbf{u}^k). \quad (3.40)$$

Equivalently, Eq.(3.40) can be rewritten as

$$\mathbf{e}^k = \mathbf{M}^{-1}\mathbf{r}^k, \quad (3.41)$$

where the multiplicative Schwarz preconditioner (Richardson Preconditioner) is defined as

$$\mathbf{M}^{-1} = \mathbf{B}_1 + \mathbf{B}_2 - \mathbf{B}_2\mathbf{A}\mathbf{B}_1. \quad (3.42)$$

Note that the multiplicative Schwarz preconditioner in Eq.(3.42) is not symmetric. To symmetrize the preconditioner, a third sub-step is needed as [5, 6]

$$\mathbf{u}^{k+\frac{1}{3}} = \mathbf{u}^k + \mathbf{B}_1(\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.43)$$

$$\mathbf{u}^{k+\frac{2}{3}} = \mathbf{u}^{k+\frac{1}{3}} + \mathbf{B}_2(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{1}{3}}), \quad (3.44)$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k+\frac{2}{3}} + \mathbf{B}_1(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{2}{3}}). \quad (3.45)$$

As a one-step scheme the symmetrized multiplicative Schwarz can be rewritten as [6]

$$\mathbf{u}^{k+1} = \mathbf{u}^k + (\mathbf{B}_1 + \mathbf{B}_2 - \mathbf{B}_2\mathbf{A}\mathbf{B}_1 - \mathbf{B}_1\mathbf{A}\mathbf{B}_2 + \mathbf{B}_1\mathbf{A}\mathbf{B}_2\mathbf{A}\mathbf{B}_1)(\mathbf{f} - \mathbf{A}\mathbf{u}^k). \quad (3.46)$$

Eq.(3.46) can be expressed in a factored form as

$$\mathbf{u}^{k+1} = \mathbf{u}^k + [\mathbf{B}_1 + (\mathbf{I} - \mathbf{B}_1\mathbf{A})\mathbf{B}_2(\mathbf{I} - \mathbf{A}\mathbf{B}_1)](\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.47)$$

and the symmetrized multiplicative Schwarz preconditioner can be expressed as

$$\mathbf{M}^{-1} = \mathbf{B}_1 + (\mathbf{I} - \mathbf{B}_1\mathbf{A})\mathbf{B}_2(\mathbf{I} - \mathbf{A}\mathbf{B}_1), \quad (3.48)$$

which can be viewed as a generalization of block Gauss-Seidel method [5, 6, 102].

On the other hand, the additive Schwarz preconditioner can be expressed as

$$\mathbf{M}^{-1} = [\mathbf{B}_1 + \mathbf{B}_2], \quad (3.49)$$

which is a generalization of a block Jacobi method [5, 6].

3.2.5 Schwarz Method for Many Subdomains

The multiplicative Schwarz scheme Eq.(3.36) and Eq.(3.37) can be generalized to the case of many overlapping subdomains $(\Omega_s, s = 1, 2, \dots, n_s)$ as [6]

$$\mathbf{u}^{k+\frac{1}{n_s}} = \mathbf{u}^k + \mathbf{B}_1(\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.50)$$

$$\mathbf{u}^{k+\frac{2}{n_s}} = \mathbf{u}^{k+\frac{1}{n_s}} + \mathbf{B}_2(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{1}{n_s}}), \quad (3.51)$$

$$\vdots$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k+\frac{(n_s-1)}{n_s}} + \mathbf{B}_{n_s}(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{(n_s-1)}{n_s}}). \quad (3.52)$$

This form of the multiplicative Schwarz scheme has a limited potential for parallelism [6, 72]. In practice however, there are often many subdomains that do not share a common interface boundary. Thus the solution on these subdomains can be updated concurrently and in parallel. This strategy can be implemented using a multi-coloring technique whereby each subdomain is identified with a color such that subdomains of the same color do not share a common interface boundary [6, 72].

If q be the number of colors used, the q -step multiplicative Schwarz scheme can be defined as [6]

$$\mathbf{u}^{k+\frac{1}{q}} = \mathbf{u}^k + \sum_{i \in Color_1} \mathbf{B}_i(\mathbf{f} - \mathbf{A}\mathbf{u}^k), \quad (3.53)$$

$$\mathbf{u}^{k+\frac{2}{q}} = \mathbf{u}^{k+\frac{1}{q}} + \sum_{i \in Color_2} \mathbf{B}_i(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{1}{q}}), \quad (3.54)$$

$$\vdots$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k+\frac{(q-1)}{q}} + \sum_{i \in Color_q} \mathbf{B}_i(\mathbf{f} - \mathbf{A}\mathbf{u}^{k+\frac{(q-1)}{q}}). \quad (3.55)$$

Generally, the convergence rate of the multi-coloring scheme depends on the number of colors. Increasing the number of colors leads to slow convergence rate of the scheme [6].

3.3 Non-Overlapping Domain Decomposition Methods

In non-overlapping domain decomposition methods or substructuring techniques, the solution domain is partitioned into a number of non-overlapping subdomains. On each subdomain, the finite element stiffness matrix and load vector are assembled independently. The subdomain local variables are split into interior and interface variables. The interior variables of each subdomain are concurrently eliminated by static condensation leading to a smaller but denser interface problem, namely the Schur complement system. The solution of the Schur complement system gives the interface variables. Once the interface variables are available, the interior variable can be obtained by solving the interior problem concurrently on each subdomain. The methodology can be described as follow [4–7].

Consider a linear second-order elliptic partial differential equation (PDE) defined on a domain Ω with given boundary conditions on $\partial\Omega$. The finite element discretization of the

PDE leads to the following sparse symmetric positive definite linear system

$$\mathbf{A}\mathbf{u} = \mathbf{f}, \quad (3.56)$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$ is the stiffness matrix, $\mathbf{u} \in \mathbb{R}^n$ is the response, and $\mathbf{f} \in \mathbb{R}^n$ is the forcing term.

Let the spatial domain Ω be partitioned into n_s non-overlapping subdomains $\{\Omega_s, 1 \leq s \leq n_s\}$ as shown schematically in Fig.(3.3). Each of the subdomains is a union of elements and such that

$$\Omega = \bigcup_{s=1}^{n_s} \Omega_s, \quad \Omega_s \cap \Omega_r = \emptyset \quad s \neq r \quad (3.57)$$

and

$$\Gamma = \bigcup_{s=1}^{n_s} \Gamma_s \text{ where } \Gamma_s = \partial\Omega_s \setminus \partial\Omega. \quad (3.58)$$

Figure 3.3: A typical domain partitioned into n_s non-overlapping subdomains

For a typical subdomain Ω_s , the solution vector $\mathbf{u}^s$ can be split into two subvectors as

$$\mathbf{u}^s = \begin{Bmatrix} \mathbf{u}_I^s \\ \mathbf{u}_\Gamma^s \end{Bmatrix}, \quad (3.59)$$

where $\mathbf{u}_I^s$ is the interior solution vector which corresponds to the nodes in the interior of the subdomain and $\mathbf{u}_\Gamma^s$ is the interface solution vector that relates to the nodes on the interface boundary between two or more neighboring subdomains.

Consequently, the equilibrium equation for a typical subdomain Ω_s can be written in a block form as

$$\begin{bmatrix} \mathbf{A}_{II}^s & \mathbf{A}_{I\Gamma}^s \\ \mathbf{A}_{\Gamma I}^s & \mathbf{A}_{\Gamma\Gamma}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s \\ \mathbf{u}_\Gamma^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_\Gamma^s \end{Bmatrix}. \quad (3.60)$$

The submatrix $\mathbf{A}_{II}^s$ relates to the stiffness matrix of the interior nodes, and the stiffness submatrices $\mathbf{A}_{I\Gamma}^s$ and $\mathbf{A}_{\Gamma I}^s$ relate to the coupling between the interior and interface boundary nodes, and the submatrix $\mathbf{A}_{\Gamma\Gamma}^s$ represents the stiffness matrix of the interface boundary nodes.

For a typical subdomain Ω_s , let $\mathbf{R}_s$ be a restriction matrix (consisting of zeros and ones) that maps the entire set of interface degrees of freedom $\mathbf{u}_\Gamma$ to the local subdomain interface degree of freedom $\mathbf{u}_\Gamma^s$ on Γ_s as

$$\mathbf{u}_\Gamma^s = \mathbf{R}_s \mathbf{u}_\Gamma. \quad (3.61)$$

In parallel implementation, $\mathbf{R}_s$ acts as a *scatter* operator while $\mathbf{R}_s^T$ acts as a *gather* operator and are not constructed explicitly.

Enforcing the transmission conditions (compatibility and equilibrium) along the interfaces boundaries by global assembly, yields the following global equilibrium equation [66]

$$\begin{bmatrix} \mathbf{A}_{II}^1 & \dots & 0 & \mathbf{A}_{I\Gamma}^1 \mathbf{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathbf{A}_{II}^{n_s} & \mathbf{A}_{I\Gamma}^{n_s} \mathbf{R}_{n_s} \\ \mathbf{R}_1^T \mathbf{A}_{\Gamma I}^1 & \dots & \mathbf{R}_{n_s}^T \mathbf{A}_{\Gamma I}^{n_s} & \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{A}_{\Gamma\Gamma}^s \mathbf{R}_s \end{bmatrix} \begin{bmatrix} \mathbf{u}_I^1 \\ \vdots \\ \mathbf{u}_I^{n_s} \\ \mathbf{u}_\Gamma \end{bmatrix} = \begin{bmatrix} \mathbf{f}_I^1 \\ \vdots \\ \mathbf{f}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{f}_\Gamma^s \end{bmatrix}. \quad (3.62)$$

Performing the Gaussian elimination, Eq.(3.62) can be recast as

$$\begin{bmatrix} \mathbf{A}_{II}^1 & \dots & 0 & \mathbf{A}_{I\Gamma}^1 \mathbf{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathbf{A}_{II}^{n_s} & \mathbf{A}_{I\Gamma}^{n_s} \mathbf{R}_{n_s} \\ 0 & \dots & 0 & \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{S}_s \mathbf{R}_s \end{bmatrix} \begin{bmatrix} \mathbf{u}_I^1 \\ \vdots \\ \mathbf{u}_I^{n_s} \\ \mathbf{u}_\Gamma \end{bmatrix} = \begin{bmatrix} \mathbf{f}_I^1 \\ \vdots \\ \mathbf{f}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{g}_\Gamma^s \end{bmatrix}, \quad (3.63)$$

where the local Schur complement matrix $\mathbf{S}_s$ and the corresponding right-hand side vector $\mathbf{g}_\Gamma^s$ are respectively defined as

$$\mathbf{S}_s = \mathbf{A}_{\Gamma\Gamma}^s - \mathbf{A}_{\Gamma I}^s [\mathbf{A}_{II}^s]^{-1} \mathbf{A}_{I\Gamma}^s, \quad (3.64)$$

$$\mathbf{g}_\Gamma^s = \mathbf{f}_\Gamma^s - \mathbf{A}_{\Gamma I}^s [\mathbf{A}_{II}^s]^{-1} \mathbf{f}_I^s. \quad (3.65)$$

The global interface problem or the Schur complement system is defined as

$$\mathbf{S} \mathbf{u}_\Gamma = \mathbf{g}_\Gamma, \quad (3.66)$$

where the global Schur complement matrix $\mathbf{S}$ and the corresponding right-hand side vector $\mathbf{g}_\Gamma$ are respectively given by

$$\mathbf{S} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{S}_s \mathbf{R}_s, \quad (3.67)$$

$$\mathbf{g}_\Gamma = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{g}_\Gamma^s. \quad (3.68)$$

The solution of the Schur complement system gives the unknowns $\mathbf{u}_\Gamma$ along the interfaces boundaries. Once these unknowns are available, the interior unknowns $\mathbf{u}_I^s$ can be obtained by solving the following interior problem on each subdomain in parallel as

$$\mathbf{A}_{II}^s \mathbf{u}_I^s = \mathbf{f}_I^s - \mathbf{A}_{\Gamma I}^s \mathbf{R}_s \mathbf{u}_\Gamma. \quad (3.69)$$

The global Schur complement of the stiffness matrix of a second-order elliptic PDE is symmetric and positive definite [4–7]. However, the local Schur complement matrix is singular for the case of floating subdomains (subdomains without enough Dirichlet boundary conditions to constrain rigid body motion at the null space), and hence care must be taken while tackling the subdomain-level (local) Schur complement system [4–7]. The Schur complement matrix is generally dense and expensive to construct explicitly [4–7].

The condition number of the Schur complement matrix is generally better than the original stiffness matrix [6, 72, 78]. For instance, if h is the finite element mesh size, the condition number of the stiffness matrix for many second order PDEs is [4–7]

$$\kappa(\mathbf{A}) = \mathcal{O}\left(\frac{1}{h^2}\right). \quad (3.70)$$

On the other hand, the condition number of the Schur complement matrix grows as [4–7, 122]

$$\kappa(\mathbf{S}) = \mathcal{O}\left(\frac{1}{hH}\right), \quad (3.71)$$

where H denotes the subdomain size. As H is much greater than h , the Schur complement matrix is better conditioned than the original stiffness matrix.

Depending on the solution method used to solve the Schur complement system Eq.(3.66), substructuring techniques are divided into direct and iterative methods [6, 7]. In the direct substructuring method, the Schur complement system is explicitly constructed and solved using a dense direct solver (usually a multi-frontal solver). The computational cost and the memory requirements for constructing the Schur complement system limit the capability of the direct substructuring method to tackle large-scale practical problems using parallel computing. On the other hand, in the iterative substructuring techniques, the interface problem is solved iteratively without explicitly constructing the Schur complement system.

3.3.1 Primal Iterative Substructuring Method

In practice, it is expensive to construct the Schur complement system explicitly. Instead an iterative method, which only requires the action of the Schur complement matrix on a vector [115], is used to solve the Schur complement system. In general the performance of the iterative method can be dramatically improved by using an efficient preconditioner [52].

Iterative substructuring can be viewed as a preconditioned iterative method for solving the Schur complement system of the form [4]

$$\mathbf{S} \mathbf{u}_r = \mathbf{g}_r. \quad (3.72)$$

For symmetric positive-definite system such as Schur complement system, the Conjugate Gradient Method (CGM) is generally used. The performance of CGM mainly depends on the spectrum of the coefficient matrix. However, the rate of convergence of the iterative method can generally be improved by transforming the original system into an equivalent system that has better spectral properties (i.e. lower condition number) [52]. This transformation is called preconditioning and the matrix used in the transformation is called the preconditioner. In other words, the transformed linear system becomes

$$\mathbf{M}^{-1}\mathbf{S} \mathbf{u}_r = \mathbf{M}^{-1}\mathbf{g}_r. \quad (3.73)$$

In general, $\kappa(\mathbf{M}^{-1}\mathbf{S})$ is much smaller than $\kappa(\mathbf{S})$ and the eigenvalues of $\mathbf{M}^{-1}\mathbf{S}$ are clustered near one [52]. This procedure is known as the Preconditioned Conjugate Gradient Method (PCGM). In practice, the explicit construction of $\mathbf{M}^{-1}$ is not needed. Instead, for a given vector $\mathbf{r}_r$, a system of the the following form is solved

$$\mathbf{M}\mathbf{z} = \mathbf{r}_r. \quad (3.74)$$

In the following sections, we review various types of popular iterative substructuring methods which are used to develop an efficient preconditioner $\mathbf{M}^{-1}$ for the Schur complement system.

Neumann-Neumann Method

Neumann-Neumann preconditioner approximates the inverse of the global Schur complement matrix by a weighted sum of the inverse of the local Schur complement matrices [71]. The implementation of the preconditioner requires a local solve of a Neumann problem in each iteration of the iterative solver. The algorithm can be described as follow [4, 5, 7].

For a typical subdomain Ω_s , the equilibrium equation can be written as

$$\begin{bmatrix} \mathbf{A}_{II}^s & \mathbf{A}_{IF}^s \\ \mathbf{A}_{FI}^s & \mathbf{A}_{FF}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s \\ \mathbf{u}_F^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_F^s \end{Bmatrix}. \quad (3.75)$$

Starting with an initial guess for the interface unknown $\mathbf{u}_{F_j}$ (where j represents the iteration count), a local Dirichlet problem with non-homogeneous boundary condition is solved to obtain the interior unknown. Hence from the first row of the Eq.(3.75), the local interior unknown $\mathbf{u}_I^s$ can be obtained as

$$\mathbf{u}_I^s = [\mathbf{A}_{II}^s]^{-1}(\mathbf{f}_I^s - \mathbf{A}_{IF}^s \mathbf{u}_F^s), \quad (3.76)$$

where

$$\mathbf{u}_F^s = \mathbf{R}_s \mathbf{u}_{F_j}. \quad (3.77)$$

The corresponding subdomain level residual vector $\mathbf{r}_F^s$ can be computed from the second row of Eq.(3.75) as

$$\mathbf{r}_F^s = \mathbf{A}_{FI}^s \mathbf{u}_I^s + \mathbf{A}_{FF}^s \mathbf{u}_F^s - \mathbf{f}_F^s. \quad (3.78)$$

Substituting Eq.(3.76) into Eq.(3.78) leads to

$$\mathbf{r}_I^s = (\mathbf{A}_{II}^s - \mathbf{A}_{II}^s [\mathbf{A}_{II}^s]^{-1} \mathbf{A}_{II}^s) \mathbf{u}_I^s - (\mathbf{f}_I^s - \mathbf{A}_{II}^s [\mathbf{A}_{II}^s]^{-1} \mathbf{f}_I^s). \quad (3.79)$$

Using the definition of the local Schur complement matrix and the corresponding right-hand side, the local residual in Eq.(3.79) can be rewritten as

$$\mathbf{r}_I^s = \mathbf{S}_s \mathbf{u}_I^s - \mathbf{g}_I^s, \quad (3.80)$$

where

$$\mathbf{S}_s = \mathbf{A}_{II}^s - \mathbf{A}_{II}^s [\mathbf{A}_{II}^s]^{-1} \mathbf{A}_{II}^s, \quad (3.81)$$

$$\mathbf{g}_I^s = \mathbf{f}_I^s - \mathbf{A}_{II}^s [\mathbf{A}_{II}^s]^{-1} \mathbf{f}_I^s. \quad (3.82)$$

The global equilibrium is enforced next by gathering the local residuals from all the subdomains as

$$\mathbf{r}_{I_j} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{r}_I^s, \quad (3.83)$$

where $\mathbf{r}_{I_j}$ is the global residual vector at the j^{th} iteration which represents the *unbalanced* force over the boundary interfaces due to the erroneous initial guess for $\mathbf{u}_{I_j}$. Note that when $\mathbf{r}_{I_j} = 0$, the system is in equilibrium.

Let $\mathbf{D}_s$ represent a diagonal scaling matrix that constitutes a decomposition of unity as

$$\sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s \mathbf{R}_s = \mathbf{I}, \quad (3.84)$$

where the diagonal entries of $\mathbf{D}_s$ are the reciprocal of the number of subdomains that share the interface boundary nodes [4, 6, 7].

The global residual (the unbalanced force) given by Eq.(3.83) can be distributed over the subdomains as

$$\mathbf{r}_\Gamma^s = \mathbf{D}_s \mathbf{R}_s \mathbf{r}_{\Gamma_j}. \quad (3.85)$$

The corresponding unknowns, $\mathbf{u}_\Gamma^s$ due to the local unbalanced force given by Eq.(3.85) can be computed by solving a local Schur complement system as

$$\mathbf{S}_s \mathbf{u}_\Gamma^s = \mathbf{r}_\Gamma^s. \quad (3.86)$$

In practice, the local Schur complement matrix $\mathbf{S}_s$ is not formed explicitly. Instead the effect of its inverse on the residual vector is computed by solving the following subdomain level Neumann problem

$$\begin{bmatrix} \mathbf{A}_{II}^s & \mathbf{A}_{I\Gamma}^s \\ \mathbf{A}_{\Gamma I}^s & \mathbf{A}_{\Gamma\Gamma}^s \end{bmatrix} \begin{Bmatrix} \mathbf{x}^s \\ \mathbf{u}_\Gamma^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{r}_\Gamma^s \end{Bmatrix}. \quad (3.87)$$

For the case of floating subdomain (subdomains without sufficient Dirichlet boundary conditions), the solution to the local Neumann problem defined in Eq.(3.87) is only unique up to an additive constant (see Eq.(3.98)) and only if the right hand side vector satisfies the compatibility condition (the residual vector is orthogonal to the null space of the subdomain stiffness matrix) [4, 7]. Therefore, a small value can be added to the diagonal entries of the subdomain stiffness matrices to ensure the solvability of the subdomain level Neu-

mann problem in Eq.(3.87) [4, 6]. Note that this regularization does not change the original problem since it only affects the preconditioner matrix. Alternatively, the computationally expensive Moore-Penrose pseudo-inverse can be used. However, the accuracy of the approximate inversion highly influences the performance of the preconditioner [6].

The new approximate solution $\mathbf{u}_{\Gamma_{j+1}}$ can be obtained by updating the initial guess $\mathbf{u}_{\Gamma_j}$ with the average local solutions $\mathbf{u}_r^s$ as

$$\mathbf{u}_{\Gamma_{j+1}} = \mathbf{u}_{\Gamma_j} + \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{u}_r^s. \quad (3.88)$$

Consequently, the corresponding error vector at the j^{th} iteration can be obtained as

$$\mathbf{e}_{\Gamma_j} = \mathbf{u}_{\Gamma_{j+1}} - \mathbf{u}_{\Gamma_j}. \quad (3.89)$$

Substituting Eq.(3.88) into Eq.(3.89) and using Eq.(3.86) gives

$$\mathbf{e}_{\Gamma_j} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{S}_s^{-1} \mathbf{D}_s \mathbf{R}_s \mathbf{r}_{\Gamma_j}. \quad (3.90)$$

From preconditioning perspective, Eq.(3.90) can be rewritten as

$$\mathbf{e}_{\Gamma_j} = \mathbf{M}_{NN}^{-1} \mathbf{r}_{\Gamma_j}, \quad (3.91)$$

where the Neumann-Neumann preconditioner formally defined as

$$\mathbf{M}_{NN}^{-1} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{S}_s^{-1} \mathbf{D}_s \mathbf{R}_s. \quad (3.92)$$

Condition Number Bound

If h is the finite element mesh size and H is a typical subdomain size, the condition number of the Neumann-Neumann method for both two and three dimensional problems grows as [4, 5, 7, 72]

$$\kappa(\mathbf{M}_{NN}^{-1}\mathbf{S}) \leq \frac{C}{H^2} \left(1 + \log \frac{H}{h}\right)^2, \quad (3.93)$$

where C is a positive coefficient independent of the geometric parameters h and H .

According to the condition number estimate in Eq.(3.93) for Neumann-Neumann method, the convergence rate of the iterative method used to solve the preconditioned system $(\mathbf{M}^{-1}\mathbf{S})$ deteriorates as the size of the subdomain becomes small (i.e., the number of subdomains grows). This fact is due to the dependency of the conditioned number on H^{-2} which is typical for one-level domain decomposition preconditioners [4, 5, 7, 78].

Balancing Domain Decomposition Method

For a small number of subdomains, the Neumann-Neumann preconditioner exhibits a good performance [6]. However, its performance deteriorates as the number of subdomains increases [6, 72]. The Balancing Domain Decomposition (BDD) is introduced to address this problem [116, 117].

The Balancing Domain Decomposition (BDD) [116, 117] corrects (*balances*) the residual vector forcing it to be in the *range* of the local Schur complement matrix (i.e., makes

the local Schur complement system *consistent* to ensure the solvability of the singular system). Additionally, the BDD provides a coarse grid correction to the one-level Neumann-Neumann method. In the preconditioning step of the iterative solver, the coarse grid serves as a mechanism to propagate information globally over the subdomains [116, 117]. This spread of information prevents the growth of the condition number as increasing the number of subdomains [116, 117]. The coarse problem consists of a few unknowns per each subdomain. This coarse grid is purely algebraic and hence no geometric information about the mesh is needed to implement the BDD method [116, 117].

The effect of the Neumann-Neumann preconditioner Eq.(3.92) on a residual vector $\mathbf{r}$ is computed as

$$\mathbf{M}_{NN}^{-1}\mathbf{r} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{w}_s, \quad (3.94)$$

where $\mathbf{w}_s$ is the solution vector of the following system

$$\mathbf{S}_s \mathbf{w}_s = \mathbf{D}_s \mathbf{R}_s \mathbf{r}. \quad (3.95)$$

As previously alluded, the local Schur complement matrix in Eq.(3.95) is singular for floating subdomains. The system has a solution (not necessarily unique) only if the system is consistent (i.e., the right-hand side vector is orthogonal to the null space of the singular matrix $\mathbf{S}_s$).

Let $\mathbf{N}_s$ be a matrix of size $n_{\Gamma_s} \times d_s$, where n_{Γ_s} is the size of the interface boundary

nodes for subdomain Ω_s , and d_s is the dimension of the null space of S_s . Let the column vector of the matrix N_s span the null space of the singular matrix S_s , as

$$\text{Range}(N_s) = \text{Kernel}(S_s), \quad (3.96)$$

when the matrix S_s is singular, the subdomain matrix is solvable only if the compatibility condition holds as [7]

$$N_s^T (D_s R_s r) = 0. \quad (3.97)$$

The solution to the Schur complement Eq.(3.95) is not unique and has the following general form

$$w_s = v_s + N_s \alpha_s, \quad (3.98)$$

where $v_s \in \mathbb{R}^{n_{r_s}}$ is a particular solution and $N_s \alpha_s$ is a general term in the null space of S_s for $\alpha_s \in \mathbb{R}^{d_s}$.

The global solution can be obtained by averaging the subdomain level solutions as

$$w = \sum_{s=1}^{n_s} R_s^T D_s^T w_s. \quad (3.99)$$

Substituting Eq.(3.98) into Eq.(3.99) gives

$$w = \sum_{s=1}^{n_s} R_s^T D_s^T v_s + \sum_{s=1}^{n_s} R_s^T D_s^T N_s \alpha_s. \quad (3.100)$$

Eq.(3.100) can be rewritten as

$$\mathbf{w} = \mathbf{v} + \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{N}_s \boldsymbol{\alpha}_s, \quad (3.101)$$

where

$$\mathbf{v} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{v}_s. \quad (3.102)$$

Premultiplying Eq.(3.101) by the global Schur complement matrix $\mathbf{S}$ to calculate the global residual, one obtains

$$\mathbf{S}\mathbf{w} = \mathbf{S}\mathbf{v} + \mathbf{S} \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{N}_s \boldsymbol{\alpha}_s. \quad (3.103)$$

Equivalently, Eq.(3.103) can be expressed as

$$\mathbf{S}\mathbf{w} = \mathbf{S}\mathbf{v} + \mathbf{S} \begin{bmatrix} \mathbf{R}_1^T \mathbf{D}_1^T \mathbf{N}_1 & \mathbf{R}_2^T \mathbf{D}_2^T \mathbf{N}_2 & \cdots & \mathbf{R}_{n_s}^T \mathbf{D}_{n_s}^T \mathbf{N}_{n_s} \end{bmatrix} \begin{Bmatrix} \boldsymbol{\alpha}_1 \\ \boldsymbol{\alpha}_2 \\ \vdots \\ \boldsymbol{\alpha}_{n_s} \end{Bmatrix}. \quad (3.104)$$

Let $\mathbf{R}_0$ represent a matrix of size $n_{r_s} \times d$ where $d = (d_1 + \cdots + d_{n_s})$ and n_s is the number of subdomains. The columns of $\mathbf{R}_0$ are defined as

$$\mathbf{R}_0 = \begin{bmatrix} \mathbf{R}_1^T \mathbf{D}_1^T \mathbf{N}_1 & \mathbf{R}_2^T \mathbf{D}_2^T \mathbf{N}_2 & \cdots & \mathbf{R}_{n_s}^T \mathbf{D}_{n_s}^T \mathbf{N}_{n_s} \end{bmatrix}. \quad (3.105)$$

In the case of non-floating subdomain, $\boldsymbol{\alpha}_s = 0$ and hence the corresponding column in the matrix $\mathbf{R}_0$ is void. However, it may be advantageous to set the corresponding column

in the matrix $\mathbf{R}_0$ to a non-zero value for computer implementation [7].

Hence, Eq.(3.104) can be rewritten as

$$\mathbf{r} = \tilde{\mathbf{r}} + \mathbf{S}\mathbf{R}_0\boldsymbol{\alpha}, \quad (3.106)$$

where

$$\mathbf{r} = \mathbf{S}\mathbf{w}, \quad \tilde{\mathbf{r}} = \mathbf{S}\mathbf{v}, \quad \boldsymbol{\alpha} = \begin{Bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{n_s} \end{Bmatrix}. \quad (3.107)$$

Consequently, the compatibility condition defined in Eq.(3.97) can now be expressed as

$$\mathbf{R}_0^T \mathbf{r} = \mathbf{0}. \quad (3.108)$$

When the residual vector is not balanced (i.e., $\mathbf{R}_0^T \mathbf{r} \neq \mathbf{0}$), a correction term ($\mathbf{S}\mathbf{R}_0\boldsymbol{\alpha}$) can be sought such that the new residual $\tilde{\mathbf{r}}$ is balanced as

$$\mathbf{R}_0^T(\tilde{\mathbf{r}}) = \mathbf{0}. \quad (3.109)$$

Substituting Eq.(3.106) into Eq.(3.109) leads to

$$\mathbf{R}_0^T(\mathbf{r} - \mathbf{S}\mathbf{R}_0\boldsymbol{\alpha}) = \mathbf{0}. \quad (3.110)$$

Therefore the following linear system is solved to obtain the vector α

$$[\mathbf{R}_0^T \mathbf{S} \mathbf{R}_0] \alpha = \mathbf{R}_0^T \mathbf{r}. \quad (3.111)$$

This system is uniquely solvable due to the positive definiteness of the global Schur complement matrix $\mathbf{S}$. The system can be rewritten in a block structure as [7]

$$\begin{bmatrix} \mathbf{R}_0^{1T} \mathbf{S} \mathbf{R}_0^1 & \cdots & \mathbf{R}_0^{1T} \mathbf{S} \mathbf{R}_0^{n_s} \\ \vdots & \cdots & \vdots \\ \mathbf{R}_0^{n_s T} \mathbf{S} \mathbf{R}_0^{n_s} & \cdots & \mathbf{R}_0^{n_s T} \mathbf{S} \mathbf{R}_0^{n_s} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_{n_s} \end{bmatrix} = \begin{bmatrix} \mathbf{R}_0^{1T} \mathbf{r} \\ \vdots \\ \mathbf{R}_0^{n_s T} \mathbf{r} \end{bmatrix}, \quad (3.112)$$

where $\mathbf{R}_0^s$ defines the columns of the matrix $\mathbf{R}_0$, see Eq.(3.105).

Thus, the vector α can be obtained as

$$\alpha = \mathbf{S}_0^{-1} \mathbf{R}_0^T \mathbf{r}, \quad (3.113)$$

where the coarse grid operator is defined as

$$\mathbf{S}_0 = \mathbf{R}_0^T \mathbf{S} \mathbf{R}_0. \quad (3.114)$$

The Neumann-Neumann preconditioner now can be applied to find any solution, since the system now is consistent (the residual vector is balanced $\tilde{\mathbf{r}}$). Thus, applying the Neumann-Neumann preconditioner, one obtains

$$\mathbf{v} = \mathbf{M}_{NN}^{-1} \tilde{\mathbf{r}}. \quad (3.115)$$

Substituting Eq.(3.106) into Eq.(3.115) gives

$$\mathbf{v} = \mathbf{M}_{NN}^{-1}(\mathbf{r} - \mathbf{S}\mathbf{R}_0\boldsymbol{\alpha}). \quad (3.116)$$

The residual needs to be balanced again in order to have a symmetric preconditioner. In other words, a correction term $\mathbf{S}\mathbf{R}_0\boldsymbol{\beta}$ is sought such that the new residual is balanced again. The residual vector can be expressed as

$$\mathbf{r} = \tilde{\mathbf{r}} + \hat{\mathbf{r}} + \mathbf{S}\mathbf{R}_0\boldsymbol{\beta}. \quad (3.117)$$

Next the correction term can be calculated such that $\hat{\mathbf{r}}$ is balanced as

$$\mathbf{R}_0^T(\hat{\mathbf{r}}) = 0. \quad (3.118)$$

Substituting Eq.(3.117) into Eq.(3.118), gives

$$\mathbf{R}_0^T(\mathbf{r} - \tilde{\mathbf{r}} - \mathbf{S}\mathbf{R}_0\boldsymbol{\beta}) = 0. \quad (3.119)$$

Solving for the vector $\boldsymbol{\beta}$, one obtains

$$\boldsymbol{\beta} = \mathbf{S}_0^{-1} \mathbf{R}_0^T(\mathbf{r} - \tilde{\mathbf{r}}). \quad (3.120)$$

Finally the solution can be written as

$$\begin{aligned}
\mathbf{u} &= \mathbf{v} + \mathbf{R}_0 \boldsymbol{\beta}, \\
&= \mathbf{v} + \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T (\mathbf{r} - \tilde{\mathbf{r}}), \\
&= \mathbf{v} + \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T (\mathbf{r} - \mathbf{S} \mathbf{v}), \\
&= \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T \mathbf{r} + (\mathbf{I} - \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T \mathbf{S}) \mathbf{v}, \\
&= \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T \mathbf{r} + (\mathbf{I} - \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T \mathbf{S}) \mathbf{M}_{NN}^{-1} (\mathbf{r} - \mathbf{S} \mathbf{R}_0 \boldsymbol{\alpha}), \\
&= \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T \mathbf{r} + (\mathbf{I} - \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T \mathbf{S}) \mathbf{M}_{NN}^{-1} (\mathbf{I} - \mathbf{S} \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T) \mathbf{r}, \\
&= [\mathbf{P}_0 + (\mathbf{I} - \mathbf{P}_0 \mathbf{S}) \mathbf{M}_{NN}^{-1} (\mathbf{I} - \mathbf{S} \mathbf{P}_0)] \mathbf{r},
\end{aligned} \tag{3.121}$$

where

$$\mathbf{P}_0 = \mathbf{R}_0 \mathbf{S}_0^{-1} \mathbf{R}_0^T. \tag{3.122}$$

Note that $\mathbf{P}_0$ denotes the $\mathbf{S}$ -orthogonal projection onto the coarse space spanned by $\mathbf{R}_0$.

The balancing domain decomposition preconditioner can be formally written as

$$\mathbf{M}_{BDD}^{-1} = \mathbf{P}_0 + (\mathbf{I} - \mathbf{P}_0 \mathbf{S}) \mathbf{M}_{NN}^{-1} (\mathbf{I} - \mathbf{S} \mathbf{P}_0), \tag{3.123}$$

where

$$\mathbf{M}_{NN}^{-1} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{S}_s^{-1} \mathbf{D}_s \mathbf{R}_s, \quad \text{and} \quad \mathbf{S} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{S}_s \mathbf{R}_s. \tag{3.124}$$

Condition Number Bound

The theoretical bound for the condition number of the BDD preconditioner for both two and three dimensional problems satisfies [5, 7, 72, 116]

$$\kappa(\mathbf{M}_{BDD}^{-1}\mathbf{S}) \leq C(1 + \log \frac{H}{h})^2, \quad (3.125)$$

where C is a positive constant (independent of the geometric parameters) and h and H are the finite element mesh size and subdomain size respectively.

Neumann-Neumann with a Coarse Grid Preconditioner

The BDD method is an efficient domain decomposition technique. However, the coarse problem is costly to build as it involves a product with the global Schur complement matrix, generally not available explicitly [66]. In addition, characterization of the null space of the singular Schur complement matrix may not be a trivial task for some problems [4].

Therefore, a geometric coarse problem based on a collection of corner nodes in the physical domain can be added to the Neumann-Neumann method [66]. The coarse grid is constructed to impose sufficient artificial Dirichlet boundary conditions to remove the singularity in the stiffness matrix of the floating subdomain. This methodology is described below [66].

For a typical subdomain Ω_s , the equilibrium equation can be written as

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{i\Gamma}^s \\ \mathbf{A}_{\Gamma i}^s & \mathbf{A}_{\Gamma\Gamma}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s \\ \mathbf{u}_\Gamma^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_\Gamma^s \end{Bmatrix}. \quad (3.126)$$

Starting with an initial guess for the global interface unknowns $\mathbf{u}_{\Gamma_j}$ (where j represents the iteration count), the local interface unknowns $\mathbf{u}_\Gamma^s$ can be obtained as

$$\mathbf{u}_\Gamma^s = \mathbf{R}_s \mathbf{u}_{\Gamma_j}. \quad (3.127)$$

Next a local Dirichlet problem with non-homogeneous boundary condition can be solved on each subdomain to obtain the interior unknowns. Thus from the first row of Eq.(3.126), the local interior unknown $\mathbf{u}_i^s$ can be obtained as

$$\mathbf{u}_i^s = [\mathbf{A}_{ii}^s]^{-1}(\mathbf{f}_i^s - \mathbf{A}_{i\Gamma}^s \mathbf{u}_\Gamma^s). \quad (3.128)$$

The corresponding subdomain level residual vector $\mathbf{r}_\Gamma^s$ can be computed from the second row of Eq.(3.126) as

$$\mathbf{r}_\Gamma^s = \mathbf{A}_{\Gamma i}^s \mathbf{u}_i^s + \mathbf{A}_{\Gamma\Gamma}^s \mathbf{u}_\Gamma^s - \mathbf{f}_\Gamma^s. \quad (3.129)$$

Substituting Eq.(3.128) into Eq.(3.129) leads to

$$\mathbf{r}_\Gamma^s = (\mathbf{A}_{\Gamma\Gamma}^s - \mathbf{A}_{\Gamma i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{A}_{i\Gamma}^s) \mathbf{u}_\Gamma^s - (\mathbf{f}_\Gamma^s - \mathbf{A}_{\Gamma i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{f}_i^s). \quad (3.130)$$

In terms of Schur complement matrix $\mathbf{S}_s$, the local residual in Eq.(3.130) can be rewritten as

$$\mathbf{r}_\Gamma^s = \mathbf{S}_s \mathbf{u}_\Gamma^s - \mathbf{g}_\Gamma^s, \quad (3.131)$$

where

$$\mathbf{S}_s = \mathbf{A}_{\Gamma\Gamma}^s - \mathbf{A}_{\Gamma i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{A}_{i\Gamma}^s, \quad (3.132)$$

$$\mathbf{g}_{\Gamma}^s = \mathbf{f}_{\Gamma}^s - \mathbf{A}_{\Gamma i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{f}_i^s. \quad (3.133)$$

The global residual vector $\mathbf{r}_{\Gamma_j}$ is obtained next by gathering the local residuals from all the subdomains as

$$\mathbf{r}_{\Gamma_j} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{r}_{\Gamma}^s. \quad (3.134)$$

Let $\mathbf{D}_s$ represent a diagonal scaling matrix that forms a decomposition of unity [4, 6, 7] as

$$\sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s \mathbf{R}_s = \mathbf{I}, \quad (3.135)$$

where the diagonal entries of $\mathbf{D}_s$ are the reciprocal of the number of subdomains that share the interface nodes [4, 6, 7].

The global residual given by Eq.(3.134) can be distributed over the subdomains as

$$\mathbf{r}_{\Gamma}^s = \mathbf{D}_s \mathbf{R}_s \mathbf{r}_{\Gamma_j}. \quad (3.136)$$

The corresponding unknowns $\mathbf{u}_{\Gamma}^s$ due to $\mathbf{r}_{\Gamma}^s$ in Eq.(3.136) can be computed by solving a local Schur complement system as

$$\mathbf{S}_s \mathbf{u}_{\Gamma}^s = \mathbf{r}_{\Gamma}^s. \quad (3.137)$$

In practice, the local Schur complement matrix S_s is never formed explicitly. Instead the following subdomain level Neumann problem is solved to obtain $\mathbf{u}_\Gamma^s$

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{i\Gamma}^s \\ \mathbf{A}_{\Gamma i}^s & \mathbf{A}_{\Gamma\Gamma}^s \end{bmatrix} \begin{Bmatrix} \mathbf{x}^s \\ \mathbf{u}_\Gamma^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{r}_\Gamma^s \end{Bmatrix}. \quad (3.138)$$

To ensure the solvability of the subdomain level Neumann problem defined in Eq.(3.138), sufficient artificial Dirichlet boundary conditions are necessary to be provided in order to remove the singularity from the stiffness matrix of the floating subdomains. Therefore, for a typical subdomain Ω_s , the interface unknown vector $\mathbf{u}_\Gamma^s$ can be split as follows

$$\mathbf{u}_\Gamma^s = \begin{Bmatrix} \mathbf{u}_r^s \\ \mathbf{u}_c^s \end{Bmatrix}, \quad (3.139)$$

where $\mathbf{u}_r^s$ is the remaining nodes (boundary nodes shared between two adjacent subdomains only) and $\mathbf{u}_c^s$ is the corner nodes (boundary nodes shared between more than two subdomains plus the nodes on the ends of interface edges) [64, 66]. The corner nodes provide a mechanism to impose the artificial Dirichlet boundary conditions to remove singularity from the local Schur complement matrix of the floating subdomains. On the other hand, the corner nodes introduces a coarse grid that connects all the subdomains to provide information transfer mechanism globally.

For a typical subdomain Ω_s , the Boolean splitting operators $\mathbf{R}_s^r$ and $\mathbf{R}_s^c$ extract the remaining interface variable $\mathbf{u}_r^s$ and corner interface unknown $\mathbf{u}_c^s$ from the subdomain interface vector $\mathbf{u}_\Gamma^s$ as

$$\mathbf{u}_r^s = \mathbf{R}_s^r \mathbf{u}_\Gamma^s, \quad (3.140)$$

and

$$\mathbf{u}_c^s = \mathbf{R}_s^c \mathbf{u}_\Gamma^s. \quad (3.141)$$

Furthermore, the Boolean restriction operator $\mathbf{B}_c^s$ that maps the global corner interface vector $\mathbf{u}_c$ into the local corner interface vector $\mathbf{u}_c^s$ is defined as

$$\mathbf{u}_c^s = \mathbf{B}_c^s \mathbf{u}_c. \quad (3.142)$$

Consequently, the following partially assembled equilibrium system can be obtained

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s & \mathbf{A}_{ic}^s \mathbf{B}_c^s \\ \mathbf{A}_{ri}^s & \mathbf{A}_{rr}^s & \mathbf{A}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{ci}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{x}_i^s \\ \mathbf{u}_r^s \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{f}_r^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{f}_c^s \end{Bmatrix}, \quad (3.143)$$

where

$$\mathbf{f}_r^s = \mathbf{R}_s^r \mathbf{f}_\Gamma^s, \quad (3.144)$$

$$\mathbf{f}_c^s = \mathbf{R}_s^c \mathbf{f}_\Gamma^s. \quad (3.145)$$

The dummy variable $\mathbf{x}_i^s$ can be concurrently eliminated from Eq.(3.143) by solving a subdomain level Dirichlet problem as

$$\mathbf{x}_i^s = -[\mathbf{A}_{ii}^s]^{-1}(\mathbf{A}_{ir}^s \mathbf{u}_r^s + \mathbf{A}_{ic}^s \mathbf{B}_c^s \mathbf{u}_c). \quad (3.146)$$

Substituting Eq.(3.146) into the Eq.(3.143) leads to the following partially assembled Schur complement system

$$\begin{bmatrix} \mathbf{S}_{rr}^s & \mathbf{S}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_r^s \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_r^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{f}_c^s \end{Bmatrix}, \quad (3.147)$$

where

$$\mathbf{S}_{\alpha\beta}^s = \mathbf{A}_{\alpha\beta}^s - \mathbf{A}_{\alpha i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{A}_{i\beta}^s, \quad (3.148)$$

where the subscripts α and β relate to r and c .

Due to the artificial Dirichlet boundary conditions imposed by the corner nodes, the local Schur complement matrix $\mathbf{S}_{rr}^s$ in Eq.(3.147) is positive-definite and hence invertible for the floating subdomains. Thus, the remaining interface unknown $\mathbf{u}_r^s$ can be obtained by solving the *fine Schur complement problem* as

$$\mathbf{S}_{rr}^s \mathbf{u}_r^s = \mathbf{f}_r^s - \mathbf{S}_{rc}^s \mathbf{B}_c^s \mathbf{u}_c. \quad (3.149)$$

Substituting the subdomain level solution $\mathbf{u}_r^s$ from Eq.(3.149) into Eq.(3.147) leads to the following global *coarse Schur complement problem*

$$\mathbf{F}_{cc} \mathbf{u}_c = \mathbf{d}_c, \quad (3.150)$$

where

$$\mathbf{F}_{cc} = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} (\mathbf{S}_{cc}^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s) \mathbf{B}_c^s \quad (3.151)$$

$$\mathbf{d}_c = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} (\mathbf{f}_c^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{f}_r^s). \quad (3.152)$$

The coarse Schur complement problem Eq.(3.150) couples the subdomains by the corner nodes constituting a global grid to transfer information across the subdomains.

Next, the local interface unknowns can be obtained as

$$\mathbf{u}_r^s = \mathbf{R}_s^{rT} \mathbf{u}_r^s + \mathbf{R}_s^{cT} \mathbf{u}_c^s. \quad (3.153)$$

The new approximate solution $\mathbf{u}_{\Gamma_{j+1}}$ can be expressed by updating the initial guess $\mathbf{u}_{\Gamma_j}$ with the average local solutions $\mathbf{u}_r^s$ as

$$\mathbf{u}_{\Gamma_{j+1}} = \mathbf{u}_{\Gamma_j} + \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{u}_r^s. \quad (3.154)$$

After some algebraic manipulations, the Neumann-Neumann with a coarse grid preconditioner can be expressed as

$$\mathbf{M}_{NNC}^{-1} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T (\mathbf{R}_s^{rT} [\mathbf{S}_{rr}^s]^{-1} \mathbf{R}_s^r) \mathbf{D}_s \mathbf{R}_s + \mathbf{R}_0^T [\mathbf{F}_{cc}]^{-1} \mathbf{R}_0, \quad (3.155)$$

where

$$\mathbf{R}_0 = \sum_{s=1}^{n_s} \mathbf{B}_c^T (\mathbf{R}_c^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{R}_r^s) \mathbf{D}_s \mathbf{R}_s. \quad (3.156)$$

Balancing Domain Decomposition by Constraints

The Balancing Domain Decomposition by Constraint (BDDC) is a non-overlapping domain decomposition preconditioner based on constrained energy minimization [67, 107, 108, 123]. The BDDC can be viewed as an evolution of the balancing domain decomposition (BDD) method. While BDD uses a multiplicative coarse problem, the BDDC method applies an additive coarse problem [108]. The use of an additive rather than multiplicative coarse problem leads to a favorable sparser coarse matrix [107].

The basic idea of BDDC is to find a set of coarse basis functions using the interface nodes and minimize the energy norm, subjected to some constraints. If primal constraints are used, the coarse basis functions have a value of unity at the corresponding coarse nodes and zero value on the remaining coarse nodes [4, 78]. The basis functions span a coarse space. Projection of the Schur complement operator onto this space leads to a coarse problem. The method can be explained as follows [7, 67, 78, 83, 107].

Let the physical domain Ω be decomposed into n_s non-overlapping subdomains. The equilibrium system of a typical subdomain Ω_s can be written as

$$\mathbf{A}^s \mathbf{u}^s = \mathbf{f}^s. \quad (3.157)$$

The discrete internal energy of subdomain Ω_s can be represented as [107]

$$E_s = \frac{1}{2} \mathbf{u}^{sT} \mathbf{A}^s \mathbf{u}^s. \quad (3.158)$$

Let ψ_s^j be the solution to the minimization problem of the subdomain internal energy E_s in Eq.(3.158) subject to the following constraints [107]

$$\mathbf{C}_s \mathbf{u}^s = \mathbf{e}_j, \quad (3.159)$$

where $\mathbf{C}_s$ represent a constraint matrix and $\mathbf{e}_j$ denotes the j^{th} column of the identity matrix. The matrix $\mathbf{C}_s$ contains constraints to couple the subdomains globally which naturally leads to a coarse problem [107, 123].

A constrained minimization problem can be solved to minimize the energy norm as

$$\text{minimize } E_s(\Psi_s) = \frac{1}{2} \Psi_s^T \mathbf{A}^s \Psi_s, \quad (3.160)$$

$$\text{subject to } \mathbf{C}_s \Psi_s = \mathbf{I}, \quad (3.161)$$

where $\mathbf{I}$ is the identity matrix and $\Psi_s = [\psi_s^1, \dots, \psi_s^{ncs}]$ and ncs is the size of the local (subdomain) constraints. These constraints make the subdomain problem well-posed.

Introducing a vector of Lagrange multipliers, the following Lagrangian function can be obtained for the above constrained minimization problem

$$\mathcal{L}(\Psi_s, \Lambda_s) = \frac{1}{2} \Psi_s^T \mathbf{A}^s \Psi_s + \Lambda_s^T (\mathbf{C}_s \Psi_s - \mathbf{I}). \quad (3.162)$$

Minimizing the Lagrangian function in Eq.(3.162) with respect to Ψ_s and Λ_s , the following linear system is obtained

$$\begin{bmatrix} \mathbf{A}^s & \mathbf{C}_s^T \\ \mathbf{C}_s & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \Psi_s \\ \Lambda_s \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{I} \end{Bmatrix}. \quad (3.163)$$

If primal constraints are used (e.g. the constraints represent continuity at the subdomain corner nodes), Lagrange multipliers are not required in order to enforce the constraints. In this case, the functions Ψ_s are *discrete harmonic functions* (i.e. the functions Ψ_s have a zero value at all the corner nodes except one where they have a value of unity, and they have minimal energy on the remaining interface nodes) [4, 78, 83, 124, 125]. Consequently, the coarse basis functions Ψ_s can be obtained via an analogy to block Cholesky factorization as explained next [78, 83].

Let the subdomain unknown $\mathbf{u}^s$ be partitioned into the interior unknown $\mathbf{u}_i^s$, remaining unknown $\mathbf{u}_r^s$ and corner unknown $\mathbf{u}_c^s$. The equilibrium of a typical subdomain Ω_s can be expressed as

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s & \mathbf{A}_{ic}^s \\ \mathbf{A}_{ri}^s & \mathbf{A}_{rr}^s & \mathbf{A}_{rc}^s \\ \mathbf{A}_{ci}^s & \mathbf{A}_{cr}^s & \mathbf{A}_{cc}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s \\ \mathbf{u}_r^s \\ \mathbf{u}_c^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_r^s \\ \mathbf{f}_c^s \end{Bmatrix}. \quad (3.164)$$

Partial assembly of the corner node unknown $\mathbf{u}_c^s$ in Eq.(3.164) leads to the following equilibrium equation

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s & \mathbf{A}_{ic}^s \mathbf{B}_c^s \\ \mathbf{A}_{ri}^s & \mathbf{A}_{rr}^s & \mathbf{A}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{ci}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s \\ \mathbf{u}_r^s \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_r^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{f}_c^s \end{Bmatrix}, \quad (3.165)$$

where $\mathbf{B}_c^s$ is a Boolean restriction operator that maps the global corner vector $\mathbf{u}_c$ to the local corner vector $\mathbf{u}_c^s$ as

$$\mathbf{u}_c^s = \mathbf{B}_c^s \mathbf{u}_c. \quad (3.166)$$

The interior variable $\mathbf{u}_i^s$ can be obtained from the first row of Eq.(3.165) as

$$\mathbf{u}_i^s = [\mathbf{A}_{ii}^s]^{-1} (\mathbf{f}_i^s - \mathbf{A}_{ir}^s \mathbf{u}_r^s - \mathbf{A}_{ic}^s \mathbf{B}_c^s \mathbf{u}_c^s). \quad (3.167)$$

Substituting $\mathbf{u}_i^s$ in the second and third rows of Eq.(3.165), the following Schur complement system is obtained

$$\begin{bmatrix} \mathbf{S}_{rr}^s & \mathbf{S}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_r^s \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{g}_r^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{g}_c^s \end{Bmatrix}, \quad (3.168)$$

where

$$\mathbf{S}_{\alpha\beta}^s = \mathbf{A}_{\alpha\beta}^s - \mathbf{A}_{\alpha i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{A}_{i\beta}^s, \quad (3.169)$$

$$\mathbf{g}_\alpha^s = \mathbf{f}_\alpha^s - \mathbf{A}_{\alpha i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{f}_i^s, \quad (3.170)$$

and α and β denote the subscripts r and c .

Equivalently, the Schur complement system in Eq.(3.168) can be expressed as

$$\tilde{\mathbf{S}}^s \tilde{\mathbf{u}}_r^s = \tilde{\mathbf{g}}^s. \quad (3.171)$$

Performing Cholesky factorization to the partially assembled Schur complement matrix $\tilde{\mathbf{S}}^s$ in Eq.(3.171), one obtains

$$Fact(\tilde{\mathbf{S}}^s) = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{S}_{rr}^s & \mathbf{0} \\ \mathbf{0} & \mathbf{F}_{cc} \end{bmatrix} \begin{bmatrix} \mathbf{I} & [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \quad (3.172)$$

where

$$\mathbf{F}_{cc} = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} (\mathbf{S}_{cc}^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s) \mathbf{B}_c^s. \quad (3.173)$$

Alternatively, $\mathbf{F}_{cc}$ can be expressed as

$$\mathbf{F}_{cc} = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{F}_{cc}^s \mathbf{B}_c^s, \quad (3.174)$$

where the local coarse grid operator is represented as

$$\mathbf{F}_{cc}^s = \mathbf{S}_{cc}^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s. \quad (3.175)$$

Inverting the factored partially assembled Schur complement matrix in Eq.(3.172) as [83]

$$[\tilde{\mathbf{S}}^s]^{-1} = \begin{bmatrix} \mathbf{I} & -[\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} [\mathbf{S}_{rr}^s]^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{F}_{cc}^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} & \mathbf{I} \end{bmatrix}. \quad (3.176)$$

Let the function Ψ_s be defined as

$$\Psi_s = \begin{bmatrix} -[\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s \\ \mathbf{I} \end{bmatrix}. \quad (3.177)$$

Then the inverse of the the partially assembled Schur complement matrix in Eq.(3.176) can be expressed as

$$[\tilde{\mathbf{S}}^s]^{-1} = \begin{bmatrix} [\mathbf{S}_{rr}^s]^{-1} & 0 \\ 0 & 0 \end{bmatrix} + \Psi_s \mathbf{F}_{cc}^{-1} \Psi_s^T. \quad (3.178)$$

Clearly, the partially assembled Schur complement problem in Eq.(3.178) consists of a local (fine) and global (coarse) components respectively defined as

$$\mathbf{T}_{sub}^s = [\mathbf{S}_{rr}^s]^{-1}, \quad (3.179)$$

$$\mathbf{T}_0^s = \Psi_s \mathbf{F}_{cc}^{-1} \Psi_s^T. \quad (3.180)$$

Note that the local coarse grid operator $\mathbf{F}_{cc}^s$ in Eq.(3.175) can be expressed in terms of the coarse basis functions Ψ_s as

$$\mathbf{F}_{cc}^s = \mathbf{S}_{cc}^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s \quad (3.181)$$

$$= \begin{bmatrix} -\mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{S}_{rr}^s & \mathbf{S}_{rc}^s \\ \mathbf{S}_{cr}^s & \mathbf{S}_{cc}^s \end{bmatrix} \begin{bmatrix} -[\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s \\ \mathbf{I} \end{bmatrix} \quad (3.182)$$

$$= \Psi_s^T \mathbf{S}_s \Psi_s. \quad (3.183)$$

Accordingly, the global coarse operator $\mathbf{F}_{cc}$ can be expressed as

$$\mathbf{F}_{cc} = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \Psi_s^T \mathbf{S}_s \Psi_s \mathbf{B}_c^s, \quad (3.184)$$

where

$$\mathbf{S}_s = \begin{bmatrix} \mathbf{S}_{rr}^s & \mathbf{S}_{rc}^s \\ \mathbf{S}_{cr}^s & \mathbf{S}_{cc}^s \end{bmatrix}. \quad (3.185)$$

Given a global residual vector $\mathbf{r}_\Gamma$, its local component $\mathbf{r}_r^s$ can be obtained as

$$\mathbf{r}_r^s = \mathbf{R}_s^r \mathbf{r}_\Gamma^s, \quad (3.186)$$

where

$$\mathbf{r}_\Gamma^s = \mathbf{D}_s \mathbf{R}_s \mathbf{r}_\Gamma. \quad (3.187)$$

Consequently, the local (fine) solution $\mathbf{u}_r^s$ is obtained as

$$\begin{aligned} \mathbf{u}_r^s &= [\mathbf{S}_{rr}^s]^{-1} \mathbf{r}_r^s, \\ &= [\mathbf{S}_{rr}^s]^{-1} \mathbf{R}_s^r \mathbf{r}_\Gamma^s. \end{aligned} \quad (3.188)$$

The coarse component $\mathbf{u}_c^s$ is

$$\mathbf{u}_c^s = \Psi_s \mathbf{F}_{cc}^{-1} \Psi_s^T \mathbf{r}_\Gamma^s. \quad (3.189)$$

For the subdomain Ω_s , the interface unknown $\mathbf{u}_\Gamma^s$ can be expressed as

$$\begin{aligned} \mathbf{u}_\Gamma^s &= \mathbf{R}_s^{rT} \mathbf{u}_r^s + \mathbf{u}_c^s, \\ &= \mathbf{R}_s^{rT} [\mathbf{S}_{rr}^s]^{-1} \mathbf{R}_s^r \mathbf{r}_\Gamma^s + \Psi_s \mathbf{F}_{cc}^{-1} \Psi_s^T \mathbf{r}_\Gamma^s \end{aligned} \quad (3.190)$$

The global interface unknown $\mathbf{u}_\Gamma$ can be constructed from the local interface unknown $\mathbf{u}_\Gamma^s$ gathered from all the subdomains as

$$\mathbf{u}_\Gamma = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T \mathbf{u}_\Gamma^s. \quad (3.191)$$

Now $\mathbf{u}_\Gamma$ can be expressed in terms of the global interface residual $\mathbf{r}_\Gamma$ as

$$\mathbf{u}_\Gamma = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T (\mathbf{R}_s^{rT} [\mathbf{S}_{rr}^s]^{-1} \mathbf{R}_s^r + \Psi_s \mathbf{F}_{cc}^{-1} \Psi_s^T) \mathbf{D}_s \mathbf{R}_s \mathbf{r}_\Gamma. \quad (3.192)$$

Therefore the BDDC preconditioner takes the following form

$$\mathbf{M}_{BDDC}^{-1} = \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^T (\mathbf{T}_{sub} + \mathbf{T}_0) \mathbf{D}_s \mathbf{R}_s, \quad (3.193)$$

where

$$\mathbf{T}_{sub} = \mathbf{R}_s^{rT} [\mathbf{S}_{rr}^s]^{-1} \mathbf{R}_s^r, \quad \text{and} \quad \mathbf{T}_0 = \Psi_s \mathbf{F}_{cc}^{-1} \Psi_s^T. \quad (3.194)$$

Condition Number Bound

If h is the finite element mesh size and H is a typical subdomain size, the condition number of the BDDC method is bounded by [67, 108]

$$\kappa(\mathbf{M}_{BDDC}^{-1} \mathbf{S}) \leq C(1 + \log(\frac{H}{h}))^2, \quad (3.195)$$

where C is a positive coefficient independent of the the number of subdomains and the size of the elements.

3.3.2 Primal-Primal Iterative Substructuring Method

In this section, we describe a novel primal version of iterative substructuring methods for the solution of the large-scale linear system arising from the finite element method. The method offers a straightforward approach to formulate a two-level scalable preconditioner. In this method, the interior and corner degrees of freedom are eliminated first to obtain a *reduced interface problem* for the remaining degrees of freedom. Next, the two-level preconditioner for the reduced interface problem is formulated by strictly enforcing the continuity condition on the corner nodes of the interface by global assembly. The continuity condition on the remaining interface nodes is satisfied weakly (in an average sense). The continuity of the solution field across the entire interface is eventually satisfied at the convergence of the iterations. This approach naturally leads to a coarse grid which connects the subdomains globally via the corner nodes. The coarse grid provides a mechanism to propagate information globally which makes the algorithm scalable with respect to subdomain size.

For a typical subdomain Ω_s , we partition the subdomain nodal vector $\mathbf{u}^s$ into a set of interior unknowns $\mathbf{u}_i^s$, remaining unknowns $\mathbf{u}_r^s$ and corner unknowns $\mathbf{u}_c^s$ as schematically shown in Fig.(3.4).

Figure 3.4: Partitioning the subdomain nodes into: interior (◊), remaining (■) and corner(●)

According to this partitioning scheme, the subdomain equilibrium equation can be represented as

$$\begin{bmatrix} A_{ii}^s & A_{ir}^s & A_{ic}^s \\ A_{ri}^s & A_{rr}^s & A_{rc}^s \\ A_{ci}^s & A_{cr}^s & A_{cc}^s \end{bmatrix} \begin{Bmatrix} u_i^s \\ u_r^s \\ u_c^s \end{Bmatrix} = \begin{Bmatrix} f_i^s \\ f_r^s \\ f_c^s \end{Bmatrix}. \quad (3.196)$$

Enforcing the transmission conditions along the boundary interfaces, the subdomain equilibrium equation can be expressed as

$$\begin{bmatrix}
\mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s \mathbf{B}_r^s & \mathbf{A}_{ic}^s \mathbf{B}_c^s \\
\sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{A}_{ri}^s & \sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{A}_{rr}^s \mathbf{B}_r^s & \sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{A}_{rc}^s \mathbf{B}_c^s \\
\sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{ci}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cr}^s \mathbf{B}_r^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cc}^s \mathbf{B}_c^s
\end{bmatrix}
\begin{Bmatrix}
\mathbf{u}_i^s \\
\mathbf{u}_r \\
\mathbf{u}_c
\end{Bmatrix}
=
\begin{Bmatrix}
\mathbf{f}_i^s \\
\sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{f}_r^s \\
\sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{f}_c^s
\end{Bmatrix}
\quad (3.197)$$

where $\mathbf{B}_r^s$ is a Boolean rectangular matrix that maps the global remaining vector $\mathbf{u}_r$ to the local remaining vector $\mathbf{u}_r^s$ as

$$\mathbf{u}_r^s = \mathbf{B}_r^s \mathbf{u}_r. \quad (3.198)$$

Similarly, the restriction operator $\mathbf{B}_c^s$ is a Boolean rectangular matrix that maps the global corner vector $\mathbf{u}_c$ to the local corner vector $\mathbf{u}_c^s$ as

$$\mathbf{u}_c^s = \mathbf{B}_c^s \mathbf{u}_c. \quad (3.199)$$

In parallel implementation both $\mathbf{B}_r^s$ and $\mathbf{B}_c^s$ act as *scatter* operators, while $\mathbf{B}_r^{sT}$ and $\mathbf{B}_c^{sT}$ act as *gather* operators.

The first block equation in Eq.(3.197) can be solved concurrently for $\mathbf{u}_i^s$ as

$$\mathbf{u}_i^s = [\mathbf{A}_{ii}^s]^{-1} (\mathbf{F}_i^s - \mathbf{A}_{ir}^s \mathbf{B}_r^s \mathbf{u}_r - \mathbf{A}_{ic}^s \mathbf{B}_c^s \mathbf{u}_c). \quad (3.200)$$

Substituting Eq.(3.200) into Eq.(3.197) leads to the following condensed system

$$\begin{bmatrix} \sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{S}_{rr}^s \mathbf{B}_r^s & \sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{S}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s \mathbf{B}_r^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_r \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{g}_r^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{g}_c^s \end{Bmatrix}, \quad (3.201)$$

where

$$\mathbf{S}_{\alpha\beta}^s = \mathbf{A}_{\alpha\beta}^s - \mathbf{A}_{\alpha i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{A}_{i\beta}^s, \quad (3.202)$$

$$\mathbf{g}_\alpha^s = \mathbf{f}_\alpha^s - \mathbf{A}_{\alpha i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{f}_i^s. \quad (3.203)$$

The interface system in Eq.(3.201) involves the remaining nodal vector $\mathbf{u}_r$ and corner node unknown $\mathbf{u}_c$ as shown in Fig.(3.5).

Figure 3.5: The interface boundary nodes split into: remaining (■) and corner(●) nodes

The corner nodal vector $\mathbf{u}_c$ in Eq.(3.201) is eliminated next to obtain the following symmetric positive definite reduced interface problem

$$(\mathbf{F}_{rr} - \mathbf{F}_{rc}[\mathbf{F}_{cc}]^{-1}\mathbf{F}_{cr})\mathbf{u}_r = \mathbf{d}_r - \mathbf{F}_{rc}[\mathbf{F}_{cc}]^{-1}\mathbf{d}_c, \quad (3.204)$$

where

$$\mathbf{F}_{\alpha\beta} = \sum_{s=1}^{n_s} \mathbf{B}_{\alpha}^{sT} \mathbf{S}_{\alpha\beta}^s \mathbf{B}_{\beta}^s, \quad (3.205)$$

$$\mathbf{d}_{\alpha} = \sum_{s=1}^{n_s} \mathbf{B}_{\alpha}^{sT} \mathbf{g}_{\alpha}^s, \quad (3.206)$$

and α and β denotes subscripts r and c . The reduced interface problem can be solved using PCGM with an appropriate preconditioner defined in the next section.

Primal-Primal Preconditioner

As alluded previously, the continuity condition on the remaining interface nodes is enforced weakly. At the corner nodes, the continuity is enforced strictly. This fact is schematically illustrated in Fig.(3.6). As the iterations converges the continuity condition is enforced strictly for the entire interface nodal vector. Consequently, the following equilibrium equation is obtained

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s & \mathbf{A}_{ic}^s \mathbf{B}_c^s \\ \mathbf{A}_{ri}^s & \mathbf{A}_{rr}^s & \mathbf{A}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{ci}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{x}_i^s \\ \mathbf{u}_r^s \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{f}_r^s \\ \mathbf{0} \end{Bmatrix}, \quad (3.207)$$

where $\mathbf{f}_r^s = \mathbf{D}_r^s \mathbf{B}_r^s \mathbf{r}_j$ and $\mathbf{r}_j$ is the residual at the j^{th} iteration of the iterative solver and $\mathbf{D}_r^s$ represents a diagonal weighting matrix which satisfies the following property

$$\sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{D}_r^s \mathbf{B}_r^s = \mathbf{I}. \quad (3.208)$$

The diagonal entries of each block of $\mathbf{D}_r^s$ are the reciprocal of the number of subdomains that share the remaining interface boundary nodes.

Figure 3.6: Partial assembly of corner nodes (●)

The dummy variable $\mathbf{x}_i^s$ can be eliminated from Eq.(3.207) in parallel by solving a sub-domain level Dirichlet problem as

$$\mathbf{x}_i^s = -[\mathbf{A}_{ii}^s]^{-1}(\mathbf{A}_{ir}^s \mathbf{u}_r^s + \mathbf{A}_{ic}^s \mathbf{B}_s \mathbf{u}_c). \quad (3.209)$$

Substituting Eq.(3.209) into the Eq.(3.207) leads to

$$\begin{bmatrix} \mathbf{S}_{rr}^s & \mathbf{S}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s \mathbf{B}_r^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_r^s \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_r^s \\ 0 \end{Bmatrix}. \quad (3.210)$$

For each subdomain, $\mathbf{u}_r^s$ can be eliminated in parallel from the first row of Eq.(3.210) as

$$\mathbf{u}_r^s = [\mathbf{S}_{rr}^s]^{-1}(\mathbf{f}_r^s - \mathbf{S}_{rc}^s \mathbf{B}_c^s \mathbf{u}_c). \quad (3.211)$$

Substituting $\mathbf{u}_r^s$ into the second row of Eq.(3.210) leads to the following coarse problem

$$\mathbf{F}_{cc} \mathbf{u}_c = \mathbf{d}_c, \quad (3.212)$$

where

$$\mathbf{F}_{cc} = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} (\mathbf{S}_{cc}^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s) \mathbf{B}_c^s, \quad (3.213)$$

$$\mathbf{d}_c = - \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{f}_r^s. \quad (3.214)$$

The continuity of the solution field on the remaining interface nodes $\mathbf{u}_r$ is satisfied next by averaging $\mathbf{u}_r^s$ for all the subdomains as

$$\mathbf{u}_r = \sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{D}_r^s \mathbf{u}_r^s. \quad (3.215)$$

After some algebraic manipulations, the primal-primal preconditioner can be expressed as

$$\mathbf{M}_{PP}^{-1} = \sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{D}_r^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{D}_r^s \mathbf{B}_r^s + \mathbf{R}_0^T [\mathbf{F}_{cc}]^{-1} \mathbf{R}_0, \quad (3.216)$$

where

$$\mathbf{R}_0 = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{D}_r^s \mathbf{B}_r^s. \quad (3.217)$$

3.3.3 Dual Iterative Substructuring Method

The Finite Element Tearing and Interconnecting (FETI) is a Lagrange multiplier based technique for solving the linear system arising from the discretization of self-adjoint elliptic PDEs [119, 120, 126–129]. In the FETI method, the solution domain is decomposed into a number of non-overlapping subdomains [130]. On each subdomain, a local stiffness matrix and a local load vector are obtained from the finite element discretization of a subdomain level problem. The continuity of the solution field along the subdomain interfaces is enforced by Lagrange multipliers [131]. The interior variables are then eliminated by solving a subdomain level Neumann problems resulting a *dual interface problem* containing Lagrange multipliers. The dual interface problem is solved using a projected PCGM algorithm equipped with lumped or Dirichlet preconditioners. In each iteration of the iterative solver, the equilibrium in each subdomain is satisfied. However, the continuity is strictly enforced only when the iterative solver converges [119, 120, 126].

In the FETI method, an algebraic coarse problem handles the issue of floating subdomains (having singular stiffness matrices). The coarse problem enables a global propagation of information across the subdomains [7, 110, 132]. In particular, the coarse problem provides a global mechanism to exchange information among non-neighboring subdomains without requiring the transmission of information through the intermediate subdomains [7, 110, 132]. The coarse problem forces the condition number of FETI method to be bounded and independent on the number of subdomains [120]. The FETI iterative substructuring method can be summarized as follows [4, 7, 119].

Let the spatial domain Ω be partitioned into n_s non-overlapping subdomains $\{\Omega_s, 1 \leq s \leq n_s\}$. For a typical subdomain Ω_s , let $\mathbf{u}_s, \mathbf{A}_s$ and $\mathbf{f}_s$ be the local solution vector, the subdomain stiffness matrix and local load vector respectively. For the entire system, the extended stiffness matrix, solution and load vectors can be expressed as follows [7]

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}^1 & & & \\ & \ddots & & \\ & & \mathbf{A}^s & \\ & & & \ddots \\ & & & & \mathbf{A}^{n_s} \end{bmatrix}, \quad \mathbf{u} = \begin{Bmatrix} \mathbf{u}^1 \\ \vdots \\ \mathbf{u}^s \\ \vdots \\ \mathbf{u}^{n_s} \end{Bmatrix}, \quad \mathbf{f} = \begin{Bmatrix} \mathbf{f}^1 \\ \vdots \\ \mathbf{f}^s \\ \vdots \\ \mathbf{f}^{n_s} \end{Bmatrix}. \quad (3.218)$$

The subdomain stiffness matrix is positive semidefinite for the case of floating subdomains. Let $\mathbf{Z}_s$ be a full rank matrix of size $n_s \times \min(1, d_s)$ whose columns span the null space of the subdomain stiffness matrix $\mathbf{A}_s$. When the subdomain stiffness matrix is positive definite, $\mathbf{Z}_s$ is a void matrix. In the block matrix form the null space matrix can be expressed as [7]

$$\mathbf{Z} = \begin{bmatrix} \mathbf{Z}^1 & & & \\ & \ddots & & \\ & & \mathbf{Z}^s & \\ & & & \ddots \\ & & & & \mathbf{Z}^{n_s} \end{bmatrix}, \quad (3.219)$$

where $\text{Range}(\mathbf{Z}) = \text{Kernel}(\mathbf{A})$ and $\text{Kernel}(\mathbf{Z}) = \{\mathbf{0}\}$.

Let $\mathbf{B}^s$ be a signed Boolean matrix that enforces that the nodal interface variables have the same values for all the subdomains shearing the same boundaries. This constrain is represented by

$$\mathbf{B}^s \mathbf{u}^s = 0. \quad (3.220)$$

The global continuity matrix $\mathbf{B}$ takes the following form

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}^1 & & & \\ & \ddots & & \\ & & \mathbf{B}^s & \\ & & & \ddots \\ & & & & \mathbf{B}^{n_s} \end{bmatrix}. \quad (3.221)$$

In FETI method, the original finite element problem is restated as follows [4, 7, 78, 133]

Find $\mathbf{u}$ such that

$$J(\mathbf{u}) = \frac{1}{2} \mathbf{u}^T \mathbf{A} \mathbf{u} - \mathbf{u}^T \mathbf{f} \rightarrow \min \quad (3.222)$$

subject to $\mathbf{B} \mathbf{u} = 0$.

By introducing a vector of Lagrange multipliers $\boldsymbol{\lambda}$, the constrained minimization problem in Eq.(3.222) can be reexpressed as a saddle point problem as

$$\mathcal{L}(\mathbf{u}, \boldsymbol{\lambda}) = \frac{1}{2} \mathbf{u}^T \mathbf{A} \mathbf{u} - \mathbf{u}^T \mathbf{f} + \mathbf{u}^T \mathbf{B}^T \boldsymbol{\lambda}. \quad (3.223)$$

The Lagrange multipliers λ *weakly* enforces the continuity condition of the nodal interface variables.

Minimizing the Lagrangian function in Eq.(3.223) with respect to u and λ leads to the following equilibrium system

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} u \\ \lambda \end{Bmatrix} = \begin{Bmatrix} f \\ 0 \end{Bmatrix}. \quad (3.224)$$

If $\mathbf{A}$ is singular, a solution vector u of the first equation in Eq.(3.224) exists if and only if [4, 7]

$$(f - \mathbf{B}^T \lambda) \in \text{Range}(\mathbf{A}). \quad (3.225)$$

The general solution to the singular system can be written as [4, 7]

$$u = \mathbf{A}^+(f - \mathbf{B}^T \lambda) + \mathbf{Z}\alpha \quad \text{if} \quad (f - \mathbf{B}^T \lambda) \perp \text{Kernel}(\mathbf{A}) \quad (3.226)$$

where $\mathbf{A}^+$ is a pseudo-inverse of $\mathbf{A}$ and $\alpha \in \mathbb{R}^d$ is to be determined. Note that, the condition $(f - \mathbf{B}^T \lambda) \perp \text{Kernel}(\mathbf{A})$ means that the action of applied forces does not excite the rigid body motions [4, 7].

Since the matrix $\mathbf{Z}$ has a full rank, and the column vectors of $\mathbf{Z}^T$ span the null space of the singular matrix $\mathbf{A}$, the solution exists when

$$\mathbf{Z}^T(f - \mathbf{B}^T \lambda) = 0. \quad (3.227)$$

Eq.(3.227) can be rewritten as

$$\mathbf{G}^T \boldsymbol{\lambda} = \mathbf{e} \quad (3.228)$$

where $\mathbf{G} = \mathbf{BZ}$ and $\mathbf{e} = \mathbf{Z}^T \mathbf{f}$.

Using the constrain $\mathbf{Bu} = 0$, Eq.(3.226) yields

$$\mathbf{BA}^+(\mathbf{f} - \mathbf{B}^T \boldsymbol{\lambda}) + \mathbf{BZ}\boldsymbol{\alpha} = 0. \quad (3.229)$$

Eq.(3.229) can be expressed as

$$\mathbf{F}\boldsymbol{\lambda} - \mathbf{G}\boldsymbol{\alpha} = \mathbf{d}, \quad (3.230)$$

where $\mathbf{F} = \mathbf{BA}^+\mathbf{B}^T$, $\mathbf{G} = \mathbf{BZ}$ and $\mathbf{d} = \mathbf{BA}^+\mathbf{f}$.

When Eq.(3.230) and Eq.(3.228) are combined, one obtains the following linear system

$$\mathbf{F}\boldsymbol{\lambda} - \mathbf{G}\boldsymbol{\alpha} = \mathbf{d}. \quad (3.231)$$

$$\mathbf{G}^T \boldsymbol{\lambda} = \mathbf{e}. \quad (3.232)$$

Let $\mathbf{P}$ be an orthogonal projection operator onto $\text{Kernel}(\mathbf{G}^T)$ defined as [4, 7]

$$\mathbf{P} = \mathbf{I} - \mathbf{G}(\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T \quad (3.233)$$

Multiplying the first equation of Eq.(3.231) by the orthogonal projector P yields

$$PF\lambda = Pd \quad (3.234)$$

The FETI method is a preconditioned conjugate gradient method applied to solve the system defined in Eq.(3.234) (as schematically shown in Fig.(3.7)) with an initial approximation λ_0 chosen such that

$$G^T \lambda_0 = e. \quad (3.235)$$

Figure 3.7: Lagrange multiples are the force required to enforce continuity constraint

Once λ is determined, the unknown coefficient vector α can be obtained from Eq.(3.230) in a least square sense as

$$\alpha = (\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T (\mathbf{F} \lambda - \mathbf{d}) \quad (3.236)$$

Any solution λ from Eq.(3.231) is unique up to an additive vector from $Kernel(\mathbf{B}^T)$ [7]. However, any of these solutions of λ are the solution to the minimization problem. Here $\mathbf{u}$ is given by Eq.(3.226) with α defined by Eq.(3.236). When the matrix $\mathbf{A}$ is not singular, the coefficient vector α is omitted. In this case $\mathbf{F} = \mathbf{B} \mathbf{A}^{-1} \mathbf{B}^T$, $\mathbf{d} = \mathbf{B} \mathbf{A}^{-1} \mathbf{f}$, $\mathbf{G} = \mathbf{0}$, $\mathbf{P} = \mathbf{I}$ and $\mathbf{e} = \mathbf{0}$.

Preconditioners for FETI

The FETI method can be viewed as a projected preconditioned conjugate gradient iterative solver for the Lagrange multipliers as [4, 7, 64]

$$\mathbf{P} \mathbf{M}^{-1} \mathbf{P}^T \mathbf{F} \lambda = \mathbf{P} \mathbf{M}^{-1} \mathbf{P}^T \mathbf{d} \quad (3.237)$$

Two types of preconditioner $\mathbf{M}^{-1}$ are available to FETI method, lumped and Dirichlet preconditioners. The lumped preconditioner approximates the local Schur complement matrix by its leading matrix as

$$\mathbf{M}_L^{-1} = \sum_{s=1}^{n_s} \mathbf{B}^s \mathbf{D}^s \mathbf{A}_{\Gamma\Gamma}^s \mathbf{D}^s \mathbf{B}^{sT}. \quad (3.238)$$

This preconditioner is not expensive to apply, but not mathematically optimal. On the other hand, the Dirichlet preconditioner is defined as

$$\mathbf{M}_D^{-1} = \sum_{s=1}^{n_s} \mathbf{B}^s \mathbf{D}^s \mathbf{S}_s \mathbf{D}^s \mathbf{B}^{sT}. \quad (3.239)$$

The Dirichlet preconditioner is mathematically optimal [134] due to the fact that it leads to the boundness of the condition number estimate [4, 7, 134]. Application of the Dirichlet preconditioner requires the solution of a local subdomain problem with non-homogeneous Dirichlet boundary conditions.

Condition Number Bound

For the second order elliptic problems, the condition number of the preconditioned coefficient matrices in Eq.(3.237), equipped with the Dirichlet preconditioner $\mathbf{M}_D^{-1}$, grows asymptotically as [4, 126]

$$\kappa(\mathbf{P} \mathbf{M}_D^{-1} \mathbf{P}^T \mathbf{F}) \leq C(1 + \log \frac{H}{h})^2, \quad (3.240)$$

where C is a positive coefficient independent of the mesh size h and subdomain size H . Clearly the condition number estimation of FETI method indicates that the method is numerically scalable with respect to problem size h and subdomain size H [129].

3.3.4 Dual-Primal Iterative Substructuring Method

The existence of non-trivial kernels of the local subdomain stiffness matrices is essential for the scalability of FETI method [4, 7, 135]. For complex problems, the characterization of these local kernels is not a trivial task [4, 7].

In the Dual-Primal Finite Element Tearing and Interconnecting (FETI-DP) [64, 81, 136–138], the continuity condition on the corner nodes (the primal variables) of the subdomains is enforced strictly in each iteration while Lagrange multipliers (the dual variables) are used to enforce the continuity constraint weakly on the remaining interface nodes. The continuity condition on the whole interface boundary is enforced only when the iterative solver converges. Strictly enforcing the continuity condition on the corner nodes at each iteration makes the local (subdomain) problems nonsingular. This fact also naturally provides a global coarse problem. The original FETI, on the other hand, is a projected preconditioned conjugate gradient which cannot start from an arbitrary guess [4, 7]. In some cases, the initial guess can be faraway from the exact solution [4, 7]. The FETI-DP, in contrast, employs the standard preconditioned conjugate gradient algorithm which can be start with any arbitrary initial guess [4, 7]. The dual-primal FETI method can be described as follows [4, 7, 64, 81, 136, 137].

Let the physical domain Ω be decomposed into n_s non-overlapping subdomains. The subdomain nodes are partitioned into interior $\mathbf{u}_i^s$, remaining $\mathbf{u}_r^s$ and corner $\mathbf{u}_c^s$ nodes as shown schematically in Fig.(3.4). The equilibrium system of a typical subdomain Ω_s can be expressed as [4, 7, 64, 81, 136, 137]

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s & \mathbf{A}_{ic}^s \\ \mathbf{A}_{ri}^s & \mathbf{A}_{rr}^s & \mathbf{A}_{rc}^s \\ \mathbf{A}_{ci}^s & \mathbf{A}_{cr}^s & \mathbf{A}_{cc}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s \\ \mathbf{u}_r^s \\ \mathbf{u}_c^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_r^s \\ \mathbf{f}_c^s \end{Bmatrix}. \quad (3.241)$$

The global equilibrium equation is given by [7, 64, 78, 83]

$$\begin{bmatrix} \mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s & \mathbf{A}_{ic}^s \mathbf{B}_c^s \\ \mathbf{A}_{ri}^s & \mathbf{A}_{rr}^s & \mathbf{A}_{rc}^s \mathbf{B}_c^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{ci}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cc}^s \mathbf{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s \\ \mathbf{u}_r^s \\ \mathbf{u}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_r^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{f}_c^s \end{Bmatrix}, \quad (3.242)$$

where $\mathbf{B}_c^s$ is a Boolean restriction operator that maps the global corner vector $\mathbf{u}_c$ to the local corner vector $\mathbf{u}_c^s$ as

$$\mathbf{u}_c^s = \mathbf{B}_c^s \mathbf{u}_c. \quad (3.243)$$

The partially assembled system in Eq.(3.242) can be rewritten in compact form as

$$\tilde{\mathbf{A}}^s \tilde{\mathbf{u}}^s = \tilde{\mathbf{f}}^s, \quad (3.244)$$

where $\tilde{\mathbf{A}}^s$ denotes the partially assembled stiffness matrix, $\tilde{\mathbf{u}}^s$ is a partially assembled unknowns nodal vector, and $\tilde{\mathbf{f}}^s$ is the associated partially assembled load vector.

Let $\mathbf{B}_r^s$ be a signed Boolean continuity matrix defined as

$$\sum_{s=1}^{n_s} \mathbf{B}_r^s \mathbf{u}_r^s = \mathbf{0}. \quad (3.245)$$

Next, the original finite element problem can be reformulated as an equivalent constrained minimization problem as

$$\frac{1}{2}\tilde{\mathbf{u}}^T \tilde{\mathbf{A}} \tilde{\mathbf{u}} - \tilde{\mathbf{u}}^T \tilde{\mathbf{f}} \rightarrow \min \quad (3.246)$$

$$\text{subject to } \mathbf{B}\mathbf{u} = 0,$$

where

$$\tilde{\mathbf{A}} = \begin{bmatrix} \tilde{\mathbf{A}}^1 & & & \\ & \ddots & & \\ & & \tilde{\mathbf{A}}^s & \\ & & & \ddots \\ & & & & \tilde{\mathbf{A}}^{n_s} \end{bmatrix}, \quad \tilde{\mathbf{u}} = \begin{bmatrix} \tilde{u}^1 \\ \vdots \\ \tilde{u}^s \\ \vdots \\ \tilde{u}^{n_s} \end{bmatrix}, \quad \tilde{\mathbf{f}} = \begin{bmatrix} \tilde{f}^1 \\ \vdots \\ \tilde{f}^s \\ \vdots \\ \tilde{f}^{n_s} \end{bmatrix}, \quad (3.247)$$

$$\mathbf{B} = [(\mathbf{0} \ \mathbf{B}_r^1 \ 0), \dots, (\mathbf{0} \ \mathbf{B}_r^s \ 0), \dots, (\mathbf{0} \ \mathbf{B}_r^{n_s} \ 0)]. \quad (3.248)$$

Introducing Lagrange multipliers to weakly enforce the compatibility constraint, the constrained minimization problem in Eq.(3.246) can be expressed as [4, 7]

$$\mathcal{L}(\tilde{\mathbf{u}}, \boldsymbol{\lambda}) = \frac{1}{2}\tilde{\mathbf{u}}^T \tilde{\mathbf{A}} \tilde{\mathbf{u}} - \tilde{\mathbf{u}}^T \tilde{\mathbf{f}} + \tilde{\mathbf{u}}^T \mathbf{B}^T \boldsymbol{\lambda}. \quad (3.249)$$

Minimizing Eq.(3.249) with respect to $\tilde{\mathbf{u}}$ and $\boldsymbol{\lambda}$ leads to the following equilibrium system [7, 64, 78, 83]

$$\begin{bmatrix}
 \mathbf{A}_{ii}^s & \mathbf{A}_{ir}^s & \mathbf{A}_{ic}^s \mathbf{B}_c^s & 0 \\
 \mathbf{A}_{ri}^s & \mathbf{A}_{rr}^s & \mathbf{A}_{rc}^s \mathbf{B}_c^s & \mathbf{B}_r^{sT} \\
 \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{ci}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{A}_{cc}^s \mathbf{B}_c^s & 0 \\
 0 & \sum_{s=1}^{n_s} \mathbf{B}_r^s & 0 & 0
 \end{bmatrix}
 \begin{Bmatrix}
 \mathbf{u}_i^s \\
 \mathbf{u}_r^s \\
 \mathbf{u}_c \\
 \lambda
 \end{Bmatrix}
 =
 \begin{Bmatrix}
 \mathbf{f}_i^s \\
 \mathbf{f}_r^s \\
 \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{f}_c^s \\
 0
 \end{Bmatrix}, \quad (3.250)$$

where λ are the nodal forces required to satisfy continuity at the remaining interface nodes as shown schematically in Fig.(3.8).

Figure 3.8: Lagrange multipliers are the forces required to connect the tore interface boundary

From the first row of Eq.(3.250), one obtains

$$\mathbf{u}_i^s = [\mathbf{A}_{ii}^s]^{-1} (\mathbf{f}_i^s - \mathbf{A}_{ir}^s \mathbf{u}_r^s - \mathbf{A}_{ic}^s \mathbf{B}_c^s \mathbf{u}_c). \quad (3.251)$$

Eliminating $\mathbf{u}_i^s$ from Eq.(3.250), leads to the following compact system

$$\begin{bmatrix} \mathbf{S}_{rr}^s & \mathbf{S}_{rc}^s \mathbf{B}_c^s & \mathbf{B}_r^{sT} \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s & \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cc}^s \mathbf{B}_c^s & 0 \\ \sum_{s=1}^{n_s} \mathbf{B}_r^s & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_r^s \\ \mathbf{u}_c \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{g}_r^s \\ \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{g}_c^s \\ 0 \end{bmatrix}, \quad (3.252)$$

where

$$\mathbf{S}_{\alpha\beta}^s = \mathbf{A}_{\alpha\beta}^s - \mathbf{A}_{\alpha i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{A}_{i\beta}^s, \quad (3.253)$$

$$\mathbf{g}_\alpha^s = \mathbf{f}_\alpha^s - \mathbf{A}_{\alpha i}^s [\mathbf{A}_{ii}^s]^{-1} \mathbf{f}_i^s. \quad (3.254)$$

The local Schur complement matrix $\mathbf{S}_{rr}^s$ associated with the remaining interface nodes in Eq.(3.252) is positive definite and hence invertible for the case of floating subdomains. Consequently, the subdomain level remaining unknown vector $\mathbf{u}_r^s$ can be obtained from Eq.(3.252) as

$$\mathbf{u}_r^s = [\mathbf{S}_{rr}^s]^{-1} (\mathbf{g}_r^s - \mathbf{S}_{rc}^s \mathbf{B}_c^s \mathbf{u}_c - \mathbf{B}_r^{sT} \lambda). \quad (3.255)$$

Substituting $\mathbf{u}_r^s$ from Eq.(3.255) into Eq.(3.252) leads to the following system

$$\begin{bmatrix} \mathbf{F}_{cc} & -\mathbf{F}_{cr} \\ \mathbf{F}_{rc} & \mathbf{F}_{rr} \end{bmatrix} \begin{bmatrix} \mathbf{u}_c \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{d}_c \\ \mathbf{d}_r \end{bmatrix}, \quad (3.256)$$

where

$$\mathbf{F}_{cc} = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} (\mathbf{S}_{cc}^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s) \mathbf{B}_c^s, \quad (3.257)$$

$$\mathbf{F}_{cr} = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{B}_r^{sT}, \quad (3.258)$$

$$\mathbf{F}_{rc} = \sum_{s=1}^{n_s} \mathbf{B}_r^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{S}_{rc}^s \mathbf{B}_c^s, \quad (3.259)$$

$$\mathbf{F}_{rr} = \sum_{s=1}^{n_s} \mathbf{B}_r^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{B}_r^{sT}, \quad (3.260)$$

$$\mathbf{d}_c = \sum_{s=1}^{n_s} \mathbf{B}_c^{sT} (\mathbf{G}_c^s - \mathbf{S}_{cr}^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{g}_r^s), \quad (3.261)$$

$$\mathbf{d}_r = \sum_{s=1}^{n_s} \mathbf{B}_r^s [\mathbf{S}_{rr}^s]^{-1} \mathbf{g}_r^s. \quad (3.262)$$

Solving for $\mathbf{u}_c$ from Eq.(3.256) gives the following coarse problem

$$\mathbf{F}_{cc} \mathbf{u}_c = (\mathbf{d}_c + \mathbf{F}_{cr} \boldsymbol{\lambda}). \quad (3.263)$$

Substituting $\mathbf{u}_c$ into Eq.(3.256) leads to the following symmetric positive-definite Lagrange multiplier system

$$(\mathbf{F}_{rr} + \mathbf{F}_{rc} [\mathbf{F}_{cc}]^{-1} \mathbf{F}_{cr}) \boldsymbol{\lambda} = \mathbf{d}_r - \mathbf{F}_{rc} [\mathbf{F}_{cc}]^{-1} \mathbf{d}_c \quad (3.264)$$

Eq.(3.264) is the dual interface problem which can be tackled iteratively by the standard preconditioned conjugate gradient method equipped with a lumped or Dirichlet preconditioner.

Preconditioners for FETI-DP

The dual interface problem in the FETI-DP method can be solved using the standard preconditioned conjugate gradient method. The preconditioned system takes the following form

$$\mathbf{M}^{-1}(\mathbf{F}_{rr} + \mathbf{F}_{rc}[\mathbf{F}_{cc}]^{-1}\mathbf{F}_{cr})\boldsymbol{\lambda} = \mathbf{M}^{-1}(\mathbf{d}_r - \mathbf{F}_{rc}[\mathbf{F}_{cc}]^{-1}\mathbf{d}_c). \quad (3.265)$$

Since the coarse problem $\mathbf{F}_{cc}^{-1}$ is already embedded within the FETI-DP operator, a one-level preconditioner such as a lumped or Dirichlet preconditioner is sufficient for numerical scalability. The lumped and Dirichlet preconditioners are respectively defined as

$$\mathbf{M}_L^{-1} = \sum_{s=1}^{n_s} \mathbf{B}_r^s \mathbf{D}_r^s \mathbf{A}_{rr}^s \mathbf{D}_r^s \mathbf{B}_r^{sT} \quad (3.266)$$

$$\mathbf{M}_D^{-1} = \sum_{s=1}^{n_s} \mathbf{B}_r^s \mathbf{D}_r^s \mathbf{S}_{rr}^s \mathbf{D}_r^s \mathbf{B}_r^{sT} \quad (3.267)$$

The lumped preconditioner is not computationally expensive to apply, but not mathematically optimal. The Dirichlet preconditioner, on the other hand, is mathematically optimal as it provides a bound on the condition number estimate [4, 78, 136].

Condition Number Bound

If h and H are the typical finite element mesh size and subdomain size respectively, the condition number of the preconditioned operator of the FETI-DP method is bounded by [4, 78, 136]

$$\kappa(\mathbf{M}_D^{-1}(\mathbf{F}_{rr} + \mathbf{F}_{rc}[\mathbf{F}_{cc}]^{-1}\mathbf{F}_{cr})) \leq C(1 + \log \frac{H}{h})^2, \quad (3.268)$$

where C is a positive coefficient independent of the the number of subdomains and the size of the elements. Clearly, the condition number estimate is bounded as the number of subdomains increases [135].

3.4 Summary

An overview of various types of domain decomposition methods is presented in this chapter. In particular, we describe the overlapping and non-overlapping domain decomposition approaches and outline the primal, dual and dual-primal iterative substructuring methods. In addition, a novel primal-primal iterative substructuring method equipped with a two-level scalable preconditioner is presented.

Domain decomposition methods can be viewed as a divide and conquer techniques for solving the linear system arising from the discretization of partial differential equations [4–7]. It involves iteratively or alternately solving subsystems defined on smaller subdomains while enforcing continuity requirements of the solution field across the subdomain interfaces [4–7].

In the overlapping domain decomposition method (Schwarz methods), the computational domain is split into a number of overlapping subdomains whereby a smaller problem is solved alternately on each subdomain. The additive Schwarz method is an embar-

rassingly parallel algorithm, but its convergence rate is slow compared to multiplicative Schwarz method. On the other hand, the classical multiplicative Schwarz method is sequential in nature and has a limited potential for parallelism as it requires the solution of one subdomain problem prior to another [6, 7]. However, the multi-coloring technique can be used to improve the parallel performance of the multiplicative Schwarz method. In this approach, each subdomain is identified with a color such that the subdomains with the same color do not have a common interface boundary. Consequently the multiplicative Schwarz algorithm is implemented sequentially for the subdomains with different colors, but concurrently for subdomains with the same colors citechan1994. In general the convergence rate depends on the number of colors as the fewer the colors the faster the convergence [6].

Non-overlapping domain decomposition methods are preconditioned iterative algorithms to solve the large-scale linear system arising from the discretization of partial differential equations. The computational domain is partitioned into a number of non-overlapping subdomains. At each iteration of the iterative solver loop, local problems are solved on each subdomain concurrently to construct a subdomain level preconditioner. This local preconditioner leads to an iterative method that is numerically scalable with respect to mesh size [4–7, 129]. Furthermore, a coarse problem with a few unknowns per each subdomain is solved in each iteration in order to make the iterative method numerically scalable with respect to subdomain size. The local part of the preconditioner is to eliminate the high frequency component of the error, while the coarse problem is to provide a global exchange of information about the error and thus quickly reducing the low frequency component of the error [4–7].

In general, the overlapping Schwarz domain decomposition methods are relatively easier to formulate and implement compared to the non-overlapping Schur complement methods. However, the computational complexity of one iteration of Schwarz algorithm can exceed the computational cost of the Schur complement algorithm by a factor, proportional to the overlap between the adjacent subdomain [7].

Chapter 4

Domain Decomposition Methods for Stochastic PDEs

4.1 Introduction

This chapter is closely based on the references [70, 74, 75]. In the SSFEM, the finite element discretization of SPDEs involves tackling a large-scale deterministic linear system. The order of the linear system in SSFEM increases significantly with the mesh resolution and the size of the stochastic dimension. The solution of this system of linear equations poses a significant computational challenge. In this chapter, iterative substructuring technique for SPDEs is presented extending the basic formulation in [68]. In particular, a parallel PCGM is introduced to tackle the interface problem in the context of domain decomposition method of SPDEs. The iterative algorithm eliminates the need of explicit construction of the *extended* Schur complement system.

4.2 Mathematical Formulation

Consider an elliptic SPDE, defined on a spatial domain Ω with given boundary conditions on $\partial\Omega$, whose differential operator (left hand side) contains spatially varying random coefficients. The finite element approximation of the SPDE yields the linear system with stochastically varying parameters as

$$\mathbf{A}(\theta)\mathbf{u}(\theta) = \mathbf{f}, \quad (4.1)$$

where $\mathbf{A}(\theta)$ denotes the stochastic stiffness matrix, $\mathbf{u}(\theta)$ is the stochastic solution vector and $\mathbf{f}$ is the applied deterministic force. In the domain decomposition methods (for example, see [4–7]), the spatial domain Ω is divided into n_s non-overlapping subdomains $\{\Omega_s\}_{s=1}^{n_s}$ and the subdomain degrees of freedom $\mathbf{u}^s(\theta)$ is split into two subsets: interior $\mathbf{u}_I^s(\theta)$ and interface $\mathbf{u}_F^s(\theta)$ degrees of freedom as shown schematically in Fig.(4.1).

Figure 4.1: Partitioning the subdomain nodes into: interior ($\diamond$) and interface ($\blacksquare$)

The equilibrium equation for a typical subdomain Ω_s is expressed as

$$\begin{bmatrix} \mathbf{A}_{II}^s(\theta) & \mathbf{A}_{IG}^s(\theta) \\ \mathbf{A}_{GI}^s(\theta) & \mathbf{A}_{GG}^s(\theta) \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s(\theta) \\ \mathbf{u}_G^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_G^s \end{Bmatrix}. \quad (4.2)$$

When the PCE can be used to represent the non-Gaussian system parameters, the above equation becomes

$$\sum_{i=0}^L \Psi_i(\theta) \begin{bmatrix} \mathbf{A}_{II,i}^s & \mathbf{A}_{IG,i}^s \\ \mathbf{A}_{GI,i}^s & \mathbf{A}_{GG,i}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s(\theta) \\ \mathbf{u}_G^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_G^s \end{Bmatrix}. \quad (4.3)$$

The transmission conditions along the subdomain boundaries are enforced next by global assembly. Using the PCE of the solution vector and Galerkin projection, we obtain the following coupled linear systems [68, 70, 74, 76, 79, 80]:

$$\begin{aligned}
& \left\langle \sum_{i=0}^L \Psi_i(\theta) \begin{bmatrix} \mathbf{A}_{II,i}^1 & \dots & 0 & \mathbf{A}_{I\Gamma,i}^1 \mathbf{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathbf{A}_{II,i}^{n_s} & \mathbf{A}_{I\Gamma,i}^{n_s} \mathbf{R}_{n_s} \\ \mathbf{R}_1^T \mathbf{A}_{\Gamma I,i}^1 & \dots & \mathbf{R}_{n_s}^T \mathbf{A}_{\Gamma I,i}^{n_s} & \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{A}_{\Gamma\Gamma,i}^s \mathbf{R}_s \end{bmatrix} \sum_{j=0}^N \Psi_j(\theta) \begin{Bmatrix} \mathbf{u}_{I,j}^1 \\ \vdots \\ \mathbf{u}_{I,j}^{n_s} \\ \mathbf{u}_{\Gamma,j} \end{Bmatrix} \right\rangle \Psi_k(\theta) \\
& = \left\langle \begin{Bmatrix} \mathbf{f}_I^1 \\ \vdots \\ \mathbf{f}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{f}_\Gamma^s \end{Bmatrix} \right\rangle \Psi_k(\theta), \quad k = 0, \dots, N. \tag{4.4}
\end{aligned}$$

where $\mathbf{R}_s$ is a restriction matrix that relates the global interface unknown $\mathbf{u}_\Gamma(\theta)$ to the local interface unknown $\mathbf{u}_\Gamma^s(\theta)$ as

$$\mathbf{u}_\Gamma^s(\theta) = \mathbf{R}_s \mathbf{u}_\Gamma(\theta). \tag{4.5}$$

In the concise form, Eq.(4.4) can be expressed as

$$\begin{bmatrix} \mathcal{A}_{II}^1 & \dots & 0 & \mathcal{A}_{I\Gamma}^1 \mathcal{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathcal{A}_{II}^{n_s} & \mathcal{A}_{I\Gamma}^{n_s} \mathcal{R}_{n_s} \\ \mathcal{R}_1^T \mathcal{A}_{\Gamma I}^1 & \dots & \mathcal{R}_{n_s}^T \mathcal{A}_{\Gamma I}^{n_s} & \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{A}_{\Gamma\Gamma}^s \mathcal{R}_s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_I^1 \\ \vdots \\ \mathcal{U}_I^{n_s} \\ \mathcal{U}_\Gamma \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_I^1 \\ \vdots \\ \mathcal{F}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{F}_\Gamma^s \end{Bmatrix}, \tag{4.6}$$

where

$$\begin{aligned}
[\mathcal{A}_{\alpha\beta}^s]_{jk} &= \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_{\alpha\beta,i}^s; \quad \mathcal{F}_{\alpha,k}^s = \langle \Psi_k \mathbf{f}_\alpha^s \rangle, \\
\mathcal{U}_I^m &= (\mathbf{u}_{I,0}^m, \dots, \mathbf{u}_{I,N}^m)^T; \quad \mathcal{U}_\Gamma = (\mathbf{u}_{\Gamma,0}, \dots, \mathbf{u}_{\Gamma,N})^T.
\end{aligned} \tag{4.7}$$

The subscripts α and β can assume the index I and Γ . The new restriction matrix $\mathcal{R}_s$ is given by

$$\mathcal{R}_s = \text{blockdiag}(\mathbf{R}_s^0, \dots, \mathbf{R}_s^N), \quad (4.8)$$

After eliminating the interior degrees of freedom, Eq.(4.6) reduces to the following *extended* Schur complement system

$$\mathcal{S} \mathcal{U}_\Gamma = \mathcal{G}_\Gamma, \quad (4.9)$$

where the extended Schur complement matrix $\mathcal{S}$ is defined by the local Schur complement matrices as

$$\mathcal{S} = \sum_{s=1}^{n_s} \mathcal{R}_s^T [\mathcal{A}_{\Gamma\Gamma}^s - \mathcal{A}_{\Gamma I}^s (\mathcal{A}_{II}^s)^{-1} \mathcal{A}_{I\Gamma}^s] \mathcal{R}_s, \quad (4.10)$$

and the right hand side vector $\mathcal{G}_\Gamma$ is defined by

$$\mathcal{G}_\Gamma = \sum_{s=1}^{n_s} \mathcal{R}_s^T [\mathcal{F}_\Gamma^s - \mathcal{A}_{\Gamma I}^s (\mathcal{A}_{II}^s)^{-1} \mathcal{F}_I^s]. \quad (4.11)$$

The solution of the extended Schur complement system in Eq.(4.9) gives the unknowns $\mathcal{U}_\Gamma$ along the interface. Once these unknowns are available, the interior unknowns $\mathcal{U}_I^s$ can be obtained by solving the following stochastic interior problem on each subdomain concurrently

$$\mathcal{A}_{II}^s \mathcal{U}_I^s = \mathcal{F}_I^s - \mathcal{A}_{\Gamma I}^s \mathcal{R}_s \mathcal{U}_\Gamma \quad (4.12)$$

4.3 The Extended Schur Complement Matrix

The extended Schur complement matrix of stochastic PDEs is generally dense. However, the block matrices forming the extended Schur complement matrix have two distinct level of sparsity structure. The first level relates to the finite element discretization whereas the second level arises due to the stochastic features of the problem. In the computer implementation of the algorithm, this multilevel sparsity structure is exploited in order to minimize the storage requirements and to reduce the unnecessary floating point operations associated with zero-valued elements. Fig.(4.2) shows the non-zero block pattern of the block matrices forming the stochastic Schur complement matrix for the first, second and third order PC expansions. The size of Schur complement matrix is $[n_\Gamma(N+1)] \times [n_\Gamma(N+1)]$ where n_Γ is the number of the global interface unknowns and $(N+1)$ is the order of PC expansion. The size of each individual block is $n_\Gamma \times n_\Gamma$ and the number of blocks is $(N+1)$.

Figure 4.2: The sparsity structure of the stochastic block matrices

Note that we do not construct or store the extended Schur complement matrix. Instead we only store the non-zero elements of the subdomain stiffness matrices $\mathcal{A}_{\alpha\beta}^s$ in Eq.(4.10). PETSc [87] sparse matrix (compressed row) format is used for efficient memory management. For better performance of PETSc matrix assembly process, the memory required for the sparse matrix storage need to be preallocated by setting the number of non-zeros entries per each row. This task is accomplished by defining an integer array of size n_α where α represents the index I and Γ . The entries of this array is obtained by looping over the rows of the $\mathcal{A}_{\alpha\beta,i}^s$ matrix in Eq.(4.7) and counting the number of non-zeros for each row. This array represents the first sparsity level of the stochastic matrix. A second array of size $(N + 1)$ containing the number of non-zeros block per row is constructed by counting the non-zeros coefficients of the $\langle \Psi_i \Psi_j \Psi_k \rangle$ (see Eq.(4.7)) which provides the second level of sparsity. Finally, an array of size $n_\alpha(N + 1)$ is formed by multiplying the first array by the corresponding element of the second array. This array contains the sparsity pattern of the stochastic submatrices $\mathcal{A}_{\alpha\beta}^s$ in Eq.(4.10). Recall that $\mathcal{A}_{\alpha\beta}^s$ relates to $\mathcal{S}$ through Eq.(4.10).

4.4 Iterative Substructuring Methods for Stochastic PDEs

For a large-scale system, the solution of the interface problem in Eq.(4.9) using direct solvers becomes impractical due to overwhelming memory requirements and poor scalability to large number of processors. Therefore, iterative solution techniques are generally adopted [52]. When an iterative solver is used to tackle the global Schur complement system, domain decomposition method is referred to as *iterative substructuring* [6, 7]. The iterative substructuring algorithm can be outlined as follows [4, 6, 7, 52]:

Algorithm 2: Iterative Substructuring Procedure

input : number of subdomains n_s
1 for $s = 1, 2, \dots, n_s$ **in parallel:**
2 do
3 assemble: $\mathcal{A}_{II}^s, \mathcal{A}_{IR}^s, \mathcal{A}_{RI}^s, \mathcal{A}_{RR}^s, \mathcal{F}_I^s, \mathcal{F}_R^s$
4 solve : $\mathcal{A}_{II}^s \mathcal{X}^s = \mathcal{F}_I^s$
5 compute : $\mathcal{G}_R^s = \mathcal{F}_R^s - \mathcal{A}_{RI}^s \mathcal{X}^s$
6 gather : $\mathcal{G}_R = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{G}_R^s$
7 iteratively solve in parallel: $\mathcal{S} \mathcal{U}_R = \mathcal{G}_R$
8 for $s = 1, 2, \dots, n_s$ **in parallel:**
9 do
10 scatter : $\mathcal{U}_R^s = \mathcal{R}_s \mathcal{U}_R$
11 solve : $\mathcal{A}_{II}^s \mathcal{U}_I^s = \mathcal{F}_I^s - \mathcal{A}_{RI}^s \mathcal{U}_R^s$
output : $(\mathcal{U}_I^1, \dots, \mathcal{U}_I^{n_s}, \mathcal{U}_R)$

4.4.1 Iterative Solution of the Interface Problem

In domain decomposition approach, the Schur complement system is typically solved using preconditioned Krylov subspace method such as Precondition Conjugate Gradient Method (PCGM) (e.g. [52]). The preconditioned Krylov subspace method circumvents the need to construct the Schur complement matrix explicitly. Instead only the action of the Schur complement matrix on a vector is needed [4, 7]. Non-overlapping domain decomposition method or iterative substructuring can be viewed as a preconditioned iterative method to solve the Schur complement system defined by Eq.(4.9) equipped with a parallel preconditioner [4, 7].

For symmetric positive-definite system such as the Schur complement system considered here, the Conjugate Gradient Method (CGM) is generally used. The performance of CGM mainly depends on the spectrum of the coefficient matrix [52]. However, the rate of convergence of the iterative method can generally be improved by transforming the original system into an equivalent system that has better spectral properties (i.e. lower condition number). This transformation is called preconditioning and the matrix used in the transformation is called the preconditioner. In other words, the transformed linear system becomes:

$$\mathcal{M}^{-1}S \mathcal{U}_r = \mathcal{M}^{-1}\mathcal{G}_r, \quad (4.13)$$

where $\mathcal{M}^{-1}$, the preconditioner, is a symmetric and invertible matrix that approximates S^{-1} , the inverse of the coefficient matrix, in the sense that the condition number of the preconditioned system $\kappa(\mathcal{M}^{-1}S)$ is much smaller than that of the original system $\kappa(S)$

and the eigenvalues of the preconditioned system $\mathcal{M}^{-1}S$ are clustered near one [52, 139]. This procedure known as Preconditioned Conjugate Gradient Method (PCGM). In practice, the explicit construction of $\mathcal{M}^{-1}$ is not needed. Instead, for a given vector r_r , a system of the the following form is solved

$$\mathcal{M}Z = r_r. \quad (4.14)$$

The combination of a good parallel preconditioning technique and the CGM solver makes the iterative solver well-suited to tackle large-scale systems in parallel computers [52]. The preconditioned conjugate gradient algorithm applied to solve the extended Schur complement system proceeds as follows [52]

Algorithm 3: The PCGM Procedure

```

input           :  $(\mathcal{U}_{\Gamma_0})$ 

1 compute         :  $\mathbf{r}_{\Gamma_0} = \mathcal{G}_\Gamma - \mathcal{S} \mathcal{U}_{\Gamma_0}$ 
2 precondition    :  $\mathcal{Z}_0 = \mathcal{M}^{-1} \mathbf{r}_{\Gamma_0}$ 
3 compute         :  $\mathcal{P}_0 = \mathcal{Z}_0$ 
4 compute         :  $\rho_0 = (\mathbf{r}_{\Gamma_0}, \mathcal{Z}_0)$ 
5 for  $j = 1, 2, \dots$ , until convergence:
6 do
7   compute       :  $\mathcal{Q}_j = \mathcal{S} \mathcal{P}_j$ 
8   compute       :  $\rho_{tmp_j} = (\mathcal{Q}_j, \mathcal{P}_j)$ 
9   compute       :  $\alpha_j = \rho_j / \rho_{tmp_j}$ 
10  update        :  $\mathcal{U}_{\Gamma_{j+1}} = \mathcal{U}_{\Gamma_j} + \alpha_j \mathcal{P}_j$ 
11  update        :  $\mathbf{r}_{\Gamma_{j+1}} = \mathbf{r}_{\Gamma_j} - \alpha_j \mathcal{Q}_j$ 
12  precondition  :  $\mathcal{Z}_{j+1} = \mathcal{M}^{-1} \mathbf{r}_{\Gamma_{j+1}}$ 
13  compute       :  $\rho_{j+1} = (\mathbf{r}_{\Gamma_{j+1}}, \mathcal{Z}_{j+1})$ 
14  compute       :  $\beta_j = \rho_{j+1} / \rho_j$ 
15  update        :  $\mathcal{P}_{j+1} = \mathcal{Z}_{j+1} + \beta_j \mathcal{P}_j$ 

output         :  $(\mathcal{U}_\Gamma)$ 

```

The PCGM algorithm indicates that the essential computational operations are calculating the matrix-vector product ($\mathcal{Q} = \mathcal{S} \mathcal{P}$) in step 7 and computing the preconditioner effect on the residual vector ($\mathcal{Z} = \mathcal{M}^{-1} \mathbf{r}_\Gamma$) in steps 2 and 12. Iterative substructuring tech-

nique allows to perform these operations at the subdomain level (local). In other words, the global matrix-vector operations can be transformed into a series of subdomain level (local) computations. This fact paves the way for concurrency or parallelism as delineated in the next sections.

4.4.2 Parallel Matrix-Vector Product

While using PCGM, the Schur complement matrix need not be constructed explicitly, only its effect on a vector is required. This matrix-vector product can be obtained by solving an auxiliary Dirichlet problem on each subdomain concurrently and then gathering the resulting vectors. For the j^{th} iteration of Algorithm (3), the matrix-vector product in step 7 is computed as

$$\mathcal{Q} = \mathcal{S}\mathcal{P}, \quad (4.15)$$

$$= \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{S}_s \mathcal{R}_s \mathcal{P}, \quad (4.16)$$

$$= \sum_{s=1}^{n_s} \mathcal{R}_s^T (\mathcal{A}_{\Gamma\Gamma}^s - \mathcal{A}_{\Gamma I}^s [\mathcal{A}_{II}^s]^{-1} \mathcal{A}_{I\Gamma}^s) \mathcal{R}_s \mathcal{P}. \quad (4.17)$$

This procedure is summarized in the following Algorithm:

Algorithm 4: Parallel Matrix-Vector Product Procedure

```

input      :  $(\mathcal{P})$ 

1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter :  $\mathcal{P}^s = \mathcal{R}_s \mathcal{P}$ 
4   compute :  $v_1 = \mathcal{A}_{II}^s \mathcal{P}^s$ 
5   solve   :  $\mathcal{A}_{II}^s v_2 = v_1$ 
6   compute :  $v_3 = \mathcal{A}_{II}^s v_2$ 
7   compute :  $v_4 = \mathcal{A}_{II}^s \mathcal{P}^s$ 
8   compute :  $Q^s = v_4 - v_3$ 
9   gather  :  $Q = \sum_{s=1}^{n_s} \mathcal{R}_s^T Q^s$ 
output    :  $(Q)$ 

```

The action of the Schur complement S on a vector $\mathcal{P}$ is accomplished by three matrix vector products and one direct solve of a local Dirichlet problem with non-homogeneous boundary condition on each subdomain. This approach is computational less expensive than constructing the dense Schur complement matrix S explicitly. A drawback associated with the approach of not constructing the Schur complement matrix explicitly is that preconditioners for the Schur complement matrix such as Jacobi preconditioner (the inverse of the diagonal of S) or probing technique (the inverse of the tridiagonal part of S) cannot be used directly.

4.4.3 Parallel Preconditioner Effect

The preconditioned residual vector Z at step 12 of Algorithm (3), is computed by solving a local system of the form $\mathcal{M}^s Z^s = r_\Gamma^s$ on each subdomain in parallel followed by a global assembly to calculate the global effect as

$$Z = \mathcal{M}^{-1} r_\Gamma, \quad (4.18)$$

$$= \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{M}_s^{-1} \mathcal{R}_s r_\Gamma, \quad (4.19)$$

where $\mathcal{M}_s^{-1}$ is a subdomain level preconditioner. This procedure is outlined in the following algorithm

Algorithm 5: Parallel Preconditioner Effect Procedure

```

input      : ( $r_\Gamma$ )

1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter  :  $r_\Gamma^s = \mathcal{R}_s r_\Gamma$ 
4   solve    :  $\mathcal{M}^s Z^s = r_\Gamma^s$ 
5   gather   :  $Z = \sum_{s=1}^{n_s} \mathcal{R}_s^T Z^s$ 
output     : ( $Z$ )

```

The working vectors r_Γ^s and Z^s are defined on the subdomain level.

4.4.4 Parallel Preconditioned Conjugate Gradient Method

Exploiting Algorithms(4 & 5), a parallel version of the PCGM algorithm can be implemented as outlined in the following algorithm. The summation steps in the following algorithm can be performed in parallel.

Algorithm 6: The Parallel PCGM Procedure

input : $(\mathcal{U}_{\Gamma_0})$
 1 compute : $\mathbf{r}_{\Gamma_0} = \mathcal{G}_{\Gamma} - \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{S}_s \mathcal{R}_s \mathcal{U}_{\Gamma_0}$
 2 precondition : $\mathcal{Z}_0 = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{M}_s^{-1} \mathcal{R}_s \mathbf{r}_{\Gamma_0}$
 3 compute : $\mathcal{P}_0 = \mathcal{Z}_0$
 4 compute : $\rho_0 = (\mathbf{r}_{\Gamma_0}, \mathcal{Z}_0)$
 5 for $j = 1, 2, \dots$, until convergence:
 6 do
 7 compute : $\mathcal{Q}_j = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{S}_s \mathcal{R}_s \mathcal{P}_j$
 8 compute : $\rho_{tmp_j} = (\mathcal{Q}_j, \mathcal{P}_j)$
 9 compute : $\alpha_j = \rho_j / \rho_{tmp_j}$
 10 update : $\mathcal{U}_{\Gamma_{j+1}} = \mathcal{U}_{\Gamma_j} + \alpha_j \mathcal{P}_j$
 11 update : $\mathbf{r}_{\Gamma_{j+1}} = \mathbf{r}_{\Gamma_j} - \alpha_j \mathcal{Q}_j$
 12 precondition : $\mathcal{Z}_{j+1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{M}_s^{-1} \mathcal{R}_s \mathbf{r}_{\Gamma_{j+1}}$
 13 compute : $\rho_{j+1} = (\mathbf{r}_{\Gamma_{j+1}}, \mathcal{Z}_{j+1})$
 14 compute : $\beta_j = \rho_{j+1} / \rho_j$
 15 update : $\mathcal{P}_{j+1} = \mathcal{Z}_{j+1} + \beta_j \mathcal{P}_j$
output : $(\mathcal{U}_{\Gamma})$

The vector $\mathcal{Q}_j$ in step 7 of Algorithm (6) is computed in parallel using Algorithm (4), and the preconditioned residual vector $\mathcal{Z}_j$ in step 12 of Algorithm (6) is obtained in parallel using Algorithm (5). All the inner products of the vectors are preformed in parallel on a

distributed data set.

Finally, A flow chart of iterative substructuring technique for stochastic PDEs is shown in Fig. (4.3).

Figure 4.3: Flow chart of iterative substructuring technique

4.5 Summary

Iterative substructuring technique for SPDEs is described in this chapter. In particular, a parallel PCGM is introduced to tackle the interface problem in the context of domain decomposition method of SPDEs. The iterative algorithm eliminates the need of explicit construction of the extended Schur complement system.

Chapter 5

One-Level Preconditioners for Stochastic PDEs

5.1 Introduction

This chapter is closely based on the references [70, 74, 75]. The preconditioning technique is the essential ingredient in enhancing the reliability, robustness and performance of the iterative methods used to tackle the interface problem arising in the domain decomposition of SPDEs. The combination of a scalable parallel preconditioner suitably customized for the stochastic systems and the CGM solver makes the iterative method well-suited to tackle the interface problem using high performance computing platforms. In this chapter, we describe the mathematical frameworks and parallel implementations of one-level preconditioners namely Lumped (L), Weighted Lumped (WL) and Neumann-Neumann (NN) to tackle the extended Schur complement system of SPDEs.

5.2 Extended Lumped Preconditioner

As previously alluded, iterative substructuring technique is a preconditioned Krylov subspace iteration method for solving the extended Schur complement system as

$$\mathcal{M}^{-1} \mathcal{S} \mathcal{U}_\Gamma = \mathcal{M}^{-1} \mathcal{G}_\Gamma, \quad (5.1)$$

where $\mathcal{M}^{-1}$ being the preconditioning matrix.

A preliminary preconditioner for the extended Schur complement system is devised by approximating the inverse of the extended Schur complement matrix by the sum of the inverse of the local interface coupling matrices as [70]

$$\mathcal{M}_L^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T [\mathcal{A}_{\Gamma\Gamma}^s]^{-1} \mathcal{R}_s. \quad (5.2)$$

The inverse of the subdomain interface coupling matrix $[\mathcal{A}_{\Gamma\Gamma}^s]^{-1}$ is not constructed explicitly. Instead the following system is solved on each subdomain in parallel followed by a global assembly in order to calculate the global effect of the preconditioner as

$$\mathcal{A}_{\Gamma\Gamma}^s \mathcal{Z}^s = r_\Gamma^s. \quad (5.3)$$

The interface coupling matrix is much more diagonally dominant than the Schur complement matrix. However, this elementary preconditioner reduces the arithmetic complexity in the preconditioning step of the PCGM iteration loop.

5.2.1 Parallel Implementation

In the framework of the parallel PCGM, the *extended* Lumped preconditioner can be implemented in parallel as outlined in the following algorithm

Algorithm 7: Extended Lumped Preconditioner Effect Procedure	
<hr/>	
input	: $(\mathbf{r}_T)$
1	for $s = 1, 2, \dots, n_s$ in parallel:
2	do
3	scatter : $\mathbf{r}_T^s = \mathcal{R}_s \mathbf{r}_T$
4	solve : $\mathcal{A}_{TT}^s \mathbf{Z}^s = \mathbf{r}_T^s$
5	gather : $\mathbf{Z} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathbf{Z}^s$
	output : $(\mathbf{Z})$

Cholesky factorization of the matrix $\mathcal{A}_{TT}^s$ is performed only once, and the solution of the local system proceeds by forward and backward substitutions. This fact highlights the efficiency of the Lumped preconditioner in reducing the arithmetic complexity in the preconditioning step.

5.3 Extended Weighted Lumped Preconditioner

The performance of the Lumped preconditioner can be improved by employing a scaling matrix $\mathcal{D}_s$, namely a partition of identity matrix (e.g [4, 6, 7] obtained as

$$\sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{R}_s = I, \quad (5.4)$$

where $\mathcal{D}_s$ is a block diagonal matrix of the following form

$$\mathcal{D}_s = \text{blockdiag}(\mathbf{D}_s^0, \dots, \mathbf{D}_s^N). \quad (5.5)$$

The diagonal entries of the deterministic weighting matrix $\mathbf{D}_s^i$ are equal to the reciprocal of the number of subdomains which contain the same interface node [4, 6, 7].

Consequently, the extended Weighted Lumped preconditioner which approximates the inverse of the global extended Schur complement matrix by a weighted sum of the inverse of the local interface coupling matrices can be expressed as

$$\mathcal{M}_{WL}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s [\mathcal{A}_{\Gamma\Gamma}^s]^{-1} \mathcal{D}_s \mathcal{R}_s. \quad (5.6)$$

5.3.1 Parallel Implementation

The parallel implementation of the extended Weighted Lumped preconditioner resembles that of the extended Lumped preconditioner but with the additional two steps to calculate the multiplication of a vector by the scaling matrix $\mathcal{D}_s$. The parallel implementation is summarized below:

Algorithm 8: Extended Weighted Lumped Preconditioner Effect Procedure

```

input      :  $(\mathbf{r}_I)$ 
1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter :  $\mathbf{r}_I^s = \mathcal{R}_s \mathbf{r}_I$ 
4   compute :  $\mathcal{Y}_I^s = \mathcal{D}_s \mathbf{r}_I^s$ 
5   solve   :  $\mathcal{A}_{II}^s \mathcal{U}_I^s = \mathcal{Y}_I^s$ 
6   compute :  $\mathcal{Z}^s = \mathcal{D}_s \mathcal{U}_I^s$ 
7   gather  :  $\mathcal{Z} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{Z}^s$ 
output    :  $(\mathcal{Z})$ 

```

5.4 Extended Neumann-Neumann Preconditioner

In this section, a one-level Neumann-Neumann domain decomposition preconditioner [4–7, 71, 74, 76] is introduced to enhance the performance of the PCGM to tackle the interface system. The global extended Schur complement matrix can be constructed by the aggregated local extended Schur complement matrices. It is therefore natural to design a preconditioner for SPDEs by the weighted average of the inverse extended subdomain Schur complement matrices. This preconditioner may be construed to be analogous to the Neumann-Neumann preconditioner devised for the deterministic PDEs [4–7], albeit with more complex structure and higher dimension due to the stochastic aspects. The construction of the Neumann-Neumann preconditioner for SPDEs is described next in details [74, 76].

In particular, we describe the details of computing preconditioned residual $\mathcal{Z} = \mathcal{M}_{NN}^{-1} r_\Gamma$ where $\mathcal{M}_{NN}^{-1}$ and r_Γ are the Neumann-Neumann preconditioner and the residual vector at a given PCGM iteration. Subsequently it is demonstrated that the Neumann-Neumann preconditioner is the weighted sum of the inverse local Schur complement matrices of the stochastic subsystems. This fact can be mathematically stated as:

$$\mathcal{M}_{NN}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{S}_s^{-1} \mathcal{D}_s \mathcal{R}_s. \quad (5.7)$$

At the j^{th} iteration of PCGM, assume $\mathcal{U}_{\Gamma_j}$ to be an approximation of the global interface variable which in turn provides the local interface variable $\mathcal{U}_\Gamma^s$ as

$$\mathcal{U}_\Gamma^s = \mathcal{R}_s \mathcal{U}_{\Gamma_j}. \quad (5.8)$$

Next we describe the procedure to compute the new residual r_{Γ_j} using $\{\mathcal{U}_\Gamma^s\}_{s=1}^{n_s}$. For each subdomain, it involves first computing the local interior variable $\mathcal{U}_I^s$ which is then used to obtain the local residual $\mathbf{r}_\Gamma^s$. The global residual $\mathbf{r}_{\Gamma_j}$ is calculated by aggregating the local residuals $\{\mathbf{r}_\Gamma^s\}_{s=1}^{n_s}$.

The computation of the interior unknown $\mathcal{U}_I^s$ translates to tackling a stochastic local problem defined by

$$\begin{bmatrix} \mathcal{A}_{II}^s & \mathcal{A}_{I\Gamma}^s \\ \mathcal{A}_{\Gamma I}^s & \mathcal{A}_{\Gamma\Gamma}^s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_I^s \\ \mathcal{U}_\Gamma^s \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_I^s \\ \mathcal{F}_\Gamma^s \end{Bmatrix}. \quad (5.9)$$

From the first row of Eq.(5.9), the solution of a stochastic Dirichlet problem computes the unknown $\mathcal{U}_I^s$ as

$$\mathcal{U}_I^s = [\mathcal{A}_{II}^s]^{-1}(\mathcal{F}_I^s - \mathcal{A}_{II}^s \mathcal{U}_I^s). \quad (5.10)$$

Consequently, the local residual $\mathbf{r}_I^s$ is computed from the second row of Eq.(5.9) as

$$\mathbf{r}_I^s = \mathcal{S}_s \mathcal{U}_I^s - \mathcal{G}_I^s, \quad (5.11)$$

where the local extended Schur complement matrix $\mathcal{S}_s$ and the corresponding right hand side vector $\mathcal{G}_I^s$ are given by

$$\mathcal{S}_s = \mathcal{A}_{II}^s - \mathcal{A}_{II}^s [\mathcal{A}_{II}^s]^{-1} \mathcal{A}_{II}^s, \quad (5.12)$$

$$\mathcal{G}_I^s = \mathcal{F}_I^s - \mathcal{A}_{II}^s [\mathcal{A}_{II}^s]^{-1} \mathcal{F}_I^s. \quad (5.13)$$

The local residual vectors $\{\mathbf{r}_I^s\}_{s=1}^{n_s}$ are then aggregated to obtain the global residual vector $\mathbf{r}_{I_j}$ as

$$\mathbf{r}_{I_j} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathbf{r}_I^s. \quad (5.14)$$

The global residual $\mathbf{r}_{I_j}$ is scattered on the subdomain interfaces to obtain the new local residuals as

$$\mathbf{r}_I^s = \mathcal{D}_s \mathcal{R}_s \mathbf{r}_{I_j}, \quad s = 1, \dots, n_s \quad (5.15)$$

Using the new local residual $\mathbf{r}_I^s$, the computation of the local interface variable $\mathcal{U}_I^s$ involves the solution of a local stochastic Neumann problem defined by

$$\begin{bmatrix} \mathcal{A}_{II}^s & \mathcal{A}_{IR}^s \\ \mathcal{A}_{RI}^s & \mathcal{A}_{RR}^s \end{bmatrix} \begin{Bmatrix} \chi^s \\ \mathcal{U}_R^s \end{Bmatrix} = \begin{Bmatrix} 0 \\ \mathbf{r}_R^s \end{Bmatrix}. \quad (5.16)$$

It is straightforward to prove that the solution of the above Neumann problem relates to tackling the local Schur complement system defined by

$$\mathcal{S}_s \mathcal{U}_R^s = \mathbf{r}_R^s. \quad (5.17)$$

It is worthwhile to point out at this stage that the local Schur complement matrix is singular for the *floating* subdomains, namely the subdomains containing insufficient Dirichlet boundary conditions. This singularity issue is circumvented by adding a small number to the diagonal entries of the subdomain stiffness matrix. This numerical artifact only affects the computation of the preconditioned residual, but does not alter the original problem to be solved.

Next the PCGM update of the solution vector $\mathcal{U}_{R_{j+1}}$ is computed by gathering the local interface vectors $\{\mathcal{U}_I^s\}_{s=1}^{n_s}$ as

$$\mathcal{U}_{R_{j+1}} = \mathcal{U}_{R_j} + \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{U}_I^s. \quad (5.18)$$

Using Eq.(5.17) and Eq.(5.15), the new solution vector $\mathcal{U}_{R_{j+1}}$ can be formally written as

$$\mathcal{U}_{R_{j+1}} = \mathcal{U}_{R_j} + \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{S}_s^{-1} \mathcal{D}_s \mathcal{R}_s \mathbf{r}_{R_j}. \quad (5.19)$$

Therefore the error vector $\mathbf{e}_{R_j}$ can be expressed as

$$\mathbf{e}_{r_j} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{S}_s^{-1} \mathcal{D}_s \mathcal{R}_s \mathbf{r}_{r_j}, \quad (5.20)$$

leading to the following expression of the extended Neumann-Neumann preconditioner for the stochastic system

$$\mathcal{M}_{NN}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{S}_s^{-1} \mathcal{D}_s \mathcal{R}_s. \quad (5.21)$$

5.4.1 Parallel Implementation

The parallel implementation of the extended Neumann-Neumann preconditioner can be outline in Algorithm(9).

Algorithm 9: Extended Neumann-Neumann Preconditioner Effect Procedure

```

input      : ( $\mathbf{r}_r$ )
1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter  :  $\mathbf{r}_r^s = \mathcal{R}_s \mathbf{r}_r$ 
4   compute  :  $\mathcal{Y}_r^s = \mathcal{D}_s \mathbf{r}_r^s$ 
5   solve    :  $\begin{bmatrix} \mathcal{A}_{II}^s & \mathcal{A}_{Ir}^s \\ \mathcal{A}_{rI}^s & \mathcal{A}_{rr}^s \end{bmatrix} \begin{Bmatrix} \mathcal{X}^s \\ \mathcal{U}_r^s \end{Bmatrix} = \begin{Bmatrix} 0 \\ \mathcal{Y}_r^s \end{Bmatrix}$ 
6   compute  :  $\mathcal{Z}^s = \mathcal{D}_s \mathcal{U}_r^s$ 
7   gather   :  $\mathcal{Z} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{Z}^s$ 
output    : ( $\mathcal{Z}$ )

```

The regularization and Cholesky factorization of the subdomain level stiffness matrix is performed only once, and the solution of the local system proceeds by forward and backward substitutions.

5.5 Summary

One-level domain decomposition algorithms are described for the iterative solution of the coupled large-scale linear systems in the spectral stochastic finite element method. The extended Neumann-Neumann preconditioner proposed here is the essential ingredient to develop two-level domain decomposition algorithms for SPDEs.

Chapter 6

Two-Level Preconditioner for Stochastic PDEs

6.1 Introduction

This chapter is closely based on the references [76, 77]. Recent advances in high performance computing systems and sensing technologies motivate computational simulations with extremely high resolution models with capabilities to quantify uncertainties for credible numerical predictions. To this end, a two-level domain decomposition method is reported in this chapter to tackle the large-scale linear system within the framework of the intrusive spectral stochastic finite element method (SSFEM). In particular, a two-level scalable preconditioner is introduced in order to iteratively solve the large-scale linear system in the intrusive SSFEM using an iterative substructuring based domain decomposition solver. The implementation of the algorithm involves solving a local problem on each subdomain

that constructs the local part of the preconditioner and a coarse problem that propagates information globally among the subdomains. The two-level preconditioner may be construed to be a probabilistic extension of the Balancing Domain Decomposition by Constraints (BDDC) [66, 78] devised for deterministic PDEs.

6.2 Solution of the Interface Problem using Two-Level Preconditioner

In the iterative substructuring technique, the interface system $S\mathcal{U}_r = \mathcal{G}_r$ is generally tackled by the preconditioned conjugate gradient method (PCGM). In the PCGM, a preconditioning matrix $\mathcal{M}^{-1}$ is employed to transform the original system into an equivalent system whereby the transformed system possesses a smaller condition number than that of the original system. Additionally the preconditioned system has eigenvalues clustered near one [52, 140, 141]. The preconditioned extended Schur complement system takes the following form

$$\mathcal{M}^{-1}S\mathcal{U}_r = \mathcal{M}^{-1}\mathcal{G}_r. \quad (6.1)$$

In this chapter, we devise a two-level preconditioner to enhance the performance of iterative substructuring techniques to tackle Eq.(6.1). The preconditioner consists of a local part to smooth some components of the error and a global part to propagate the error globally over the subdomains. The general form of the two-level preconditioner is defined as

$$\mathcal{M}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{M}_s^{-1} \mathcal{R}_s + \mathcal{R}_0^T \mathcal{M}_0^{-1} \mathcal{R}_0. \quad (6.2)$$

Within the parallel PCGM algorithm, the two-level preconditioner can be implemented using Algorithm(10) [74, 79].

Algorithm 10: The Parallel PCGM Procedure

```

input           :  $(\mathcal{U}_{\Gamma_0})$ 

1 compute       :  $\mathbf{r}_{\Gamma_0} = \mathcal{G}_\Gamma - \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{S}_s \mathcal{R}_s \mathcal{U}_{\Gamma_0}$ 

2 precondition :  $\mathcal{Z}_0 = [\sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{M}_s^{-1} \mathcal{R}_s + \mathcal{R}_0^T \mathcal{M}_0^{-1} \mathcal{R}_0] \mathbf{r}_{\Gamma_0}$ 

3 compute       :  $\mathcal{P}_0 = \mathcal{Z}_0$ 

4 compute       :  $\rho_0 = (\mathbf{r}_{\Gamma_0}, \mathcal{Z}_0)$ 

5 for  $j = 1, 2, \dots$ , until convergence:

6 do
7   compute       :  $\mathcal{Q}_j = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{S}_s \mathcal{R}_s \mathcal{P}_j$ 
8   compute       :  $\rho_{tmpj} = (\mathcal{Q}_j, \mathcal{P}_j)$ 
9   compute       :  $\alpha_j = \rho_j / \rho_{tmpj}$ 
10  update        :  $\mathcal{U}_{\Gamma_{j+1}} = \mathcal{U}_{\Gamma_j} + \alpha_j \mathcal{P}_j$ 
11  update        :  $\mathbf{r}_{\Gamma_{j+1}} = \mathbf{r}_{\Gamma_j} - \alpha_j \mathcal{Q}_j$ 
12  precondition :  $\mathcal{Z}_{j+1} = [\sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{M}_s^{-1} \mathcal{R}_s + \mathcal{R}_0^T \mathcal{M}_0^{-1} \mathcal{R}_0] \mathbf{r}_{\Gamma_{j+1}}$ 
13  compute       :  $\rho_{j+1} = (\mathbf{r}_{\Gamma_{j+1}}, \mathcal{Z}_{j+1})$ 
14  compute       :  $\beta_j = \rho_{j+1} / \rho_j$ 
15  update        :  $\mathcal{P}_{j+1} = \mathcal{Z}_{j+1} + \beta_j \mathcal{P}_j$ 

output         :  $(\mathcal{U}_\Gamma)$ 

```

Neither the extended Schur complement matrix in step 7, nor the two-level preconditioner in step 12 need to be formed explicitly. The effect of the extended Schur complement matrix on a given vector is obtained by computing three subdomain level ma-

trix vector products and solving local stochastic Dirichlet problems as outlined in Algorithm(11) [74, 79]. Whereas the preconditioner effect on the residual is calculated by solving local stochastic Neumann problems and a global coarse problem.

Algorithm 11: Dirichlet-Solver Procedure

```

input      :  $(\mathcal{P})$ 

1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter :  $\mathcal{P}^s = \mathcal{R}_s \mathcal{P}$ 
4   compute :  $v_1 = \mathcal{A}_{II}^s \mathcal{P}^s$ 
5   solve   :  $\mathcal{A}_{II}^s v_2 = v_1$ 
6   compute :  $v_3 = \mathcal{A}_{II}^s v_2$ 
7   compute :  $v_4 = \mathcal{A}_{II}^s \mathcal{P}^s$ 
8   compute :  $Q^s = v_4 - v_3$ 
9   gather  :  $Q = \sum_{s=1}^{n_s} \mathcal{R}_s^T Q^s$ 

output    :  $(Q)$ 

```

Preconditioners for Stochastic PDEs

For stochastic PDEs, the convergence rate of the PCGM equipped with efficient preconditioners should not be hampered by the level of uncertainty and order of the stochastic dimension. Furthermore, the PCG solvers must also demonstrate a scalable performance in relation to the physical problem size and number of subdomains. Such performance can be achieved by a two-level preconditioner suitably customized for the stochastic system as

delineated next.

Extended One-Level Preconditioner

Previously, a one-level Neumann-Neumann preconditioner for stochastic PDEs is introduced in Chapter 5. The extended Neumann-Neumann preconditioner is defined as

$$\mathcal{M}_{NN}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s^T \mathcal{S}_s^{-1} \mathcal{D}_s \mathcal{R}_s, \quad (6.3)$$

where

$$\mathcal{D}_s = \text{blockdiag}(\mathbf{D}_s^0, \dots, \mathbf{D}_s^N), \quad (6.4)$$

and $\mathbf{D}_s^k$ is a diagonal scaling matrix defined by

$$\sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{D}_s^k \mathbf{R}_s = \mathbf{I}. \quad (6.5)$$

The diagonal entries of $\mathbf{D}_s^k$ are the reciprocal of the number of subdomains that share the interface nodes [4–7].

The implementation of the extended Neumann-Neumann preconditioner entails solving a subdomain level stochastic Neumann problem. This step calculates the effect of the inverse of the local Schur complement matrix $\mathcal{S}_s^{-1}$ on the local residual vector $\mathbf{r}_I^s$ as

$$\begin{bmatrix} \mathcal{A}_{II}^s & \mathcal{A}_{I\Gamma}^s \\ \mathcal{A}_{\Gamma I}^s & \mathcal{A}_{\Gamma\Gamma}^s \end{bmatrix} \begin{Bmatrix} \mathcal{X}^s \\ \mathcal{U}_\Gamma^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{r}_\Gamma^s \end{Bmatrix}, \quad (6.6)$$

where $\mathbf{r}_I^s = \mathcal{R}_s \mathcal{D}_s \mathbf{r}_{\Gamma_j}$ and $\mathbf{r}_{\Gamma_j}$ denotes the global residual at the j^{th} iteration of the PCGM.

The PCGM equipped with a one-level Neumann-Neumann preconditioner exhibits a convergence rate that is almost insensitive to the level of uncertainty in the system parameters [74, 75]. As no mechanism for global information exchange exists in the one-level Neumann-Neumann preconditioner, its performance deteriorates for relatively large number of subdomains. For scalability, the global communication is required to propagate information across the subdomains [4–7]. Another difficulty in the implementation of the one-level Neumann-Neumann preconditioner is that the local stochastic Neumann problem defined in Eq.(6.6) is singular for *floating* subdomains. In practice, the singularity of the local stiffness matrix is avoided by altering its diagonal entries with a small positive constant and the local Neumann problem is solved approximately [6, 7]. However, such approximation may adversely affect the overall convergence rate of the algorithm [6].

6.3 Extended Two-Level Preconditioner

In the one-level Neumann-Neumann preconditioner, the information is only exchanged among the neighboring subdomains. To provide a mechanism for a global transfer of information, a coarse problem is required [4, 5, 7]. To this end, we describe a mathematical framework for a two-level preconditioner for the iterative substructuring to devise an iterative solver for the large-scale linear system in the intrusive SSFEM. This method bears similarity with a version of the Balancing Domain Decomposition by Constraints (BDDC) for deterministic PDEs [66, 78]. The two-level preconditioner is formulated by adding a coarse grid to the one-level Neumann-Neumann preconditioner as described next.

The interface nodes of each subdomain $\{\Omega_s\}_{s=1}^{n_s}$ are partitioned into a set of remaining nodes (boundary nodes shared only between two adjacent subdomains) and corner nodes (boundary nodes shared among more than two subdomains plus the nodes at the ends of interface edges) [64, 66, 67, 78] as shown in Fig.(6.1).

Figure 6.1: Partitioned interface nodes into remaining (■) and corner (●) nodes.

Let $\mathcal{R}_s^r$ and $\mathcal{R}_s^c$ be the Boolean operators that split the local interface unknowns $\mathcal{U}_F^s$ into

remaining $\mathcal{U}_r^s$ and corner $\mathcal{U}_c^s$ variables respectively as

$$\begin{Bmatrix} \mathcal{U}_r^s \\ \mathcal{U}_c^s \end{Bmatrix} = \begin{bmatrix} \mathcal{R}_s^r \\ \mathcal{R}_s^c \end{bmatrix} \mathcal{U}_\Gamma^s \quad (6.7)$$

where

$$\mathcal{R}_s^r = \text{blockdiag}(\mathbf{R}_s^{r,0}, \dots, \mathbf{R}_s^{r,N}),$$

$$\mathcal{R}_s^c = \text{blockdiag}(\mathbf{R}_s^{c,0}, \dots, \mathbf{R}_s^{c,N}).$$

The deterministic restriction operators $\mathbf{R}_s^{r,k}$ and $\mathbf{R}_s^{c,k}$ for the k^{th} polynomial chaos basis are defined as

$$\mathbf{u}_{r,k}^s = \mathbf{R}_s^{r,k} \mathbf{u}_{\Gamma,k}^s,$$

$$\mathbf{u}_{c,k}^s = \mathbf{R}_s^{c,k} \mathbf{u}_{\Gamma,k}^s.$$

According to the partition defined in Eq.(6.7), the subdomain level Neumann problem given by Eq.(6.6), can be rewritten as

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \\ \mathcal{A}_{ci}^s & \mathcal{A}_{cr}^s & \mathcal{A}_{cc}^s \end{bmatrix} \begin{Bmatrix} \mathcal{X}^s \\ \mathcal{U}_r^s \\ \mathcal{U}_c^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathcal{F}_r^s \\ \mathcal{F}_c^s \end{Bmatrix}, \quad (6.8)$$

where

$$\mathcal{F}_r^s = \mathcal{R}_s^r \mathbf{r}_\Gamma^s,$$

$$\mathcal{F}_c^s = \mathcal{R}_s^c \mathbf{r}_\Gamma^s.$$

Performing a partial assembly to enforce the continuity condition at the corner nodes, we obtain the following linear system

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \mathcal{B}_c^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \mathcal{B}_c^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{ci}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cr}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cc}^s \mathcal{B}_c^s \end{bmatrix} \begin{bmatrix} \mathcal{X}^s \\ \mathcal{U}_r^s \\ \mathcal{U}_c \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{F}_r^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{F}_c^s \end{bmatrix}, \quad (6.9)$$

where $\mathcal{B}_c^s$ is a restriction operator that maps the global corner unknown $\mathcal{U}_c$ into its local components $\{\mathcal{U}_c^s\}_{s=1}^{n_s}$ as

$$\mathcal{U}_c^s = \mathcal{B}_c^s \mathcal{U}_c, \quad (6.10)$$

where

$$\mathcal{B}_c^s = \text{blockdiag}(\mathbf{B}_{c,0}^s, \dots, \mathbf{B}_{c,N}^s),$$

and $\mathbf{B}_{c,k}^s$ is defined by

$$\mathbf{u}_{c,k}^s = \mathbf{B}_{c,k}^s \mathbf{u}_{c,k}.$$

Eliminating the local variables $\mathcal{X}^s$ and $\mathcal{U}_r^s$ in Eq.(6.9), we obtain the following symmetric positive definite coarse problem

$$F_{cc} \mathcal{U}_c = d_c, \quad (6.11)$$

where

$$F_{cc} = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s,$$

$$d_c = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{F}_c^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{F}_r^s),$$

and $\mathcal{S}_{\alpha\beta}^s = \mathcal{A}_{\alpha\beta}^s - \mathcal{A}_{\alpha i}^s [\mathcal{A}_{ii}^s]^{-1} \mathcal{A}_{i\beta}^s$ where α and β stand for the index r and c .

The corner nodes artificially enforce Dirichlet boundary conditions to eliminate the singularity arising from the subdomain Schur complement matrix $\mathcal{S}_{rr}^s$ of the floating subdomains. The remaining interface variables $\mathcal{U}_r^s$ can be obtained next for each subdomain as

$$\mathcal{S}_{rr}^s \mathcal{U}_r^s = \mathcal{F}_r^s - \mathcal{S}_{rc}^s \mathcal{U}_c^s. \quad (6.12)$$

Once the local interface variables $\mathcal{U}_r^s$ and $\mathcal{U}_c^s$ are available, the global interface unknowns $\mathcal{U}_\Gamma$ can be aggregated as

$$\mathcal{U}_\Gamma = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s (\mathcal{R}_s^r \mathcal{U}_r^s + \mathcal{R}_s^c \mathcal{U}_c^s). \quad (6.13)$$

Substituting Eq.(6.11) and Eq.(6.12) into Eq.(6.13) and performing some algebraic manipulations, the two-level preconditioner can be expressed as

$$\mathcal{M}_{NNC}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{R}_s^{rT} [\mathcal{S}_{rr}^s]^{-1} \mathcal{R}_s^r \mathcal{D}_s \mathcal{R}_s + \mathcal{R}_0^T [\mathcal{F}_{cc}]^{-1} \mathcal{R}_0, \quad (6.14)$$

where the restriction operator $\mathcal{R}_0$ mapping from fine to coarse grid, is defined by

$$\mathcal{R}_0 = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{R}_s^c - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{R}_s^r) \mathcal{D}_s \mathcal{R}_s.$$

Evidently, the two-level Neumann-Neumann preconditioner in Eq.(6.14) is equipped with a coarse operator $[\mathcal{F}_{cc}]^{-1}$ to scatter information globally.

6.4 Parallel Implementation

The precondition extended Schur complement system in Eq.(6.1) is solved iteratively using PCGM (see Algorithm(10)) equipped with the aforementioned two-level Neumann-Neumann preconditioner defined in Eq.(6.14). The preconditioned residual vectors at steps 2 and 12 of Algorithm (10) are computed in parallel as outlined in Algorithm(12).

Algorithm 12: Two-Level Neumann-Neumann Preconditioner Procedure

```

input      :  $(\mathbf{r}_r)$ 

1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter :  $\mathbf{r}_r^s = \mathcal{D}_s \mathcal{R}_s \mathbf{r}_r$ 
4   compute :  $\mathcal{F}_r^s = \mathcal{R}_s^T \mathbf{r}_r^s$ 
5   compute :  $\mathcal{F}_c^s = \mathcal{R}_s^c \mathbf{r}_r^s$ 
6   solve   :  $\mathcal{S}_{rr}^s v_1^s = \mathcal{F}_r^s$ 
7   update  :  $d_c^s = \mathcal{F}_c^s - \mathcal{S}_{cr}^s v_1^s$ 
8   gather  :  $d_c = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} d_c^s$ 
9   solve   :  $F_{cc} Z_c = d_c$ 
10 for  $s = 1, 2, \dots, n_s$  in parallel:
11 do
12   scatter :  $Z_c^s = \mathcal{B}_c^s Z_c$ 
13   update  :  $v_2^s = \mathcal{F}_r^s - \mathcal{S}_{rc}^s Z_c^s$ 
14   solve   :  $\mathcal{S}_{rr}^s Z_r^s = v_2^s$ 
15   update  :  $Z^s = \mathcal{R}_s^T Z_r^s + \mathcal{R}_s^{cT} Z_c^s$ 
16   gather  :  $Z = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s Z^s$ 

output    :  $(Z)$ 

```

The implementation of Algorithm (12) requires solution of two local fine problems (steps 6 and 14) and a global coarse problem (step 9). The fine problems correspond to

the local stochastic Neumann problems are solved using Algorithm (13).

Algorithm 13: Neumann-Solver Procedure

input : $(\mathcal{F}_r^s)$
1 solve : $\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s \end{bmatrix} \begin{Bmatrix} \mathcal{X}_i^s \\ \mathcal{Z}_r^s \end{Bmatrix} = \begin{Bmatrix} 0 \\ \mathcal{F}_r^s \end{Bmatrix}$
output : $(\mathcal{Z}_r^s)$

The size of the coarse problem in step 9 of Algorithm (12) is relatively small. However, an explicit construction of the coarse Schur complement matrix F_{cc} is computationally intensive. In our implementation, the coarse problem is solved using a parallel PCGM with the Lumped preconditioner as

$$\mathcal{M}_c^{-1} F_{cc} \mathcal{Z}_c = \mathcal{M}_c^{-1} d_c, \quad (6.15)$$

where

$$\mathcal{M}_c^{-1} = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cc}^s \mathcal{B}_c^s. \quad (6.16)$$

A flow-chart of the two-level extended Neumann-Neumann algorithm is shown in Fig.(6.2)

Figure 6.2: Flow chart of parallel implementation of the two-level extended Neumann-Neumann algorithm

6.5 Summary

We formulated a novel two-level domain decomposition preconditioner for the iterative substructuring of stochastic PDEs. Within the framework of the intrusive SSFEM, the two-level preconditioner is constructed by adding a coarse problem to the one-level Neumann-Neumann preconditioner. A collection of corner nodes at the subdomain interfaces constitute the coarse grid. Consequently, a coarse problem is solved at each iteration to spread information across all the subdomains. This information exchange achieved by the coarse

grid makes the preconditioner scalable. The two-level preconditioner may be construed to be a probabilistic extension of the Balancing Domain Decomposition by Constraints (BDDC) devised for deterministic PDEs.

Chapter 7

Primal-Primal Domain Decomposition Method for Stochastic PDEs

7.1 Introduction

This chapter is closely based on the references [79, 80]¹. In this chapter, we describe a novel primal version of the iterative substructuring technique for the solution of the large-scale linear system arising from the stochastic finite element method. The algorithm offers a straightforward approach to formulate a two-level scalable preconditioner. In the primal-primal method, a *reduced interface problem* corresponding to the remaining interface nodes is solved iteratively using PCGM equipped with a two-level preconditioner.

In the preconditioning step of the primal-primal technique, the continuity condition is strictly enforced on the corner nodes, while weakly satisfied (in an average sense) on the

¹The paper [79] received an award at the HPCS2010 conference for outstanding technical contribution.

remaining interface nodes. The iterative method converges when the continuity of the solution field is satisfied across the entire interface. This approach naturally leads to a coarse problem connecting the subdomains globally via the corner nodes which makes the algorithm scalable.

7.2 Primal-Primal Method for Stochastic PDEs

Let the physical domain Ω be decomposed into n_s non-overlapping subdomains $\{\Omega_s\}_{s=1}^{n_s}$, and the subdomain nodal vector $\mathbf{u}^s(\theta)$ be partitioned into a set of interior $\mathbf{u}_i^s(\theta)$, corner $\mathbf{u}_c^s(\theta)$ and remaining unknowns $\mathbf{u}_r^s(\theta)$, as schematically shown in Fig.(7.1).

Figure 7.1: Partitioning the subdomain nodes into: interior ($\diamond$), remaining ($\blacksquare$) and corner($\bullet$)

For a typical subdomain Ω_s , the equilibrium equation can be expressed as

$$\begin{bmatrix} \mathbf{A}_{ii}^s(\theta) & \mathbf{A}_{ir}^s(\theta) & \mathbf{A}_{ic}^s(\theta) \\ \mathbf{A}_{ri}^s(\theta) & \mathbf{A}_{rr}^s(\theta) & \mathbf{A}_{rc}^s(\theta) \\ \mathbf{A}_{ci}^s(\theta) & \mathbf{A}_{cr}^s(\theta) & \mathbf{A}_{cc}^s(\theta) \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s(\theta) \\ \mathbf{u}_r^s(\theta) \\ \mathbf{u}_c^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_r^s \\ \mathbf{f}_c^s \end{Bmatrix}. \quad (7.1)$$

Expanding the stochastic system parameters and the solution process by PCE and then performing Galerkin projection, Eq.(7.1) can be expressed as

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \\ \mathcal{A}_{ci}^s & \mathcal{A}_{cr}^s & \mathcal{A}_{cc}^s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_i^s \\ \mathcal{U}_r^s \\ \mathcal{U}_c^s \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_i^s \\ \mathcal{F}_r^s \\ \mathcal{F}_c^s \end{Bmatrix}, \quad (7.2)$$

where

$$[\mathcal{A}_{\alpha\beta}^s]_{jk} = \sum_{l=0}^L \langle \Psi_l \Psi_j \Psi_k \rangle \mathbf{A}_{\alpha\beta,l}^s, \quad \mathcal{F}_{\alpha,k}^s = \langle \Psi_k \mathbf{f}_{\alpha}^s \rangle, \quad \mathcal{U}_{\alpha}^s = (\mathbf{u}_{\alpha,0}^s, \dots, \mathbf{u}_{\alpha,N}^s)^T.$$

The subscripts α and β represent the index i, r and c .

The continuity condition is enforced next by global assembly of the remaining and corner variables as

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s \mathcal{B}_r^s & \mathcal{A}_{ic}^s \mathcal{B}_c^s \\ \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{A}_{ri}^s & \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{A}_{rr}^s \mathcal{B}_r^s & \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{A}_{rc}^s \mathcal{B}_c^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{ci}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cr}^s \mathcal{B}_r^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cc}^s \mathcal{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_i^s \\ \mathcal{U}_r \\ \mathcal{U}_c \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_i^s \\ \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{F}_r^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{F}_c^s \end{Bmatrix}, \quad (7.3)$$

where $\mathcal{B}_r^s$ is a Boolean rectangular matrix that maps the global remaining vector $\mathcal{U}_r$ to the local remaining vector $\mathcal{U}_r^s$ as

$$\mathcal{U}_r^s = \mathcal{B}_r^s \mathcal{U}_r. \quad (7.4)$$

Similarly, the restriction operator $\mathcal{B}_c^s$ is a Boolean rectangular matrix that maps the global corner vector $\mathcal{U}_c$ to the local corner vector $\mathcal{U}_c^s$ as

$$\mathcal{U}_c^s = \mathcal{B}_c^s \mathcal{U}_c. \quad (7.5)$$

The interior unknowns $\mathcal{U}_i^s$ can be obtained concurrently from Eq.(7.3) as

$$\mathcal{U}_i^s = [\mathcal{A}_{ii}^s]^{-1} (\mathcal{F}_i^s - \mathcal{A}_{ir}^s \mathcal{B}_r^s \mathcal{U}_r - \mathcal{A}_{ic}^s \mathcal{B}_c^s \mathcal{U}_c). \quad (7.6)$$

Substituting Eq.(7.6) into Eq.(7.3) leads to the following Schur complement system corresponding to the remaining and corner nodes of the interface boundary, as shown schematically in Fig.(7.2).

$$\begin{bmatrix} \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{S}_{rr}^s \mathcal{B}_r^s & \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{S}_{rc}^s \mathcal{B}_c^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s \mathcal{B}_r^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cc}^s \mathcal{B}_c^s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_r \\ \mathcal{U}_c \end{Bmatrix} = \begin{Bmatrix} \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{G}_r^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{G}_c^s \end{Bmatrix}, \quad (7.7)$$

where

$$\mathcal{S}_{\alpha\beta}^s = \mathcal{A}_{\alpha\beta}^s - \mathcal{A}_{\alpha i}^s [\mathcal{A}_{ii}^s]^{-1} \mathcal{A}_{i\beta}^s, \quad (7.8)$$

$$\mathcal{G}_\alpha^s = \mathcal{F}_\alpha^s - \mathcal{A}_{\alpha i}^s [\mathcal{A}_{ii}^s]^{-1} \mathcal{F}_i^s. \quad (7.9)$$

Figure 7.2: Fully assembled system: remaining (■) and corner(●) nodes

Eliminating the corner unknowns $\mathcal{U}_c$ in Eq.(7.7) gives the following symmetric positive definite *reduced interface problem*

$$(\mathcal{F}_{rr} - \mathcal{F}_{rc}[\mathcal{F}_{cc}]^{-1}\mathcal{F}_{cr})\mathcal{U}_r = \mathcal{d}_r - \mathcal{F}_{rc}[\mathcal{F}_{cc}]^{-1}\mathcal{d}_c, \quad (7.10)$$

where

$$\mathcal{F}_{\alpha\beta} = \sum_{s=1}^{n_s} \mathcal{B}_{\alpha}^s \mathcal{S}_{\alpha\beta}^s \mathcal{B}_{\beta}^s, \quad (7.11)$$

$$\mathcal{d}_{\alpha} = \sum_{s=1}^{n_s} \mathcal{B}_{\alpha}^s \mathcal{G}_{\alpha}^s, \quad (7.12)$$

The reduced interface problem defined in Eq.(7.10) can be solved iteratively using PCGM equipped with two-level preconditioner defined in the next section.

7.3 Primal-Primal Preconditioner

The two-level preconditioner for the reduced interface problem is constructed by strictly enforcing the continuity condition on the corner nodes, while for the remaining nodes the continuity is satisfied in an average sense. This fact is schematically illustrated in Fig.(7.3). As the iterations converge, the continuity condition at all interface nodes (both corner and remaining boundary nodes) is satisfied strictly.

Figure 7.3: Partial assembly of the corner nodes (●)

Performing a global assembly of the corner variables leads to the following system:

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \mathcal{B}_c^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \mathcal{B}_c^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{ci}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cr}^s \mathcal{B}_r^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cc}^s \mathcal{B}_c^s \end{bmatrix} \begin{bmatrix} \mathcal{X}_i^s \\ \mathcal{U}_r \\ \mathcal{U}_c \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{F}_r^s \\ 0 \end{bmatrix}, \quad (7.13)$$

where

$$\mathcal{F}_r^s = \mathcal{D}_r^s \mathcal{B}_r^s \mathbf{r}_j, \quad (7.14)$$

and $\mathbf{r}_j$ is the residual at the j^{th} iteration of the iterative solver and $\mathcal{D}_r^s$ represents a block diagonal matrix defined as

$$\mathcal{D}_r^s = \text{blockdiag}(\mathbf{D}_{r,0}^s, \dots, \mathbf{D}_{r,N}^s), \quad (7.15)$$

where $\mathbf{D}_{r,k}^s$ is a weighting matrix that satisfies the following property

$$\sum_{s=1}^{n_s} \mathbf{B}_r^{sT} \mathbf{D}_r^s \mathbf{B}_r^s = \mathbf{I}. \quad (7.16)$$

The diagonal entries of the scaling matrix $\mathbf{D}_r^s$ are the reciprocal of the number of sub-domains that share the corresponding remaining interface boundary nodes.

Eliminating the local unknown vector $\mathcal{X}_i^s$ from Eq.(7.13) leads to the following partially assembled extended Schur complement system

$$\begin{bmatrix} \mathcal{S}_{rr}^s & \mathcal{S}_{rc}^s \mathcal{B}_c^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s \mathcal{B}_r^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cc}^s \mathcal{B}_c^s \end{bmatrix} \begin{bmatrix} \mathcal{U}_r^s \\ \mathcal{U}_c \end{bmatrix} = \begin{bmatrix} \mathcal{F}_r^s \\ 0 \end{bmatrix}. \quad (7.17)$$

Next, the local remaining unknown vector $\mathcal{U}_r^s$ can be eliminated concurrently from Eq.(7.17) leading to the following global coarse problem

$$F_{cc}\mathcal{U}_c = d_c, \quad (7.18)$$

where

$$F_{cc} = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s, \quad (7.19)$$

$$d_c = - \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{F}_r^s. \quad (7.20)$$

The continuity of the solution field over the remaining interface nodes is satisfied next by averaging the local results as

$$\mathcal{U}_r = \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{D}_r^s \mathcal{U}_r^s. \quad (7.21)$$

After some algebraic manipulations, the stochastic primal-primal preconditioner can be expressed as

$$\mathcal{M}_{SPPM}^{-1} = \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{D}_r^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{D}_r^s \mathcal{B}_r^s + R_0^T [F_{cc}]^{-1} R_0, \quad (7.22)$$

where

$$R_0 = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{D}_r^s \mathcal{B}_r^s. \quad (7.23)$$

Clearly, the primal-primal preconditioner consists of subdomain level problems $[\mathcal{S}_{rr}^s]^{-1}$ and a global coarse problem $[F_{cc}]^{-1}$.

7.4 Parallel Implementation

The PCGM equipped with the primal-primal preconditioner is employed in parallel to tackle the reduced interface problem as

$$\mathcal{M}_{SPPM}^{-1}(F_{rr} - F_{rc}[F_{cc}]^{-1}F_{cr})\mathcal{U}_r = \mathcal{M}_{SPPM}^{-1}(d_r - F_{rc}[F_{cc}]^{-1}d_c). \quad (7.24)$$

At the j^{th} iteration of the parallel PCGM, the multiplication of the coefficient matrix by a vector is obtained using the following algorithm:

Algorithm 14: Parallel Matrix-Vector Product for Primal-Primal Method

```

input      :  $(\mathcal{P})$ 

1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter  :  $\mathcal{P}^s = \mathcal{B}_r^s \mathcal{P}$ 
4   compute  :  $v_1^s = \mathcal{S}_{cr}^s \mathcal{P}^s$ 
5   gather   :  $V_1 = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} v_1^s$ 
6 solve      :  $F_{cc} V_2 = V_1$ 
7 for  $s = 1, 2, \dots, n_s$  in parallel:
8 do
9   scatter  :  $v_2^s = \mathcal{B}_c^s V_2$ 
10  compute  :  $v_3^s = \mathcal{S}_{rc}^s v_2^s$ 
11  update   :  $\mathcal{Q}^s = \mathcal{S}_{rr}^s \mathcal{P}^s - v_3^s$ 
12  gather   :  $\mathcal{Q} = \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} \mathcal{Q}^s$ 

output    :  $(\mathcal{Q})$ 

```

Multiplication of the extended Schur complement matrix by a vector in steps 4, 10 and 11 of Algorithm (14) is computed by solving a corresponding Dirichlet problem as

$$v_\alpha^s = \mathcal{S}_{\alpha\beta}^s v_\beta^s, \quad (7.25)$$

$$v_\alpha^s = (\mathcal{A}_{\alpha\beta}^s - \mathcal{A}_{\alpha i}^s [\mathcal{A}_{ii}^s]^{-1} \mathcal{A}_{i\beta}^s) v_\beta^s. \quad (7.26)$$

This procedure is outlined in the following algorithm:

Algorithm 15: Dirichlet-Solver Procedure	
input	: $(v_\beta^s, \mathcal{A}_{i\beta}^s, \mathcal{A}_{\alpha i}^s, \mathcal{A}_{\alpha\beta}^s, \mathcal{A}_{ii}^s)$
1 compute	: $v_1^s = \mathcal{A}_{i\beta}^s v_\beta^s$
2 solve	: $\mathcal{A}_{ii}^s v_2^s = v_1^s$
3 compute	: $v_3^s = \mathcal{A}_{\alpha i}^s v_2^s$
4 compute	: $v_4^s = \mathcal{A}_{\alpha\beta}^s v_\beta^s$
5 compute	: $v_\alpha^s = v_4^s - v_3^s$
output	: (v_α^s)

The global problem in step 6 of Algorithm (14) is solved iteratively using PCGM equipped with lumped preconditioner as

$$\mathcal{M}_{cc}^{-1} F_{cc} V_2 = \mathcal{M}_{cc}^{-1} V_1, \quad (7.27)$$

where

$$\mathcal{M}_{cc}^{-1} = \sum_{s=1}^{n_s} B_c^{sT} \mathcal{A}_{cc}^s B_c^s. \quad (7.28)$$

The effect of the primal-primal preconditioner is computed using the procedure outlined in the following algorithm:

Algorithm 16: Primal-Primal Preconditioner Effect Procedure

```

input      :  $(r_\Gamma)$ 

1 for  $s = 1, 2, \dots, n_s$  in parallel:
2 do
3   scatter :  $\mathcal{F}_r^s = \mathcal{B}_r^s r_\Gamma$ 
4   compute :  $v_1^s = \mathcal{D}_r^s \mathcal{F}_r^s$ 
5   solve   :  $\mathcal{S}_{rr}^s v_2^s = v_1^s$ 
6   compute :  $d_c^s = \mathcal{S}_{cr}^s v_2^s$ 
7   gather  :  $d_c = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} d_c^s$ 
8 solve     :  $F_{cc} Z_c = d_c$ 
9 for  $s = 1, 2, \dots, n_s$  in parallel:
10 do
11  scatter :  $Z_c^s = \mathcal{B}_c^s Z_c$ 
12  update  :  $v_3^s = v_1^s + \mathcal{S}_{rc}^s Z_c^s$ 
13  solve   :  $\mathcal{S}_{rr}^s Z_r^s = v_3^s$ 
14  compute :  $Z^s = \mathcal{D}_r^s Z_r^s$ 
15  gather  :  $Z = \sum_{s=1}^{n_s} \mathcal{B}_r^{sT} Z^s$ 
output    :  $(Z)$ 

```

The local problems in steps 5 and 13 of Algorithm (16) constitute a subdomain level Neumann problem which can be solved using the following algorithm:

Algorithm 17: Neumann-Solver Procedure

input : $(\mathcal{F}_r^s)$
 1 **solve** : $\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s \end{bmatrix} \begin{Bmatrix} \mathcal{X}_i^s \\ \mathcal{U}_r^s \end{Bmatrix} = \begin{Bmatrix} 0 \\ \mathcal{F}_r^s \end{Bmatrix}$
output : $(\mathcal{U}_r^s)$

The global coarse stochastic problem in step 8 of Algorithm (16) is solved iteratively using PCGM solver equipped with lumped preconditioner as

$$\mathcal{M}_{cc}^{-1} F_{cc} \mathcal{Z}_c = \mathcal{M}_{cc}^{-1} d_c, \quad (7.29)$$

where

$$\mathcal{M}_{cc}^{-1} = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cc}^s \mathcal{B}_c^s. \quad (7.30)$$

Finally, we summarize the parallel implementation of the PCGM to solve the reduced interface problem using the primal-primal preconditioner in the following flow chart.

Figure 7.4: Flow chart of parallel implementation of the primal-primal method

7.5 Summary

A novel primal-primal iterative substructuring technique is introduced to solve the large-scale linear system arising from the finite element discretization of stochastic PDEs. The algorithm offers a direct approach to formulate a two-level scalable preconditioner. Throughout the iteration, the primal-primal preconditioner strictly enforces the continuity condition on the corner nodes of the interface, while weakly satisfying the continuity condition over the remaining part of the interface. This approach naturally leads to a coarse grid connecting the subdomains globally and provides a mechanism to propagate information across the subdomains which makes the algorithm scalable.

Chapter 8

Dual-Primal Domain Decomposition Method for Stochastic PDEs

8.1 Introduction

This chapter is closely based on the references [79, 80, 86]. In this chapter, we report a probabilistic version of the dual-primal domain decomposition method for the intrusive SSFEM in order to exploit high performance computing platforms for uncertainty quantification. In particular, we formulate a probabilistic version of the dual-primal finite element tearing and interconnect (FETI-DP) technique to solve the large-scale linear systems in the intrusive SSFEM. In the probabilistic setting, the operator of the dual interface system in the dual-primal approach contains a coarse problem. The introduction of the coarse problem leads to a scalable performance of the dual-primal iterative substructuring method for uncertainty quantification of large-scale computational models.

For deterministic PDEs, BDDC [78, 107, 108] and FETI-DP [64, 81] are perhaps the most popular non-overlapping domain decomposition techniques for the iterative solution of large-scale deterministic linear systems. BDDC provides a two-level preconditioner for the solution of the so-called *primal interface problem* (Schur complement system). On the contrary, FETI-DP iteratively solves a system of Lagrange multipliers arises in the so-called *dual interface system*. The coarse problem essential for scalability is built in the preconditioner of the BDDC, while it is embedded within the operator of FETI-DP. For deterministic systems, it has already been demonstrated that the condition number and thus the parallel performance of BDDC and FETI-DP are quite similar [65, 67, 78, 83–85]. Indeed, the preconditioned operators in BDDC and its counterpart in FETI-DP have the same algebraic structure with identical eigenvalues except possibly for zero and one [67]. This fact indicates that the convergence properties of both BDDC and FETI-DP are identical when using the same primal constraints [83]. It is therefore natural to ask whether the similarity of BDDC and FETI-DP extends to stochastic systems.

8.2 Dual-Primal Domain Decomposition Method for SPDEs

Using a general framework of iterative substructuring techniques [68, 70, 74–77, 79, 80], we formulate a probabilistic version of FETI-DP for the iterative solution of the deterministic linear system in the SSFEM [79, 80]. In the dual-primal method for stochastic systems, the spatial domain is partitioned into a number of non-overlapping subdomains. The polynomial chaos expansions is employed to represent the solution process. For each

subdomain, the solution vector is divided into the interior and interface unknowns [64, 81]. The interface unknowns are further split into sets of corner and remaining variables. In each iteration of PCGM for the probabilistic dual interface system, global assembly for the chaos coefficients of the solution process at the corner nodes is performed to exactly enforce the continuity conditions. On the other hand, Lagrange multipliers are utilized to weakly satisfy the continuity of the polynomial chaos coefficients on the remaining nodes of the interface. Consequently, a probabilistic coarse problem is embedded in the operator of the dual interface problem of FETI-DP. The introduction of the coarse problem in the probabilistic framework leads to a scalable performance of FETI-DP iterative substructuring based solver for large-scale stochastic systems. The methodology can be described as follows.

The physical domain Ω is partitioned into n_s non-overlapping subdomains such that $\Omega = \bigcup_{s=1}^{n_s} \Omega_s$. For a typical subdomain Ω_s , we divide the nodal solution vector as the interior unknown $\mathbf{u}_i^s(\theta)$, remaining $\mathbf{u}_r^s(\theta)$ and interface corner $\mathbf{u}_c^s(\theta)$ as shown in Fig.(8.1).

Figure 8.1: Partitioning the boundary nodes into: remaining (■) and corner(●) nodes

Accordingly, the subdomain problem can be expressed as

$$\begin{bmatrix} \mathbf{A}_{ii}^s(\theta) & \mathbf{A}_{ir}^s(\theta) & \mathbf{A}_{ic}^s(\theta) \\ \mathbf{A}_{ri}^s(\theta) & \mathbf{A}_{rr}^s(\theta) & \mathbf{A}_{rc}^s(\theta) \\ \mathbf{A}_{ci}^s(\theta) & \mathbf{A}_{cr}^s(\theta) & \mathbf{A}_{cc}^s(\theta) \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s(\theta) \\ \mathbf{u}_r^s(\theta) \\ \mathbf{u}_c^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_r^s \\ \mathbf{f}_c^s \end{Bmatrix}. \quad (8.1)$$

Expanding the stochastic system parameters and the solution process by PCE and then performing Galerkin projection, Eq.(8.1) can be expressed as

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \\ \mathcal{A}_{ci}^s & \mathcal{A}_{cr}^s & \mathcal{A}_{cc}^s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_i^s \\ \mathcal{U}_r^s \\ \mathcal{U}_c^s \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_i^s \\ \mathcal{F}_r^s \\ \mathcal{F}_c^s \end{Bmatrix}, \quad (8.2)$$

where

$$[\mathcal{A}_{\alpha\beta}^s]_{jk} = \sum_{l=0}^L \langle \Psi_l \Psi_j \Psi_k \rangle \mathbf{A}_{\alpha\beta,l}^s, \quad \mathcal{F}_{\alpha,k}^s = \langle \Psi_k \mathbf{f}_{\alpha}^s \rangle, \quad \mathcal{U}_{\alpha}^s = (\mathbf{u}_{\alpha,0}^s, \dots, \mathbf{u}_{\alpha,N}^s)^T,$$

and the subscripts α and β indicate i , r and c .

Let $\mathcal{B}_c^s$ be a block-diagonal matrix used to scatter the global corner solution vector $\mathcal{U}_c$ to its local component as

$$\mathcal{U}_c^s = \mathcal{B}_c^s \mathcal{U}_c \quad (8.3)$$

where

$$\mathcal{B}_c^s = \text{blockdiag}(\mathbf{B}_{c,0}^s, \dots, \mathbf{B}_{c,N}^s), \quad (8.4)$$

and

$$\mathbf{u}_{c,j}^s = \mathbf{B}_{c,j}^s \mathbf{u}_{c,j}. \quad (8.5)$$

Next, introducing the Lagrange multipliers Λ to satisfy the weak compatibility constraint on the remaining part of the interface and performing a global assembly of the polynomial chaos coefficients of the solution process at the corner nodes, we obtain the following system

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \mathcal{B}_c^s & 0 \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \mathcal{B}_c^s & \mathcal{B}_r^{sT} \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{ci}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cr}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cc}^s \mathcal{B}_c^s & 0 \\ 0 & \sum_{s=1}^{n_s} \mathcal{B}_r^s & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathcal{U}_i^s \\ \mathcal{U}_r^s \\ \mathcal{U}_c \\ \Lambda \end{bmatrix} = \begin{bmatrix} \mathcal{F}_i^s \\ \mathcal{F}_r^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{F}_c^s \\ 0 \end{bmatrix}, \quad (8.6)$$

where $\mathcal{B}_r^s$ is a block diagonal jump operator such that

$$\sum_{s=1}^{n_s} \mathcal{B}_r^s \mathcal{U}_r^s = 0,$$

and

$$\Lambda = \left\{ \lambda_0, \dots, \lambda_N \right\}^T.$$

The Lagrange multiplier system for the polynomial chaos coefficients of the solution process can be obtain from Eq.(8.6) as

$$(\bar{F}_{rr} + \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{F}_{cr})\Lambda = \bar{d}_r - \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{d}_c, \quad (8.7)$$

where

$$\begin{aligned} \bar{F}_{rr} &= \sum_{s=1}^{n_s} \mathcal{B}_r^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT}, & \bar{F}_{rc} &= \sum_{s=1}^{n_s} \mathcal{B}_r^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s \mathcal{B}_c^s, \\ \bar{F}_{cc} &= \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s, & \bar{F}_{cr} &= \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT}, \\ \bar{d}_c &= \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{G}_c^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{G}_r^s), & \bar{d}_r &= \sum_{s=1}^{n_s} \mathcal{B}_r^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{G}_r^s, \end{aligned}$$

and

$$\begin{aligned} S_{\alpha\beta}^s &= A_{\alpha\beta}^s - A_{\alpha i}^s [A_{ii}^s]^{-1} A_{i\beta}^s, \\ G_{\alpha}^s &= F_{\alpha}^s - A_{\alpha i}^s [A_{ii}^s]^{-1} F_i^s. \end{aligned}$$

The extended Lagrange multipliers system defined by Eq.(8.7) is symmetric and positive definite (e.g. [11, 52, 64, 81]) and thus can be solved iteratively using PCGM. Similar to the deterministic version of FETI-DP [64, 81], the coarse problem $\bar{F}_{cc}^{-1}$ required for global communication is already embedded within the operator. In this case, the extended lumped [70, 75] or the extended Dirichlet preconditioner is sufficient for scalability. Physically, the extended Lagrange multiplier system relates to the nodal forces required to satisfy the compatibility condition of the polynomial chaos coefficients of the solution process at the remaining interface nodes as shown in Fig.(8.2).

Figure 8.2: Lagrange multipliers: enforcing continuity of the polynomial chaos coefficients of the solution process

Once the Lagrange multipliers are computed, the polynomial chaos coefficients associated with the corner nodes can be recovered as

$$\bar{F}_{cc}\mathcal{U}_c = (\bar{d}_c + \bar{F}_{cr}\Lambda) \quad (8.8)$$

The subdomain level variables $\mathcal{U}_i^s$ and $\mathcal{U}_r^s$ can be obtained in parallel from the following

local linear system

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_i^s \\ \mathcal{U}_r^s \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_i^s - \mathcal{A}_{ic}^s \mathcal{B}_c^s \mathcal{U}_c \\ \mathcal{F}_r^s - \mathcal{A}_{rc}^s \mathcal{B}_c^s \mathcal{U}_c - \mathcal{B}_r^{sT} \Lambda \end{Bmatrix}. \quad (8.9)$$

8.3 Preconditioners for the Probabilistic FETI-DP

The preconditioned extended Lagrange multipliers system takes the following form

$$\mathcal{M}(\bar{F}_{rr} + \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{F}_{cr})\Lambda = \mathcal{M}(\bar{d}_r - \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{d}_c), \quad (8.10)$$

where $\mathcal{M}$ is a one-level extended Dirichlet preconditioner defined as

$$\mathcal{M}_D = \sum_{s=1}^{n_s} \mathcal{B}_r^s \mathcal{D}_r^s \mathcal{S}_{rr}^s \mathcal{D}_r^s \mathcal{B}_r^{sT}, \quad (8.11)$$

where

$$\mathcal{D}_r^s = \text{blockdiag}(\mathbf{D}_r^{s,0}, \dots, \mathbf{D}_r^{s,N}), \quad (8.12)$$

and $\mathbf{D}_r^{s,k}$ is a diagonal averaging matrix defined as

$$\sum_{s=1}^{n_s} \mathbf{R}_r^{sT} \mathbf{D}_r^{s,k} \mathbf{R}_r^s = \mathbf{I}. \quad (8.13)$$

The implementation of the extended Dirichlet preconditioner within the PCGM involves solving a local stochastic Dirichlet problem as explained below.

We consider the following local system

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s \end{bmatrix} \begin{Bmatrix} \mathcal{X}_i^s \\ \mathcal{D}_r^s \mathcal{B}_r^{sT} \mathbf{r}_r \end{Bmatrix} = \begin{Bmatrix} 0 \\ \mathcal{Z}_r^s \end{Bmatrix}, \quad (8.14)$$

where $\mathbf{r}_r$ is the global residual vector at the j^{th} iteration of PCGM.

A stochastic local Dirichlet problem is solved to compute $\mathcal{X}_i^s$ as

$$\mathcal{X}_i^s = -[\mathcal{A}_{ii}^s]^{-1} \mathcal{A}_{ir}^s \mathcal{D}_r^s \mathcal{B}_r^{sT} \mathbf{r}_r. \quad (8.15)$$

Substituting Eq.(8.15) into the second row of Eq.(8.14), we obtain

$$\mathcal{Z}_r^s = (\mathcal{A}_{rr}^s - \mathcal{A}_{ri}^s [\mathcal{A}_{ii}^s]^{-1} \mathcal{A}_{ir}^s) \mathcal{D}_r^s \mathcal{B}_r^{sT} \mathbf{r}_r. \quad (8.16)$$

Finally the global preconditioned residual is aggregated as

$$\mathcal{Z}_r = \sum_{s=1}^{n_s} \mathcal{B}_r^s \mathcal{D}_r^s \mathcal{Z}_r^s. \quad (8.17)$$

8.4 Parallel Implementation

In this section, we detail the parallel implementation of the PCGM to solve the Lagrange multiplier system of the chaos coefficients. The distributed implementation of the matrix-vector product $\mathcal{Q}_j = (\bar{F}_{rr} + \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{F}_{cr})\mathcal{P}_j$ is listed in Algorithm (18).

Algorithm 18: Parallel Matrix-Vector Product for Dual-Primal Method

```

input      :  $(\mathcal{P})$ 

1 for  $s = 1, 2, \dots, n_s$  in parallel:

2 do
3   scatter :  $\mathcal{P}^s = \mathcal{B}_r^{sT} \mathcal{P}$ 
4   solve   :  $\mathcal{S}_{rr}^s v_1^s = \mathcal{P}^s$ 
5   compute :  $v_2^s = \mathcal{S}_{cr}^s v_1^s$ 
6   gather  :  $V_2 = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} v_2^s$ 
7 solve    :  $\bar{F}_{cc} V_3 = V_2$ 
8 for  $s = 1, 2, \dots, n_s$  in parallel:

9 do
10  scatter :  $v_3^s = \mathcal{B}_c^s V_3$ 
11  compute :  $v_4^s = \mathcal{S}_{rc}^s v_3^s$ 
12  update  :  $v_5^s = \mathcal{P}^s + v_4^s$ 
13  solve   :  $\mathcal{S}_{rr}^s Q^s = v_5^s$ 
14  gather  :  $Q = \sum_{s=1}^{n_s} \mathcal{B}_r^s Q^s$ 

output    :  $(Q)$ 
  
```

The steps 4 and 13 of Algorithm (18) are implemented by solving a local stochastic

Neumann problem as outlined in Algorithm (19).

Algorithm 19: Neumann-Solver Procedure

input : $(\mathcal{F}_r^s)$

1 **solve** : $\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s \end{bmatrix} \begin{Bmatrix} \mathcal{X}_i^s \\ \mathcal{U}_r^s \end{Bmatrix} = \begin{Bmatrix} 0 \\ \mathcal{F}_r^s \end{Bmatrix}$

output : $(\mathcal{U}_r^s)$

The multiplication of the extended Schur complement matrix by a vector in steps 5 and 11 of Algorithm (18) involves solving a stochastic local Dirichlet problem as outlined in Algorithm (20).

Algorithm 20: Dirichlet-Solver Procedure

input : $(v_\beta^s, \mathcal{A}_{i\beta}^s, \mathcal{A}_{\alpha i}^s, \mathcal{A}_{\alpha\beta}^s, \mathcal{A}_{ii}^s)$

1 **compute** : $v_1^s = \mathcal{A}_{i\beta}^s v_\beta^s$

2 **solve** : $\mathcal{A}_{ii}^s v_2^s = v_1^s$

3 **compute** : $v_3^s = \mathcal{A}_{\alpha i}^s v_2^s$

4 **compute** : $v_4^s = \mathcal{A}_{\alpha\beta}^s v_\beta^s$

5 **compute** : $v_\alpha^s = v_4^s - v_3^s$

output : (v_α^s)

Note that steps 12, 13 and 14 of Algorithm (18) can be explained as follows. Recall that the local vector v_4^s in step 11 of Algorithm (18) can be written explicitly as

$$v_4^s = \mathcal{S}_{rc}^s \mathcal{B}_c^s [\bar{F}_{cc}]^{-1} \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT} \mathcal{P}.$$

Accordingly, the local vector v_5^s in step 12 of Algorithm (18) takes the following form

$$\begin{aligned} v_5^s &= \mathcal{P}^s + v_4^s, \\ &= \mathcal{B}_r^{sT} \mathcal{P} + \mathcal{S}_{rc}^s \mathcal{B}_c^s [\bar{F}_{cc}]^{-1} \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT} \mathcal{P}. \end{aligned}$$

It follows that in step 13 of Algorithm (18), the local vector Q^s can be recast as

$$\begin{aligned} Q^s &= [\mathcal{S}_{rr}^s]^{-1} v_5^s, \\ &= [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT} \mathcal{P} + [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s \mathcal{B}_c^s [\bar{F}_{cc}]^{-1} \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT} \mathcal{P}. \end{aligned}$$

Finally, the global vector Q in step 14 of Algorithm (18) representing the the matrix-vector product $Q = (\bar{F}_{rr} + \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{F}_{cr})\mathcal{P}$ is computed as

$$\begin{aligned} Q &= \sum_{s=1}^{n_s} \mathcal{B}_r^s Q^s, \\ &= \left(\sum_{s=1}^{n_s} \mathcal{B}_r^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT} + \sum_{s=1}^{n_s} \mathcal{B}_r^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s \mathcal{B}_c^s [\bar{F}_{cc}]^{-1} \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT} \right) \mathcal{P}. \end{aligned}$$

The probabilistic coarse problem in step 7 of Algorithm (18) is solved in parallel using PCGM with the extended Lumped preconditioner as

$$\mathcal{M}_{cc} \bar{F}_{cc} V_3 = \mathcal{M}_{cc} V_2, \quad (8.18)$$

where

$$\mathcal{M}_{cc} = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{A}_{cc}^s \mathcal{B}_c^s. \quad (8.19)$$

A flow-chart of the probabilistic FETI-DP algorithm is shown in Fig.(8.3)

Figure 8.3: Flow chart of parallel implementation of FETI-DP algorithm

8.5 Summary

A novel dual-primal iterative substructuring technique is formulated to tackle the coupled deterministic linear systems in the intrusive spectral stochastic finite element discretization of large-scale SPDEs. In the dual-primal approach for SPDEs, the continuity of the polynomial chaos coefficients is strictly enforced at the interface corner nodes at each iteration of PCGM. For the remaining nodes on the interface, the Lagrange multipliers are used to weakly satisfy the continuity condition of the chaos coefficients during the PCGM

iterations. The continuity of the polynomial chaos coefficients is satisfied along the entire interface as the PCGM converges. The proposed method may be viewed as the probabilistic version of FETI-DP.

Chapter 9

Numerical Results: Two-Dimensional Problems

9.1 Introduction

The numerical results presented in this chapter are from the references [75, 77, 86]. One of the most attractive features of domain decomposition method is its ability to offer parallel scalable algorithms [7, 72]. The iterative algorithm is said to be *scalable* when its convergence rate does not deteriorate as the number of subdomains increases (or the size of subdomain H decreases) [4, 5, 7, 64]. On the other hand, the iterative algorithm is said to be *optimal* when its convergence rate is independent of the mesh size h [4, 5]. However, the iterative algorithm is said to be *quasi-optimal* when its convergence rate only depends on the ratio of the subdomain size and element size (H/h) (i.e. the number of unknowns associated with one subdomain [4]). It is worth emphasizing the fact that an optimal or scal-

able preconditioner does not necessarily mean the computationally fastest preconditioner or a preconditioner with minimum computational complexity for a given problem [72].

To this end, we measure the numerical scalability of the algorithms: (a) firstly with respect to mesh size h whereby we fix the number of subdomains used to solve the problem and increase the spatial mesh resolution; (b) secondly, with respect to subdomain size H whereby we fix the spatial problem size and increase number of subdomains used to tackle the problem; (c) thirdly, with respect to the ratio of the number of elements to the number of subdomains (H/h) whereby we fix problem size per subdomain and increase the overall problem size by increasing the number of subdomains. For all these scalability measurements, we report the results for different order of PCE to measure the sensitivity of the algorithms to the order of PC representation.

The absolute performance or the parallel scalability of the algorithms is measured in terms of the *strong* and *weak* scalability [61, 142]. For the strong scalability test, we fix the global problem size and increase the number of CPUs used to solve the problem in order to reduce the total execution time. For the weak scalability test, we fix the problem size per subdomain and increase the global size of the problem by increasing the number of subdomains whereby the goal is to solve n -times larger problem using n -times larger computer (processors or cores) in nearly a constant CPU time.

For the numerical implementations, the PCGM solver is initialized with $\mathcal{U}_{r_0} = 0$ and the iterations are terminated when the ratio of the L_2 norms of the current residual to the

initial residual is less than 10^{-6} defined as

$$\frac{\|\mathcal{G}_r - S\mathcal{U}_r^k\|_2}{\|\mathcal{G}_r - S\mathcal{U}_{r_0}\|_2} \leq 10^{-6}. \quad (9.1)$$

For efficient memory usage and minimum floating point operation, the numerical implementation of the algorithm exploits the multi-level sparsity structure of the coefficient matrix of the stochastic system, namely (a) the sparsity structure due to the finite element discretization and (b) the block sparsity structure due to the orthogonal representation and projection of the stochastic processes. PETSc [87] and MPI [88] parallel libraries are used for efficient parallel implementation of the proposed algorithm. The graph partitioning tool METIS [89] is used for optimal decomposition of the finite element mesh. The finite element meshes are generated using Gmsh software [143].

Firstly, we investigate the parallel performance of the one-level domain decomposition preconditioners, namely the extended Lumped (L), Weighted Lumped (WL) and Neumann-Neumann (NN) domain decomposition preconditioners for flow through random media with spatially varying non-Gaussian random parameters. Secondly, we contrast the numerical and parallel scalabilities of the one-level preconditioner (NN) with the two-level preconditioner (NNC) for flow through random media and elasticity problems with spatially varying non-Gaussian material properties. Thirdly, we compare the convergence properties, numerical and parallel scalabilities of the two-level preconditioner (NNC) with probabilistic FETI-DP method using illustrations from flow through random media and linear elasticity with spatially varying non-Gaussian material properties.

The numerical experiments are performed on a Linux cluster (SUSE Linux Enterprise Server 11 SP1) consists of 22 nodes with an InfiniBand interconnect (2 Quad-Core 3.0 GHz Intel Xeon processors and 32 GB of memory per node). PETSc version 2.3.3 and Open-MPI version 1.4.3 libraries are compiled with GNU compiler GCC version 4.3.4 without any optimization flags.

9.2 One-Level Preconditioner

In this section, we study the performance of the one-level extended preconditioners (L, WL and NN) with respect to the level of uncertainty, the order of stochastic dimension, the spatial problem size, number of subdomains and fixed problem size per subdomain.

9.2.1 Flow Through Random Media

For the numerical illustrations, we consider a two-dimensional steady-state flow through random media with random hydraulic conductivity coefficient defined as

$$\nabla \cdot (\kappa(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) = f(\mathbf{x}, \theta), \quad \mathbf{x} \in \Omega \quad (9.2)$$

$$u(\mathbf{x}, \theta) = 0, \quad \mathbf{x} \in \partial\Omega, \quad (9.3)$$

where the coefficient $\kappa(\mathbf{x}, \theta)$ is modeled as a lognormal stochastic process obtained from underlying Gaussian process with an exponential covariance function and the forcing term is assumed to be a deterministic quantity defined as $f(\mathbf{x}, \theta) = 1.0$.

Finite Element Discretization and Mesh Decomposition

The maximum size of the finite element mesh considered consists of 512,154 elements and 256,081 nodes. The response is expanded using four-dimensional ($L = 3$) third order PCE ($N = 34$) leading to a linear system of order 8,962,835. Typical finite element mesh is depicted in Fig.(9.1(a)). The computational domain partitioned into 160 subdomains is plotted in Fig.(9.1(b)).

Figure 9.1: Finite element discretization and mesh decomposition

Stochastic Field Representation

The hydraulic conductivity coefficient $\kappa(\mathbf{x}, \theta)$ is modeled as a lognormal stochastic process obtained from the underlying Gaussian process with an exponential covariance function given by

$$C_{\alpha\alpha}(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp \left(\frac{-|x_1 - y_1|}{b_1} + \frac{-|x_2 - y_2|}{b_2} \right), \quad (9.4)$$

where the numerical values used in the investigation are $\sigma = 0.3$ and $b_1 = b_2 = 1.0$.

The generalized eigenvalue problem associated with KLE decomposition is solved using FEM with a coarse mesh consists of 21,800 elements and 10,904 nodes. Fig.(9.2) shows the monotonic decay of the eigenvalues of the exponential covariance function. The first fourth eigenvalues correspond to about 90% energy of the random process. Fig.(9.3) shows the eigenfunctions associated with the first four eigenvalues. Fig.(9.4) shows some selected PC coefficients of the lognormal process.

Figure 9.2: The decay of the eigenvalues of the exponential covariance function

Figure 9.3: The first fourth eigenfunctions of the exponential covariance function

Figure 9.4: Selected PC coefficients of the hydraulic conductivity

Stochastic Characteristics of the Solution Process

The mean and standard deviation of the hydraulic head are plotted in Fig.(9.5(a)) and Fig.(9.5(b)) respectively. The maximum coefficient of variation (CoV) of the solution field is about 25% underscoring the effect of uncertainty. Some of the chaos coefficients of the solution process are shown in Fig.(9.6). Although the response is a positive quantity, some of these chaos coefficients have negative amplitudes.

Figure 9.5: The mean and the standard deviation of the hydraulic head

Figure 9.6: Selected PC coefficients of the hydraulic head

Solution Convergence

Typical relative residual decay of PCGM equipped with Extended Lumped (L), Weighted Lumped (WL) and Neumann-Neumann (NN) preconditioners are plotted in Fig.(9.7). The WL preconditioner shows better convergence rate than the preliminary L preconditioner. This fact highlights the benefit of the weighting matrix in accelerating the convergence rate of the WL preconditioner. The NN preconditioner shows the fastest convergence rate with a smooth decay of the relative residual.

Figure 9.7: The history of the relative PCGM residual

Effect of The Coefficient of Variation

For a fixed problem size $n = 16,808$, fixed number of subdomains $n_s = 16$ and fixed order of PCE $N = 15$, we investigate the performance of the one-level preconditioners with respect to the coefficient of variation (CoV) of the diffusion coefficient. In Fig.(9.8), the PCGM iteration counts versus $CoVs$ are plotted for various preconditioners. Increasing the CoV of the system parameter up to 60% does not degrade the performance of L and NN preconditioners as the number of PCGM iteration is nearly constant. For the WL

preconditioner, we notice a slight growth in the iteration counts as the CoV increases.

Figure 9.8: Iteration counts with respect to the CoV

Numerical scalability

The scalability is measured (e.g. [6, 64, 142]) (a) firstly with respect to the size of the mesh h whereby we fix the number of subdomains and increase the spatial mesh resolution; (b) secondly, with respect to subdomain size H whereby we fix the spatial problem size and increase number of subdomains used to tackle the problem; (c) thirdly, with respect to the ratio of the number of elements to that of subdomains (H/h) whereby we increase the total problem size by increasing the number of subdomains while maintaining a fixed problem size per subdomain. For these scalability tests, we report the results for different order of PCE to measure the sensitivity of the algorithms to the order of PC representation.

I. Scalability with respect to mesh size (h)

For this scalability study, the number of subdomains is fixed to 128, the finite element mesh resolution is refined. Fig.(9.9) depicts the results for the one-level preconditioners for the

first, second and third PCEs. Fig.(9.10), the same results are plotted again for L, WL and NN preconditioners separately against various PCEs. In general, increasing mesh resolution leads to nearly linear increase in iteration counts of PCGM solver. The NN preconditioner requires less number of iteration than those required by L and WL preconditioners. In contrast to WL preconditioner, the performances of L and NN preconditioners are nearly independent of the order of PCE as the numbers of iterations remain almost constant for a given mesh size. For a spatial problem size of order n , the first, second and third order PCE involve solving problem sizes of order $(5 \times n)$, $(15 \times n)$ and $(35 \times n)$ respectively.

(a) 1st order PCE

(b) 2nd order PCE

(c) 3rd order PCE

Figure 9.9: Iteration counts with respect to mesh size for fixed number of subdomains: Different order of PCE

Figure 9.10: Iteration counts with respect to mesh size for fixed number of subdomains: Different preconditioners

II. Scalability with respect to the number of subdomains (H)

Next we maintain the problem size in the spatial dimension to $n = 127,552$ while increasing the number of subdomains. In Fig.(9.11), we present the results for the first, second and third order PCEs for L, WL and NN preconditioners. In Fig.(9.12), the same results are plotted separately for various orders of PCE for L, WL and NN preconditioners. As

the number of subdomains is increased, the iteration counts grow linearly for the one-level preconditioners. The NN preconditioner demands less number of iterations compared to L and WL preconditioners.

(a) 1st order PCE

(b) 2nd order PCE

(c) 3rd order PCE

Figure 9.11: Iteration counts with respect to the number of subdomains for fixed problem size: Different order of PCE

Figure 9.12: Iteration counts with respect to the number of subdomains for fixed problem size: Different preconditioners

III. Scalability with respect to fixed problem size per subdomain (H/h)

Fig.(9.13) demonstrates the performance of the one-level preconditioners when the problem size per subdomain remains the same, but the total problem size increases due to the additional subdomains for various orders of PCE. The same results are plotted again for L, WL and NN preconditioners separately in Fig.(9.14). These performance results indi-

cate that for fixed problem size per subdomain, the number of iterations of the one-level preconditioners increases almost linearly as the number of subdomains is increased.

(a) 1st order PCE

(b) 2nd order PCE

(c) 3rd order PCE

Figure 9.13: Iteration counts with respect to the number of subdomains for fixed problem size per subdomain: Different order of PCE

Figure 9.14: Iteration counts with respect to the number of subdomains for fixed problem size per subdomain: Different preconditioners

Parallel scalability

In order to investigate the absolute performance of the algorithm, its parallel scalability is measured in terms of the *strong* and *weak* scalabilities [61, 142]. For the strong scalability test, we maintain a constant global problem size, but increase the number of processors/cores to tackle the problem in order to reduce the total execution time. For the

weak scalability test, the problem size per subdomain is fixed, but the total problem size is increased by adding more subdomains. The goal of the weak scalability test is to tackle n -times larger system by exploiting n -times larger processors or cores while maintaining nearly a constant execution time (e.g. [142, 144]).

I. Strong scalability

Fig.(9.15) shows the total execution times for the one-level preconditioners for various numbers of processors. The results are presented for the first, second and third order of PCE. Increasing number of processors greatly reduces the total execution time. For the specific problem size considered here, the optimal number of CPUs is 64 in the case of the first order PCE. In this case, if the number of CPUs is increased further, the communication overhead predominates over the cost of floating point operation. For the second and third order PCEs, the execution time steadily decreases up to 176 CPUs. This is because the computational cost consistently dominates the communication cost while tackling the system of increasingly larger size.

Figure 9.15: Strong scalability

II. Weak scalability

Fig.(9.16) shows the weak scalability of the one-level preconditioners for the first, second and third order PCEs. The results indicate that for the fixed problem size per processor, the total execution time grows almost linearly while using larger number of processors. The NN and WL preconditioners exhibit better performance than L preconditioner.

(a) 1st order PCE

(b) 2nd order PCE

(c) 3rd order PCE

Figure 9.16: Weak scalability

9.3 Two-Level Preconditioner

In this section, we contrast the algorithmic performance of the one-level Neumann-Neumann preconditioner (NN) and two-level Neumann-Neumann preconditioner (NNC) to highlight the beneficial effect of the coarse problem. For the numerical investigation, we consider flow through random media and linear elasticity problems with spatially varying non-Gaussian material properties.

9.3.1 Flow Through Random Media

Convergence Study

A typical relative residual decay of PCGM equipped with NN and NNC preconditioners are shown in Fig.(9.17). Evidently, the PCGM equipped with NNC preconditioner converges in fewer iterations compared to that of the NN preconditioner.

Figure 9.17: The history of the relative PCGM residual

Numerical Scalability

For the numerical scalability study, we report the iteration counts of the PCGM while (a) decreasing the finite element mesh size (h) for fixed number of subdomain partitions; (b) increasing number of subdomains ($1/H$) for fixed spatial mesh resolution (c) increasing the total problem size by including more subdomains with fixed number of elements (H/h).

I. Scalability with respect to mesh size (h)

Fig.(9.18) plots the results for the NN and NNC preconditioners for 128 subdomains and third order PCE while increasing the finite element mesh resolution. Clearly, adding a coarse problem to NN preconditioner significantly reduces the number of iterations for fixed number of subdomains. Increasing problem size does not deteriorate the performance of the NNC preconditioner as the iteration counts remain constant. This fact indicates the numerical scalability of the NNC preconditioner with respect to the problem size.

Figure 9.18: Iteration counts versus mesh size for fixed number of subdomains

II. Scalability with respect to the number of subdomains (H)

Fig.(9.19) plots the performance results of the NN and NNC preconditioners for the fixed spatial problem size and fixed order of PCE with increasing number of subdomains. The NNC preconditioner demands fewer iterations to converge compared to NN preconditioner. For the NNC preconditioner, the number of iterations does not grow with the number of subdomains. This fact indicates the numerical scalability of the NNC preconditioner in

relation to the number of subdomains.

Figure 9.19: Iteration counts versus the number of subdomains for fixed problem size

III. Scalability with respect to fixed problem size per subdomain (H/h)

For fixed problem size per subdomain, the total problem size is increased next by adding more subdomains. The corresponding results are shown in Fig.(9.20). Increasing number of subdomains demonstrates a linear growth in the iteration counts for the NN preconditioner. But the iteration counts remain constant for the NNC preconditioner. This fact indicates the scalability of the NNC preconditioner in relation to the fixed problem size per subdomain.

Figure 9.20: Iteration counts versus the number of subdomains for fixed problem size per subdomain

Parallel Scalability

I. Strong scalability

The strong scalability of the NN and NNC preconditioners is plotted in Fig.(9.21). For fixed problem size (strong scalability), the total execution time for both the NN and NNC preconditioners reduce steadily as expected.

Figure 9.21: Strong scalability

II. Weak scalability

The weak scalability of the NN and NNC preconditioners is presented Fig.(9.22). For fixed problem size per subdomain (weak scalability), the total execution time increases almost linearly in both the preconditioners as we add more processors.

Figure 9.22: Weak scalability

It is worthwhile to point out that the NNC preconditioner takes longer to execute than the NN preconditioner. This is due to the extra computation incurred in solving the coarse problem at each iteration. Although the total execution time for the PCGM with the NN preconditioner is lower, the PCGM convergence criterion may not be satisfied with the NN preconditioner. The iteration count of the PCGM with the NN preconditioner increases rapidly with the number of subdomains. Furthermore, a scalable preconditioner does not necessarily mean the preconditioner with the minimum computational complexity [72], but it ensures convergence while tackling increasingly larger problems. More efficient algorithms that minimize the computational complexities of the coarse problem will reduce the total execution time of the PCGM equipped with the NNC preconditioner. This aspect

will be the subject of future investigations.

9.3.2 Two-Dimensional Elasticity

A plane-stress problem is considered next to study the performance of both the NN and NNC preconditioners for two-dimensional elasticity problems. The geometry of the problem is shown in Fig.(9.23).

Figure 9.23: The geometry of the two-dimensional plane-stress problem
(all dimensions in cm)

For plane-stress problem, the uncertain constitutive matrix can be represented as (e.g. [11])

$$\mathbf{D}(\mathbf{x}, \theta) = \frac{E(\mathbf{x}, \theta)}{1 - \nu^2(\mathbf{x}, \theta)} \begin{bmatrix} 1 & \nu(\mathbf{x}, \theta) & 0 \\ \nu(\mathbf{x}, \theta) & 1 & 0 \\ 0 & 0 & \frac{1 - \nu(\mathbf{x}, \theta)}{2} \end{bmatrix}, \quad (9.5)$$

where $E(\mathbf{x}, \theta)$ and $\nu(\mathbf{x}, \theta)$ are Young's modulus and Poisson's ratio respectively. For

simplicity and clarity of presentation, we assume Poisson's ratio to be a spatially invariant deterministic quantity. The spatial uncertainty of the Young's modulus is modeled as a stochastic process. The methodology for simultaneous treatment of uncertainties in Young's modules and Poisson's ratio is described in details in [38]. However, the proposed algorithm is general and capable of handling arbitrary non-Gaussian models. We represent the Young's modules as a lognormal process defined as

$$E(\mathbf{x}, \theta) = E_0(\mathbf{x}) \exp(g(\mathbf{x}, \theta)), \quad (9.6)$$

where $E_0(\mathbf{x})$ is the mean of Young's modulus assumed to be 20×10^9 and $g(\mathbf{x}, \theta)$ is the underlying Gaussian process with a squared exponential covariance function of the following form [92, 101]

$$C_{gg}(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp \left(\frac{-(x_2 - x_1)^2 - (y_2 - y_1)^2}{b^2} \right).$$

For the numerical investigation, two random variables are used to represent the underlying Gaussian process while the lognormal process is expanded using two-dimensional third order PCE (e.g [145]). The Gaussian process is assumed to have zero mean and σ and b are 0.35 and 12.65 respectively. Some of the chaos coefficients of the lognormal process are plotted in Fig.(9.24)

Figure 9.24: Selected PC coefficients of the Young's modules

Stochastic Characteristics of the Solution Process

The physical domain and its typical decomposition are shown in Fig.(9.25a) and Fig.(9.25b) respectively. Fig.(9.26a) and Fig.(9.26b) show the mean and standard deviation of the magnitude of the displacement field, respectively. At the free end, the coefficient of variation (CoV) is about 30% underscoring the effect of uncertainty. We show a set of selected

polynomial chaos coefficients of the magnitude of the displacement field in Fig.(9.27).

Figure 9.25: Finite element discretization and domain decomposition

Figure 9.26: The mean and standard deviation of the magnitude of the displacement field

Figure 9.27: Selected PC coefficients of the magnitude of the displacement field

Numerical Scalability

Fig.(9.28) demonstrates the performance of both the NN and NNC preconditioners by fixing the problem size and number of subdomains, but increasing the order of PCE of the solution process. Increasing the order of PCE exhibits a linear growth in the iteration

counts for the NN preconditioner. However the iteration counts remain steady for the NNC preconditioner. This fact demonstrates that the NNC preconditioner is scalable to the order of PCE.

Figure 9.28: Iteration counts versus the order of PCE

In Fig.(9.29), the iteration counts for the PCGM with NN and NNC preconditioners, for fixed number of subdomains ($n_s = 64$) and the second order PCE, are plotted while refining the finite element mesh. Evidently, the problem size does not degrade the efficiency of the NNC preconditioner as the number of iterations required for convergence remains the same. The iteration counts increase almost linearly for the NN preconditioner as the problem size grows. The NNC preconditioner takes fewer iterations to converge compared to the NN preconditioner.

Figure 9.29: Iteration counts versus mesh size for fixed number of subdomains

In Fig.(9.30), we maintain the problem size in the spatial domain to 111,651 nodes with 223,316 elements but add more subdomains for the second order PCE of the solution process. The results demonstrates that the NN preconditioner is scalable to the number of subdomains.

Figure 9.30: Iteration counts versus the number of subdomains for fixed problem size

The performance of the NN and NNC preconditioners is shown in Fig.(9.31) for fixed

problem size per subdomain. Again these results highlight the fact that the NNC preconditioner is scalable to fixed problem size per subdomain. The performance of the NN preconditioner degrades rapidly as the number of subdomains grows.

Figure 9.31: Iteration counts versus the number of subdomains for fixed problem size per subdomain

Parallel Scalability

Fig.(9.32) and Fig.(9.33) demonstrate the strong and weak scalabilities for both NN and NNC preconditioners respectively. For a fixed mesh resolution, both the NN and NNC preconditioners steadily reduce the execution time when we exploit more processors to tackle the problem. For the weak scalability tests, the execution times for both the NN and NNC preconditioners increase linearly. As alluded to previously, the extra computation involved in solving the coarse problem leads to the higher execution time for the PCGM with the NNC preconditioner than that of the NN preconditioner.

Figure 9.32: Strong scalability

Figure 9.33: Weak scalability

9.4 Dual-Primal Domain Decomposition Method

In this section, we contrast the convergence properties, numerical and parallel scalabilities of both the probabilistic NNC and FETI-DP for flow through random media and linear elasticity problems with spatially varying system parameters modeled as non-Gaussian stochastic processes.

9.4.1 Flow Through Random Media and Elasticity Problems

Convergence Properties

The convergence rate of the probabilistic NNC and FETI-DP methods for flow through random media and elasticity problems are shown in Fig.(9.34). Clearly, the convergence rates of both the methods are similar. However, the probabilistic NNC method requires slightly higher iteration counts to converge compared to the probabilistic FETI-DP method. This discrepancy between the iteration counts of the two methods may be attributed to the fact that the initial residual in the probabilistic NNC method is bigger than that of the probabilistic FETI-DP method.

Figure 9.34: The history of the relative PCGM residual

In Fig.(9.35), we plot the iteration counts for the probabilistic NNC and FETI-DP solvers versus the order of PCE used for the solution process. The iteration counts required for convergence are nearly independent of the order of the PCE for both the probabilistic NNC and FETI-DP methods. In general, the probabilistic NNC and FETI-DP solvers for elasticity

require higher iteration counts to converge compare to Poisson's problem. This fact can be mainly attributed to the size of the coarse problem. In two-dimensional cases, there are two unknowns per each corner node for elasticity while one unknown per corner node for Poisson's problem.

Figure 9.35: Iteration counts with respect to the order of PCE

For fixed number of subdomains and order of PCE, we show the number of iterations required for the probabilistic NNC and FETI-DP methods in Fig.(9.36). The iteration counts for both the flow through random media and elasticity problems remain almost constant as we increase mesh resolution. This fact indicates that both the probabilistic NNC and FETI-DP methods are scalable with respect to the problem size. Once again the probabilistic NNC method requires more iteration than that of probabilistic FETI-DP method. The difference between the iteration counts of the probabilistic NNC and FETI-DP methods becomes larger in the elasticity problem. As alluded to previously, this behavior is attributed to the size of the coarse problem which is bigger in elasticity than that in Poisson's problem.

Figure 9.36: Iteration counts with respect to mesh size for fixed number of subdomains

Next we fix the spatial problem size and order of PCE while increasing the number of subdomains/processors used to tackle the problem. The corresponding results are shown in Fig.(9.37). Note that the iteration counts for both the methods are not significantly influenced by the number of subdomains.

Figure 9.37: Iteration counts with respect to number of subdomains for fixed mesh size

Next we fix the order of PCE and problem size per subdomain and increase the total problem size by adding more subdomains. Fig.(9.38) shows the iteration counts versus the number of subdomains. Clearly, the iteration counts for both probabilistic NNC and FETIDP methods do not change significantly with respect to the number of subdomains (or the global problem size).

Figure 9.38: Iteration counts with respect to the number of subdomains for fixed problem size per subdomain

Fig.(9.39) shows the reduction in the total execution time for both probabilistic NNC and FETI-DP methods when we increase the number of processors to tackle a fixed problem size. The spatial problem size considered for flow through random media and elasticity problems is 127,552 and 111,651 respectively. Both probabilistic NNC and FETI-DP methods exhibit similar behaviors for flow through random media and elasticity problems.

Figure 9.39: Strong scalability

Next we compare the weak scalability of the probabilistic NNC and FETI-DP algorithms by increasing the overall problem size for fixed problem size per subdomain. Note the linear growth in the total execution time for both probabilistic NNC and FETI-DP algorithms for both flow through random media and elasticity problems as shown in Fig.(9.40). This fact indicates that the probabilistic NNC and FETI-DP algorithms are weakly scalable.

Figure 9.40: Weak scalability

9.5 Summary

We investigate the convergence rate, numerical and parallel scalabilities of the one-level and two-level domain decomposition algorithms for two-dimensional flow through random media and elasticity problems with spatially varying non-Gaussian system parameters. The parallel performances of the algorithms are studied with respect to the level of uncertainty, order of stochastic dimension, spatial problem size, number of subdomains and fixed problem size per subdomain. The numerical results demonstrate that:

- The performance of the probabilistic algorithms are nearly independent of the level of uncertainty and the size of the stochastic dimension.
- The one-level domain decomposition algorithms demonstrate scalability for moderate range of processors for the problem size considered in the investigation.

- The two-level preconditioner equipped with coarse problem exhibits a scalable performance with respect to the spatial problem size, number of subdomains and fixed problem size per subdomain.
- The probabilistic dual-primal approach shows similar convergence properties and parallel performance to the probabilistic BDDC type two-level domain decomposition preconditioner.

Chapter 10

Numerical Results: Three-Dimensional Problems

10.1 Introduction

The numerical results in this chapter are taken from the references [146, 147]. Constructing scalable domain decomposition algorithms for large-scale linear systems arising from three-dimensional problems is more challenging than that for two-dimensional problems. The difficulty arises due to the complicated coupling among the subdomains in three dimensions and the complex geometry of the interface boundary [7]. On the other hand, the resulting linear systems from finite element discretization of three-dimensional problems are often very ill-conditioned [4]. Therefore, simple domain decomposition preconditioners are inefficient especially for elasticity problems in three dimensions [4]. Uncertainty quantification by polynomial chaos approach adds additional complexities to the problem due to the

block structure of the stochastic submatrices and the coupling among the polynomial chaos coefficients in three dimensions. Direct extension of the Schur complement based domain decomposition algorithms developed for two-dimensional to three-dimensional problems is feasible, but maintaining the same performance and convergence properties is not always guaranteed [4, 6]. It has been demonstrated that iterative substructuring techniques can achieve a scalable performance only when equipped with a coarse problem that is required for global communication [4–7, 114]. The coarse grid for three-dimensional problems is often more complicated to construct than that for the two-dimensional cases [137, 148].

In the following sections, we apply the probabilistic Neumann-Neumann with coarse problem (NNC), Primal-Primal Domain Decomposition Method (PP-DDM) and Dual-Primal Domain Decomposition Method (DP-DDM) to quantify uncertainty in three-dimensional SPDEs. In our implementation, we select the primal constraints as the unknowns at the corner nodes of the subdomains (i.e. vertices only). This approach for constructing the coarse problem does not guarantee convergence for three-dimensional elasticity problems. In order to achieve better convergence properties for elasticity problems in three dimensions, the averages over faces or edges must be considered as additional constraints to the coarse problem. This aspect however, is not considered in the thesis and will be the subject of future investigations.

Firstly, we consider three-dimensional flow through random media and heat transfer problems with non-Gaussian system parameters. Next, we tackle three-dimensional elasticity problem having random constitutive properties. The parallel performance is investigated

with respect to mesh size, number of subdomain and fixed problem size per subdomain.

The numerical experiments are performed using MPI and PETSc libraries on a Linux cluster (CentOS release 5.6) consists of 1200 compute nodes with 6 cores and 36 GBytes of memory per node with InfiniBand interconnect [149]. PETSc version 3.1 and MVAPICH2 version 1.6 libraries are compiled with Intel compiler version 12.0.4.

10.2 Three-Dimensional Flow Through Random Media

In this section, a three-dimensional steady-state flow through random media with a spatially varying non-Gaussian hydraulic conductivity coefficient is considered. The flow is modelled by three-dimensional stochastic Poisson equation as

$$\begin{aligned}\nabla \cdot (\kappa(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) &= f(\mathbf{x}), \quad \mathbf{x} \in D, \\ u(\mathbf{x}, \theta) &= 0, \quad \mathbf{x} \in \partial D.\end{aligned}$$

The hydraulic conductivity coefficient is modeled as a lognormal stochastic process obtained from the underlying Gaussian field with zero mean and an exponential covariance function defined as [11, 145]

$$C_{gg}(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp \left(\frac{-|x_1 - x_2|}{b_x} + \frac{-|y_1 - y_2|}{b_y} + \frac{-|z_1 - z_2|}{b_z} \right), \quad (10.1)$$

where σ is the standard deviation of the process and b_x , b_y and b_z are the correlation lengths in x , y and z directions respectively. For numerical investigations, we use $\sigma = 0.6$ and

$$f(\mathbf{x}) = 1.0.$$

A typical finite element mesh of the computational domain is presented in Fig.(10.1(a)). A decomposition of the spatial domain into 128 subdomains is shown in Fig.(10.1(b)). The finite element mesh considered for the eigenvalue problem associated with KLE of the underlying Gaussian process consists of 26,614 linear tetrahedral elements and 5,654 nodes.

Figure 10.1: Finite element discretization and mesh decomposition

Stochastic Field Representation

Fig.(10.2) shows the first 20 eigenvalues of the exponential covariance function defined in Eq.(10.1), for different correlation lengths. Evidently, the eigenvalues exhibit larger decay rate as the correlation length increases. These results suggest that the decay rate of the eigenvalues is inversely proportional to the correlation length. For small correlation length (e.g. $b_x = b_y = b_z = b = 0.1$), the decay rate of the eigenvalues is almost invisible. When the eigenvalues decay slowly, large number of terms in KLE is required to represent the

stochastic process. Stated alternatively, the decay rate of the eigenvalues can be used as a guideline to determine the number of random variables required in KLE to sufficiently approximate a stochastic process.

Figure 10.2: Eigenvalues λ_i of the covariance function

For correlation lengths ($b_x = b_y = b_z = b = 1$) and ($b_x = b_y = b_z = b = 10$), selected eigenfunctions $\phi_i(\mathbf{x})$ of the exponential covariance kernel are shown in Fig.(10.3) and Fig.(10.4) respectively. As the index i increases, the eigenfunctions $\phi_i(\mathbf{x})$ exhibit higher oscillations. These results emphasize the fact that the more random variables we use in KLE, the more scales of fluctuation we incorporate in the representation of the stochastic process. Clearly, a finer finite element mesh resolution is required to accurately capture high frequency oscillations as indicated in Fig.(10.3f) and Fig.(10.4f).

Figure 10.3: Selected eigenfunctions: $b_x = b_y = b_z = 1$

Figure 10.4: Selected eigenfunctions: $b_x = b_y = b_z = 10$

Some of the chaos coefficients of the lognormal process are plotted in Fig.(10.5) and Fig.(10.6) for correlation lengths ($b_x = b_y = b_z = 1$) and ($b_x = b_y = b_z = 10$) respectively. The number of terms in KLE is taken to be $L = 4$. In Fig.(10.5a) and Fig.(10.6a), the first chaos coefficient l_0 representing the mean of the lognormal processes is defined as [145, 150]

$$l_0(\mathbf{x}) = \exp \left[g_0(\mathbf{x}) + \frac{1}{2} \sum_{j=1}^L g_j^2(\mathbf{x}) \right], \quad (10.2)$$

where $g_0(\mathbf{x})$ represents the mean of the underlying Gaussian processes, $g_j(\mathbf{x}) = \sqrt{\lambda_i} \phi_i(\mathbf{x})$, $\sqrt{\lambda_i}$ are the eigenvalues and $\phi_i(\mathbf{x})$ are eigenfunctions of the covariance kernel. Note that in the limit as ($L \rightarrow \infty$), Eq.(10.2) converges to

$$l_0 = \exp \left[g_0(\mathbf{x}) + \frac{1}{2} \sigma_g^2 \right]. \quad (10.3)$$

For $g_0(\mathbf{x}) = 0$ and $\sigma_g = 0.6$, the exact mean of the lognormal process defined in Eq.(10.3) become $l_0 = 1.1972$.

As shown in Fig.(10.5a) and Fig.(10.6a) the first chaos coefficient l_0 is almost constant. For $b = 1$ the first PC coefficient l_0 underestimates the exact value of the mean. In contrast, the first PC coefficient l_0 sufficiently approximates the mean of the lognormal process for $b = 10$. Fig.(10.2) demonstrated that for small correlation length such as $b = 1$, the eigenvalues decay slowly and thus more terms in KLE are needed to adequately approximate the process. For this reason, higher dimensional PCE is required to sufficiently approximate the lognormal process using KLE of a Gaussian process with small correlation lengths.

The PC coefficients l_j where $j > 0$ for small correlation length in Fig.(10.5) show finer structure compared to that for larger correlation length in Fig.(10.6).

Figure 10.5: Selected PC coefficients of the hydraulic conductivity:

$$b_x = b_y = b_z = 1$$

Figure 10.6: Selected PC coefficients of the hydraulic conductivity:

$$b_x = b_y = b_z = 10$$

Realizations of the underlying Gaussian and lognormal processes are plotted in Fig.(10.7) and Fig.(10.8) for different correlation lengths. Evidently, the Gaussian process is not strictly positive. On the contrary, the lognormal process is strictly positive. This fact indicates that Gaussian process is inadequate to model uncertainty in a strictly positive quantity such as the hydraulic conductivity coefficient. Note that the fluctuations of the Gaussian and lognormal processes are around the corresponding mean values.

Figure 10.7: Samples of the random hydraulic conductivity field:

$$b_x = b_y = b_z = 1$$

Figure 10.8: Samples of the random hydraulic conductivity field:

$$b_x = b_y = b_z = 10$$

10.2.1 Stochastic Features of the Solution Field

Fig.(10.9) and Fig.(10.10) show the mean and standard deviation of the hydraulic head using different orders of PCE for two different correlation lengths. The first order PCE represents the Gaussian contribution to the solution process whereas the higher orders PC coefficients contain non-Gaussian effects. As the order of PCE increases the solution converges in terms of the mean and standard deviation.

Figure 10.9: The mean and standard deviation of the hydraulic head for different order of PCE: $b_x = b_y = b_z = 1$

Figure 10.10: The mean and standard deviation of the hydraulic head for different order of PCE: $b_x = b_y = b_z = 10$

Some of the chaos coefficients of the hydraulic head are plotted in Fig.(10.11) and Fig.(10.12) for two correlation lengths. The chaos coefficients u_j exhibit oscillations whose fluctuations increase with increasing the index j . Finer structure can be observed for the case of $(b_x = b_y = b_z = 1)$ compared to that for $(b_x = b_y = b_z = 10)$. One can see that the higher the index j the smaller the magnitude of the chaos coefficients. As mentioned before, higher order PC coefficients correspond to the non-Gaussian components of the response process.

Figure 10.11: Selected PC coefficients of the hydraulic head:

$$b_x = b_y = b_z = 1$$

Figure 10.12: Selected PC coefficients of the hydraulic head:

$$b_x = b_y = b_z = 10$$

10.2.2 Numerical Scalability

I. Effect of PCE order

For the fixed problem size $n = 106,456$ and number of subdomains $n_s = 128$, Fig.(10.13) shows the iteration counts for the probabilistic two-level methods NNC, PP-DDM and DP-DDM versus the order of PCE used to represent the solution process. The probabilistic NNC and PP-DDM methods exhibit similar performances. Both the NNC and PP-DDM methods require more iteration to converge than that of DP-DDM. Nevertheless, the iteration counts required by the probabilistic two-level methods are nearly independent of the order of PCE. This fact demonstrates that the probabilistic two-level techniques are scalable to the order of PCE.

Figure 10.13: Iteration counts versus the order of PCE

In Fig.(10.14), we plot the total execution time for the probabilistic two-level techniques as the order of PCE increases. Clearly, all the two-level methods require almost the same time to run. Note that for a given spatial problem size n the first, second and third order

PCE involve solving problem size of order $(5 \times n)$, $(15 \times n)$ and $(35 \times n)$ respectively.

Undoubtedly, this rapid increase in the problem size demands longer running time.

Figure 10.14: Running time versus the order of PCE

II. Scalability with respect to mesh size (h)

For the fixed number of subdomains $n_s = 128$ and second order PCE, Fig.(10.15) plots the iteration counts of the probabilistic two-level methods against the finite element mesh resolution. Evidently, the size of the problem does not affect the performance of the two-level methods as the iteration counts required for convergence remain nearly constant. Again the NNC and PP-DDM methods show similar performances, and the DP-DDM requires less number of iterations to converge.

Figure 10.15: Iteration counts with respect to mesh size for fixed number of subdomains

III. Scalability with respect to the number of subdomains (H)

Fig.(10.16) shows the iteration counts versus number of subdomains for fixed problem size $n = 106,456$ and second order PCE. Increasing number of subdomains does not degrade the performance of the probabilistic two-level methods as the number of iterations required for convergence remains almost constant. This fact suggests that the probabilistic two-level methods are scalable with respect to number of subdomains [129].

Figure 10.16: Iteration counts with respect to number of subdomains for fixed problem size

IV. Scalability with respect to fixed problem size per subdomain (H/h)

In Fig.(10.17), we plot the iteration counts of the probabilistic two-level methods for fixed problem size per subdomain $n \approx 1,300$ and second order PCE while increasing the global problem size by adding more subdomains. The iteration counts remain bounded as we increase the total problem size by using more subdomains with fixed problem size per subdomain.

Figure 10.17: Iteration counts with respect to number of subdomains for fixed problem size per subdomain

10.2.3 Parallel Scalability

I. Strong scalability

The strong scalabilities of the probabilistic two-level domain decomposition methods are shown in Fig.(10.18) for problem size $n = 106,456$ and second order PCE. As we use more processors to tackle the problem, the total execution time steadily decreases up to 256 processors. For this specific problem, as increasing the number of processors further, the communication overhead predominates over the cost of floating point operation and no reduction in the total execution time can be gained.

Figure 10.18: Strong scalability

II. Weak scalability

In Fig.(10.19), we show the weak scalabilities of the probabilistic two-level methods for fixed spatial problem size per subdomain $n \approx 1,300$ and second order PCE. All the methods exhibit almost the same performance in terms of total execution time. The run time increases almost linearly as we increase the total problem size by adding more processors/subdomains.

Figure 10.19: Weak scalability

10.3 Application to Large-Scale Heat Transfer Problem

In this section, we apply the probabilistic two-level iterative substructuring techniques to quantify uncertainty in three-dimensional heat transfer problem in a crankshaft defined as

$$\nabla \cdot (\kappa(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) = f(\mathbf{x}, \theta), \quad \mathbf{x} \in \Omega \quad (10.4)$$

$$u(\mathbf{x}, \theta) = 0, \quad \mathbf{x} \in \partial\Omega_D, \quad (10.5)$$

where the thermal diffusivity coefficient $\kappa(\mathbf{x}, \theta)$ is modeled as a lognormal stochastic process obtained from the underlying Gaussian process with a given covariance function. The volumetric heat source is assumed to be spatially invariant deterministic quantity $f(\mathbf{x}, \theta) = 1.0$. The geometry of the crankshaft is shown in Fig.(10.20).

Figure 10.20: The geometry of the crankshaft (all dimensions in cm)

10.3.1 Finite Element Discretization and Mesh Decomposition

The crankshaft shown in Fig.(10.21(a)) is discretized using 92,429 linear tetrahedral finite elements and 545,663 nodes. The response is expanded using four-dimensional ($L = 4$) third order PCE ($N = 34$) yielding a linear system of order 3,235,015. The partitioned domain into 160 subdomains using METIS graph partitioning tool [89] is depicted in Fig.(10.21(b)) and the crankshaft is assumed to be insulated on the top surfaces.

Figure 10.21: Finite element discretization and mesh decomposition

10.3.2 Stochastic Field Representation

The uncertain thermal diffusivity coefficient $\kappa(\mathbf{x}, \theta)$ is modeled as a lognormal stochastic process obtained from the underlying Gaussian process as

$$\kappa(\mathbf{x}, \theta) = \exp(g(\mathbf{x}, \theta)). \quad (10.6)$$

The Gaussian process $g(\mathbf{x}, \theta)$ has a zero mean and an exponential covariance function defined as [92, 101]

$$C_{gg}(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp \left(\frac{-|x_1 - x_2|}{b_x} + \frac{-|y_1 - y_2|}{b_y} + \frac{-|z_1 - z_2|}{b_z} \right). \quad (10.7)$$

The following numerical values used in the investigation are $\sigma = 0.3$ and $b_x = b_y = b_z = 60$.

For computational efficiency, the eigenvalue analysis for KLE is performed on an extended domain which encapsulates the original geometry over which the problem is defined. The extended domain is discretized using 31,705 elements and 7,706 nodes. This mesh is coarse compared to the original finite element mesh of the problem. In addition, the PC coefficients of the lognormal process are computed on the same mesh. Then the finite element shape functions are used to extrapolate the PC coefficients from the coarse to the fine mesh used in the analysis. This approach avoids unnecessary complication for KLE involving the fine mesh.

In our implementation, we use LAPACK dense eigenvalue problem solver [151]. For the stochastic process with small correlation length, the contributions of higher order fluctuations become significant. Thus the eigenvalue analysis for KLE must be carried out on the fine mesh. In this context, parallel solvers for the eigenvalue problem can be useful [152].

In Fig.(10.22), we show the first four eigenfunctions of the covariance kernel. Fig.(10.23) and Fig.(10.24) show a set of selected chaos coefficients of the lognormal process (diffusivity coefficient) on the coarse and fine domains respectively.

Figure 10.22: The first four eigenfunctions of the covariance function

Figure 10.23: Selected PC coefficients of the diffusivity field on the extended domain

Figure 10.24: Selected PC coefficients of the diffusivity field on the original domain

10.3.3 Stochastic Features of the Solution Field

The mean and standard deviation of the temperature process are plotted in Fig.(10.25(a)) and Fig.(10.25(b)) respectively. The standard deviation has the same trend as the mean. The maximum coefficient of variation in the middle of the crankshaft is 21%. Some of the chaos coefficients of the temperature process are shown in Fig.(10.26). The chaos coeffi-

cients exhibit decay in magnitude as the index of the coefficients increases. In Fig.(10.27), we show Lagrange multipliers λ_j corresponding to the first four PC coefficient of the temperature process. Clearly, the larger the index j , the smaller the magnitude of Lagrange multipliers λ_j .

Figure 10.25: The mean and the standard deviation of the temperature field

Figure 10.26: Selected PC coefficients of the temperature field

(a) Lagrange multipliers: λ_0 (b) Lagrange multipliers: λ_1 (c) Lagrange multipliers: λ_2 (d) Lagrange multipliers: λ_3

Figure 10.27: Lagrange multipliers corresponding to the first four PC coefficient of the temperature field

10.3.4 Numerical Scalability

I. Effect of the order of PCE

In Fig.(10.28), we show the performances of the probabilistic two-level methods as we increase the order of PCE of the solution process. Increasing the order of PCE leads to a mild growth in the iteration counts of the probabilistic NNC and PP-DDM. However, the iteration counts remain constant for the probabilistic DP-DDM.

Figure 10.28: Iteration counts versus the order of PCE

II. Scalability with respect to mesh size (h)

In Fig.(10.29), we show the iteration counts of the probabilistic two-level methods when we fix the number of subdomains and order of PCE, but refine the finite element mesh. Evidently, the iteration counts required for convergence are nearly independent of the finite element mesh resolution. The probabilistic NNC and PP-DDM techniques exhibit similar performances. The probabilistic DP-DDM requires less number of iterations compared to the NNC and PP-DDM techniques.

Figure 10.29: Iteration counts with respect to mesh size for fixed number of subdomains

III. Scalability with respect to the number of subdomains (H)

For fixed spatial mesh resolution and order of PCE, Fig.(10.30) shows the iteration counts of the probabilistic two-level methods for increasing number of subdomains. Once again, the probabilistic NNC and PP-DDM show similar performances while DP-DDM demands less number of iterations to converge. Nevertheless, the performances of all the probabilistic two-level methods are nearly independent of the number of subdomains. This fact indicates that the probabilistic two-level techniques show a scalable performance with respect to the number of subdomains.

Figure 10.30: Iteration counts with respect to the number of subdomains
for fixed problem size

IV. Scalability with respect to fixed problem size per subdomain (H/h)

Fig.(10.31) demonstrates the performances of the probabilistic two-level domain decomposition techniques when the problem size per subdomain is kept constant, but the total problem size is increased by adding more subdomains [64, 153]. The iteration counts increase almost linearly as we add more subdomains with fixed problem size.

Figure 10.31: Iteration counts with respect to the number of subdomains
for fixed problem size per subdomain

10.3.5 Parallel Scalability

I. Strong scalability

For fixed problem size, Fig.(10.32) shows the execution time for the probabilistic two-level methods when we increase the number of processors to tackle the problem. All the methods exhibit similar performances. Increasing the number of processors from 16 to 64 leads to about 80% reduction in the total execution time. However, increasing the number of processors further does not significantly reduce the total execution time as the computational cost dominates over the communication cost.

Figure 10.32: Strong scalability

II. Weak scalability

Fig.(10.33) shows the total execution time for the probabilistic two-level methods when we fix the problem size per subdomain and increase the global size of the problem by using more subdomains. The results indicate that for fixed problem size per processor, the total execution time grows almost linearly as we add more subdomains, thereby increasing the overall problem size.

Figure 10.33: Weak scalability

10.3.6 Performance Study for Large-Scale Systems

In this section, we demonstrate the ability of the probabilistic two-level methods to tackle a large-scale problem using increasingly large number of subdomains/processors. In particular, we refine the finite element mesh of the crankshaft to generate 2,074,627 elements and 337,826 nodes. The response is expanded using four-dimensional ($L = 4$) second order PCE ($N = 14$) leading to a linear system of order 5,067,390. We tackle the problem using the probabilistic dual-primal technique and the performance results are shown in Table.(10.1). These results are generated on a Linux cluster consists of 1200 compute nodes with 6 cores and 36 GBytes of memory per node with InfiniBand interconnect [149].

Table 10.1: Iteration counts and timing for the probabilistic DP-DDM

No. of Processors	No. of Iterations	Time in sec.
128	16	5364.56
256	19	3712.71
512	25	2800.07
640	20	1890.88
768	22	1776.71

10.4 Three-Dimensional Elasticity Problem

In this section a homogeneous, isotropic, linear elastic three-dimensional cantilever beam subjected to a self-weight loading is investigated. In Fig.(10.34), we show the dimensions and boundary conditions of the physical problem.

Figure 10.34: The geometry of three-dimensional cantilever beam (all dimensions in m)

For simplicity and clarity of presentation, we assume Poisson's ratio to be a spatially invariant deterministic quantity $\nu = 0.35$. The spatial uncertainty of the Young's modulus is modeled as a stochastic process as

$$E(\mathbf{x}, \theta) = E_0(\mathbf{x}) \exp(g(\mathbf{x}, \theta)), \quad (10.8)$$

where $E_0(\mathbf{x})$ is the mean of Young's modulus assumed to be 70 GPa and $g(\mathbf{x}, \theta)$ is the underlying Gaussian process with covariance function defined in Eq.(10.1). Consequently, the uncertain constitutive matrix can be represented as (e.g. [11, 154])

$$D(\mathbf{x}, \theta) = E(\mathbf{x}, \theta) \frac{(1 - \nu)}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix} 1 & \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ \frac{\nu}{1-\nu} & 1 & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} \end{bmatrix}.$$

The lognormal process and response are represented using four-dimensional ($L = 4$) second order PCE ($N = 14$). We only consider a relatively small size problem. The finite element mesh used in the analysis consists of 10,376 nodes and 62,233 elements. Direct extension of the probabilistic dual-primal method to three-dimensional elasticity problem is implemented. The performance results for fixed problem size are shown in Table(10.2). Although the iteration counts remain nearly constant, the code takes about 3.5 H to run (when using 64 processors) which is relatively long for the problem size considered. Increasing number of subdomains further does not improve the performance of iterative solver.

Table 10.2: Iteration counts and timing for 3D elasticity problem

No. of Processors	No. of Iterations	Time in sec.
16	18	60210.33
32	13	18565.41
64	17	12536.05
128	21	17997.63

In Fig.(10.35), we show the magnitude, x , y and z components of the mean and standard deviation of displacement field. As predicted the maximum deflection occurs at the free end of the cantilever. The maximum coefficient of variation in the magnitude of the displacement field is about 45% which highlights the effect of uncertainty. The boundary conditions at the fixed end of the cantilever are satisfied with zero uncertainty. The components of the displacement vector exhibit more complex features than the magnitude.

Fig.(10.36) displays the magnitude and components of selected chaos coefficients of the displacement field. These PC coefficients represent the non-Gaussian contributions to the displacement field.

Selected Lagrange multipliers of the chaos coefficients of the displacement field are depicted in Fig.(10.37). As the index j increase, Lagrange multipliers λ_j exhibit decay in magnitude. Physically, the extended Lagrange multipliers relate to the nodal forces required to satisfy the compatibility condition of the polynomial chaos coefficients of the displacement field at the remaining interface nodes.

(a) mean: magnitude

(b) standard deviation: magnitude

(c) mean: x-component

(d) standard deviation: x-component

(e) mean: y-component

(f) standard deviation: y-component

(g) mean: z-component

(h) standard deviation: z-component

(a) u_8 : magnitude (b) u_{13} : magnitude (c) u_8 : x-component (d) u_{13} : x-component (e) u_8 : y-component (f) u_{13} : y-component (g) u_8 : z-component (h) u_{13} : z-component

Figure 10.37: Selected Lagrange multipliers for the chaos coefficients of the displacement field

Discussion

For three-dimensional elasticity problems, it is sometimes necessary to include edges and faces of the interface boundary into the coarse grid to achieve a rate of convergence that is independent on the number of subdomains (see Fig.(10.38)) [4, 6, 137, 148].

Figure 10.38: The interface boundary Γ in three dimensions: Vertices (●),

Edges (—) and Faces(≡)

(adapted from Ref. [6])

In the domain decomposition methods for two-dimensional PDEs, the coarse grid is constructed based on a set of corner nodes. The corner nodes are selected such that the subdomain systems are non-singular. For three-dimensional elasticity problems however, the use of only the corner nodes to build the coarse problem may not be sufficient to ensure the solvability of the local problems and to achieve a scalable performance [135]. Therefore, some essential modifications in the construction of the coarse problem must

be considered for elasticity problems in three dimensions. Such modifications may involve using additional constraints such as averages over faces and first-order moments over edges [81, 83, 135, 155, 156]. The implementation of the additional constraints can be performed by using optional Lagrange multipliers in the dual domain decomposition approach [81, 157] or transformation of basis in the primal domain decomposition approach [155, 156]. This aspect however, is not considered in the thesis and will be the subject of future investigations.

10.5 Summary

We investigate the convergence rate, numerical and parallel scalabilities of the two-level domain decomposition algorithms for three-dimensional flow through porous media and elasticity problems with spatially varying non-Gaussian system parameters. The numerical results demonstrate that:

- The two-level methods exhibit a scalable performance with respect to the spatial problem size, number of subdomains and fixed problem size per subdomain for three-dimensional flow through porous media.
- The probabilistic dual-primal approach shows almost similar convergence properties and parallel performance to the probabilistic BDDC type two-level preconditioners.
- For elasticity problems in three dimensions, additional constraints must be considered to achieve better convergence rate and scalability for large number of subdomains.

Chapter 11

Time-Domain Decomposition for Stochastic ODEs

11.1 Introduction

This chapter is closely based on the references [158, 159]. For a fixed mesh resolution, spatial domain decomposition techniques cannot reduce the total solution time beyond a critical number of subdomains as the interprocessor communication overhead and memory bandwidth requirement predominate over floating point operations. In order to exploit the remaining idle processors in multi-processor computers, the recent research initiatives have been directed towards achieving time domain parallelism (e.g.,[90, 91]). Roughly speaking, the time domain parallelism involves the decomposition of the total simulation time into a number of time-slices, whereby a coarse integration is carried out serially. Next the system is integrated using a fine step size within each of these coarse time-slices. The solu-

tion from the coarse integration at the beginning of each time-slice are used as approximate initial conditions. A correction to these initial conditions is then made iteratively at the interface points. The solution converges when the error at each interface point reduces to a prescribed error tolerance.

Sufficient care must be taken to extend any algorithm for ODEs to the case of SDEs. The interpretation of the solutions of Ito SDEs is problematical in the classical sense as the solution is continuous everywhere but not differentiable anywhere in *almost sure* sense [160]. In contrast to the ODEs, the solution techniques of SDEs are more susceptible to numerical approximations. This is due to the fact that the Riemann sum approximating a deterministic integral in an ODE solver can be evaluated at any arbitrary point within the discretization interval. On the contrary, the integrals in an Ito SDE involving the Wiener process are evaluated at the left end point in the time interval [160].

In this chapter, we extend a parallel ODEs solver to tackle Ito SDEs describing noisy nonlinear oscillatory systems. In particular, a parallel version of Euler-Maruyama time integration scheme is described in the framework of parareal algorithm. More specifically, we study the ability of the stochastic parareal scheme to track sample paths of noisy nonlinear systems. For numerical illustration, we consider a Duffing oscillator driven by combined harmonic and random excitations. The stochastic parareal scheme is used to simulate the trajectories of two qualitatively different noisy limit cycle oscillations (LCOs) of the Duffing system. The efficiency and limitation of the stochastic parareal algorithm with respect to the strength of the random noise are brought out through an extensive numerical ex-

perimentation. Furthermore, we demonstrate the scalability of the algorithm through its distributed implementation using Message Passing Interface (MPI) [88].

11.2 Numerical Solution of Ito SDEs

In the framework of Ito SDEs, nonlinear oscillators driven by broadband random noise can be represented as

$$dx = f(x, t)dt + G(x, t)dw, \quad (11.1)$$

where x and $f(x, t)$ denote n -dimensional state vector and random vector function respectively, $G(x, t)$ is a $n \times m$ - matrix valued random functions and w is m -dimensional vector Wiener process. It is well-known fact that the interpretation of the solutions of Eq.(11.1) is problematical in the classical sense as the solution $x(t)$ is continuous everywhere but not differentiable anywhere with probability one.

One of the simplest time marching schemes of an Ito SDE is the Euler-Maruyama scheme [160]. This scheme leads to the following discrete representation of Eq.(11.1)

$$x_{i+1} = x_i + f(x_i, t_i)\Delta t + \sqrt{\Delta t} G(x_i, t_i) \xi_i, \quad i = 0, \dots, n \quad (11.2)$$

where Δt is the integration time step, dw defining Brownian path increment in Eq.(11.1) is replaced by $w(t_{i+1}) - w(t_i) = \sqrt{\Delta t} \xi_i$ and the elements of $\xi_i \sim \mathcal{N}(0, 1)$ are independent random numbers sampled from a unit standard Gaussian random variable $\mathcal{N}(0, 1)$.

At this stage, we recall that the accuracy of a numerical integration of SDEs is measured using the notion of weak and strong convergence [160, 161]. The following metric $\epsilon^{weak}(\Delta t)$ is generally used as an indicator of weak convergence:

$$\epsilon^{weak}(\Delta t) = \sup_{0 \leq t_n \leq T} |E(\phi(\mathbf{x}_n)) - E(\phi(\mathbf{x}(t_n)))| \leq C\Delta t^\beta \quad (11.3)$$

where E denotes expectation operator, ϕ is some polynomial, C being some positive constant and β is the order of convergence. Loosely speaking, the weak convergence implies that only certain statistical moments of the approximate and exact solution require to match with reasonable accuracy. On other hand, the strong convergence criterion is employed to estimate the *closeness* of the numerical approximation to the exact (strong) solution as given by [160, 161]:

$$\epsilon^{strong}(\Delta t) = \sup_{0 \leq t_n \leq T} E(|\mathbf{x}_n - \mathbf{x}(t_n)|) \leq C\Delta t^\beta. \quad (11.4)$$

In general the strong convergence criterion is computationally expensive to satisfy than the weak convergence criterion [160, 161].

The current investigation relates to the strong convergence criterion as we approximate the sample paths (strong solutions) of noisy non-linear dynamical systems using a stochastic version of the parareal scheme. For convergence study, we conduct numerical experiments to evaluate the performance of the stochastic parareal scheme in relation its sequential counterpart. For a simple linear SDE, the theoretical convergence study is available in reference [162]. By contrast, a similar theoretical convergence analysis for the nonlinear SDE can be technically challenging. Therefore we compromise on analytical concern and

undertake numerical experiment as adopted by others (e.g. [161]).

11.3 Parareal Algorithm for SDEs

In this section, we provide a concise description of a parareal algorithm adapted to Ito SDEs. The parareal algorithm was presented in reference [90] as a numerical method to solve ODEs in parallel computers. The mathematical analysis of this method was provided in reference [91]. However, the adaptation and applicability of the parareal algorithm in the context of SDEs are not widely reported in the open literature except the work in reference [162] which deals only with simple linear SDEs.

We present the adaptation of this parallel algorithm for ODEs to Ito SDEs in the framework of Euler-Murayama scheme. A parallel version of Euler-Murayama scheme involves splitting the time integration interval into n_c number of time slices as shown in Figure (11.1).

Figure 11.1: Schematic Diagram: S_i is the time slice i and $X(\omega_j, t)$ denotes j -th realization

This approach tackles n_c SDEs over these time slices in parallel. Therefore Eq.(11.2) can be rewritten over each time slice as

$$\mathbf{x}_{i+1,s} = \mathbf{x}_{i,s} + \mathbf{f}(\mathbf{x}_{i,s}, t_i) \Delta t + \sqrt{\Delta t} \mathbf{G}(\mathbf{x}_{i,s}, t_i) \xi_{i,s}^f, \quad s = 1, \dots, n_c, \quad i = 0, \dots, n_f \quad (11.5)$$

where the superscript f indicates the *fine grid*. Each of these initial value problems will be termed as the *fine integral*.

To start the fine scale integrator over each time slice, n_c initial conditions at the interface points must be specified. An approximation to these initial conditions is generated by solving the Ito SDE in Eq.(11.2) over a coarse scale time grid with step size ΔT . The Euler-Murayama numerical integration method for the coarse scale time grid can be expressed using explicit scheme as [160, 161]

$$\mathbf{X}_{i+1} = \mathbf{X}_i + \mathbf{f}(\mathbf{X}_i, T_i)\Delta T + \sqrt{\Delta T} \mathbf{G}(\mathbf{X}_i, T_i) \xi_i^c, i = 0, \dots, n_c \quad (11.6)$$

or using *semi-implicit* scheme as [160, 161, 163]

$$\mathbf{X}_{i+1} = \mathbf{X}_i + \mathbf{f}(\mathbf{X}_{i+1}, T_{i+1})\Delta T + \sqrt{\Delta T} \mathbf{G}(\mathbf{X}_i, T_i) \xi_i^c, i = 0, \dots, n_c \quad (11.7)$$

where the superscript c relates to the *coarse grid*. In the semi-implicit method, the drift coefficient $\mathbf{f}(\mathbf{X}, T)$ is evaluated at the end of the integration step (i.e. implicitly) and the diffusion coefficient $\mathbf{G}(\mathbf{X}, T)$ is computed at the beginning of the integration step (i.e. explicitly) [161]. Note that the *fully-implicit* scheme where both the drift and diffusion coefficients are evaluated implicitly does not converge to the correct strong solution of the Ito SDEs [160, 161]. To achieve parallel efficiency, the coarse integral is performed using a relatively large time step ΔT . For convergence and stability, the semi-implicit scheme is preferable than the explicit method for the coarse integral.

In the numerical implementation of this two-scale integrator, the fine and coarse integrator must remain on the same Brownian path. This condition enforces that $\xi_{i,s}^f$ is equal to ξ_i^c at the interface points. The convergence is achieved when the errors at the interface points of the coarse and fine integrators reduce to a prescribed tolerance after a certain number of

iterations. The adapted parareal scheme for Ito SDEs is summarized next.

Fine Scale Integration

The fine scale integration is carried out over each time slice concurrently as

$$\mathbf{x}_{i+1,s}^k = \mathbf{x}_{i,s}^k + \mathbf{f}(\mathbf{x}_{i,s}^k, t_i) \Delta t + \sqrt{\Delta t} \mathbf{G}(\mathbf{x}_{i,s}^k, t_i) \xi_{i,s}^f, \quad s = 1, \dots, n_c, \quad i = 0, \dots, n_f \quad (11.8)$$

where $k = 1, \dots, n_{iter}$ denotes the number of iterations. The initial conditions at the interface points is approximated by solving the coarse integral and given by

$$\mathbf{x}_{0,s}^k = \mathbf{X}_{s-1}^k. \quad (11.9)$$

At the end of each fine integral, the error at each interface point is evaluated as

$$\Delta_s^{k+1} = \mathbf{x}_{n_f,s}^k - \mathbf{X}_s^k + \Delta_s^k, \quad (11.10)$$

where

$$\Delta_s^0 = 0. \quad (11.11)$$

The method converges as $\Delta^k = \sum_{k=1}^{n_{iter}} \Delta_s^k$ tends to zero (i.e. the difference in the coarse and fine integration results are indistinguishable in the graphical scale)

Coarse Scale Integration

At the interface points, the coarse integral is used to approximate the initial conditions for the fine integral. For the k -th iteration, the coarse integral as an explicit scheme is given by

$$\mathbf{X}_{i+1}^k = \mathbf{X}_i^k + \mathbf{f}(\mathbf{X}_i^k, T_i) \Delta T + \sqrt{\Delta T} \mathbf{G}(\mathbf{X}_i^k, T_i) \xi_i^c, \quad i = 0, \dots, n_c \quad (11.12)$$

When a semi-implicit scheme is used, the coarse integral takes the following form

$$\mathbf{X}_{i+1}^k = \mathbf{X}_i^k + \mathbf{f}(\mathbf{X}_{i+1}^k, T_{i+1}) \Delta T + \sqrt{\Delta T} \mathbf{G}(\mathbf{X}_i^k, T_i) \xi_i^c, \quad i = 0, \dots, n_c \quad (11.13)$$

with the initial condition

$$\mathbf{X}_0^k = \mathbf{X}(T = T_0). \quad (11.14)$$

In contrast to the fine integral, the coarse integral is carried out serially. Furthermore, it is *not* an ordinary SDE solver as, after each step of coarse integration, a correction is performed as

$$\mathbf{X}_{i+1}^k = \mathbf{X}_{i+1}^k + \Delta_{i+1}^k, \quad (11.15)$$

where Δ_{i+1}^k is substituted from Eq.(11.10).

11.4 Parallel Implementation

The adapted parareal algorithm for SDEs is implemented in parallel as listed in Algorithm (21). The parallel implementation of the algorithm requires two SDEs solvers: a coarse integrator $\mathcal{G}_{\Delta T}$ with a time step ΔT and a fine integrator $\mathcal{F}_{\Delta t}$ with a time step Δt . These numerical time integrators can be explicit or implicit and of any order such as Runge-Kutta [164] or Newmark methods [165]. As can be seen from Algorithm (21), the selection of the time integration method does not influence the parallel implementation, but only

affects the stability and accuracy of the numerical scheme. For simplicity, we consider a semi-implicit Euler scheme for the coarse grid and an explicit Euler scheme for the fine grid. Message Passing Interface (MPI) libraries [88] are used to implement the algorithm on parallel computers.

Algorithm 21: The Parareal Procedure

```

input  $\mathbf{X}_0$  :  $(\mathbf{X}_0)$ 

1 if  $rank = 0$  then
2   generate  $\xi^f \sim \mathcal{N}(0, 1)$ 
3   scatter  $\xi^f \mapsto \xi^c$ 
4   solve  $\mathbf{X}_{s+1}^0 = \mathcal{G}_{\Delta T}(\mathbf{X}_s^0, \xi^c)$ 
5   scatter  $\mathbf{X}_s^0 \mapsto \mathbf{x}_{0,s+1}^0$ 

6 for  $k = 1, 2, \dots$ , until convergence:
7 do
8   for  $s = 1, 2, \dots, n_c$  in parallel :
9     do
10    solve  $\mathbf{x}_{i+1,s}^k = \mathcal{F}_{\Delta t}(\mathbf{x}_{i,s}^k, \xi^f)$ 
11    compute  $\Delta_s^k = \mathbf{x}_{n_f,s}^{k-1} - \mathbf{X}_s^{k-1} + \Delta_s^{k-1}$ 
12    gather  $\Delta^k \leftarrow \Delta_s^k$ 
13    if  $rank = 0$  then
14      solve  $\mathbf{X}_{s+1}^k = \mathcal{G}_{\Delta T}(\mathbf{X}_s^k, \xi^c)$ 
15      correct  $\mathbf{X}_{s+1}^k = \mathbf{X}_{s+1}^k + \Delta_{s+1}^k$ 
16      scatter  $\mathbf{X}_s^k \mapsto \mathbf{x}_{0,s+1}^k$ 

output  $\mathbf{x}_s$  :  $(\mathbf{x}_s)$ 

```

11.5 Numerical Results

For the numerical demonstration, we consider a Duffing oscillator (see [166–168]) driven by combined deterministic and random excitations as

$$\ddot{u} + c\dot{u} + k_1u + k_3u^3 = \Gamma \cos(\omega t) + \sigma \xi(t), \quad (11.16)$$

where $u(t)$ is the displacement, c denotes the damping coefficient, k_1 and k_3 represent the stiffness coefficients, Γ is the amplitude and ω denotes the frequency of the input, $\xi(t)$ is a Gaussian white noise with unit strength and σ denotes the strength of random noise. For a slight change in the model parameters, the Duffing oscillator displays a range of dynamical response [166–168]. Therefore it serves as a paradigm model to test the performance of the parareal algorithm without undue mathematical complexity.

Eq.(11.16) can be recast in the form of Eq.(11.1) as

$$\begin{pmatrix} dx_1 \\ dx_2 \end{pmatrix} = \begin{pmatrix} x_2 \\ -[cx_2 + k_1x_1 + k_3x_1^3 - \Gamma \cos(\omega t)] \end{pmatrix} dt + \begin{bmatrix} 0 & 0 \\ 0 & \sigma \end{bmatrix} \begin{pmatrix} 0 \\ dw \end{pmatrix} \quad (11.17)$$

where $x_1 = u$ and $x_2 = \dot{u}$.

Temporal explicit discretization with time step Δt over the fine grid leads to the following discrete state evolution equations:

$$\begin{aligned} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix}_{i+1} &= \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix}_i + \begin{bmatrix} 0 & \Delta t \\ -\Delta t(k_1 + k_3 x_1^2) & -\Delta t c \end{bmatrix}_i \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix}_i + \\ &\quad \begin{Bmatrix} 0 \\ \Delta t \Gamma \cos(\omega t) \end{Bmatrix}_i + \begin{Bmatrix} 0 \\ \sigma dw \end{Bmatrix}, \end{aligned} \quad (11.18)$$

where $dw = w(t_{i+1}) - w(t_i)$ is the Brownian path increment.

The semi-implicit discrete representation of the coarse grid integral with time step ΔT is defined as

$$\begin{aligned} \begin{bmatrix} 1 & -\Delta T \\ \Delta T(k_1 + k_3 X_1^2) & 1 + \Delta T c \end{bmatrix}_{i+1} \begin{Bmatrix} X_1 \\ X_2 \end{Bmatrix}_{i+1} &= \begin{Bmatrix} X_1 \\ X_2 \end{Bmatrix}_i + \\ &\quad \begin{Bmatrix} 0 \\ \Delta T \Gamma \cos(\omega T) \end{Bmatrix}_i + \begin{Bmatrix} 0 \\ \sigma dW \end{Bmatrix}, \end{aligned} \quad (11.19)$$

where $dW = W(t_{i+1}) - W(t_i)$ is Brownian path increment.

The following system parameters are considered for the numerical investigation: $c = 0.3$, $k_1 = -1$, $k_3 = 1$, $\omega = 1.25$. Two values of Γ are considered: $\Gamma = 0.30$ and $\Gamma = 0.37$. The underlying unforced (autonomous) system has three *fixed points* at $u = 0, \pm 1$ [166–168]. The fixed point at $u = 0$ is unstable whereas the fixed points at $u = \pm 1$ are stable. In the absence of noise ($\sigma = 0$), the harmonically forced Duffing system exhibits a period-two (period $T = \frac{4\pi}{\omega}$) and period-five (period $T = \frac{10\pi}{\omega}$) subharmonic oscillations for $\Gamma = 0.30$

and $\Gamma = 0.37$ respectively [168].

Next we investigate the performance of the stochastic parareal scheme to track the noisy limit cycle oscillations for $\Gamma = 0.30$ and $\Gamma = 0.37$ by varying the strength of random noise σ . We have taken the following integration parameters: $\Delta T = 0.63$, $\Delta t = 0.003$ for the integration interval $[0, \frac{40\pi}{\omega}]$.

Case I: Noisy period two subharmonic motion $\Gamma = 0.30$

Fig.(11.2) presents the system response corresponding to the noise free case ($\sigma = 0.0$). The figure shows the starting initial conditions $\mathbf{X}^{k=0}$ for the fine scale integral obtained using the coarse integrator given by Eq.(11.19) and the solution on the fine grid $\mathbf{x}^{k=n_{iter}}$ obtained from Eq.(11.18) where n_{iter} represents the number of iterations required to converge as indicated in the figure ($n_{iter} = 59$). The method converges as $\sum_{k=1}^{k=n_{iter}} \Delta_s^k$ tends to zero (i.e. the difference in the coarse and fine integration results are indistinguishable in the graphical scale). Therefore the continuity of the coarse and fine scale integral is enforced at the interface points $\mathbf{X}_s = \mathbf{x}_{n_f, s}$.

Figure 11.2: Performance of The Stochastic Parareal Integrator:

$$\Gamma = 0.3, \sigma = 0$$

The phase plane diagrams showing the convergence of the solution with respect to the iteration number k are presented in Fig.(11.3). As expected, the convergence of the parareal algorithm improves as the iteration number increases.

Figure 11.3: Convergence of the parareal algorithm ($k = 1, k = 3, k = 5,$
 $k = 23, k = 35$ and $k = 59$): $\Gamma = 0.3, \sigma = 0$

Next we investigate the efficacy of the parareal integrator on capturing the trajectories (samples paths) of the Duffing system perturbed by combined harmonic and random inputs. Fig.(11.4) shows the results for mild noise strength corresponding to $\sigma = 0.1\Gamma$. The three panels in the plot present the response of the Duffing oscillator for three different random samples. In the figure, we show the starting initial conditions for the parallel fine scale integration scheme and the converged parareal solution after n_{iter} . Although the results presented for three different random samples, the starting initial conditions generated from the coarse integrator are almost the same. This fact can be attributed to the large time step ΔT used in the coarse integration method which affects the accuracy of the numerical scheme. Depending on the random sample, the transitions of the trajectories take place between two potential wells located at $u = \pm 1$ due to random perturbation. Interestingly the parareal method is able to capture the sample paths even when the starting initial conditions, denoted by the green lines, are grossly erroneous indicating the solution confined to the opposite potential wells. The results obtained from the parallel and sequential schemes (not shown) are almost identical and indistinguishable in the plot.

Figure 11.4: Samples of the response of the Duffing oscillator:

$$\Gamma = 0.3, \sigma = 0.1\Gamma$$

Fig.(11.5) shows the response of the Duffing oscillator for the case of medium noise strength: $\sigma = 0.5\Gamma$. Despite starting with significantly erroneous initial conditions, the parareal method again effectively tracks the sample paths. Of course, the response is now significantly affected by the random noise as observed from the noisy phase portrait. Once again, the solutions obtained from the parallel and sequential scheme match identically in the scale of the graph.

(a) Time history

(b) Phase portrait

(c) Time history

(d) Phase portrait

(e) Time history

(f) Phase portrait

Figure 11.5: Samples of the response of the Duffing oscillator:

$$\Gamma = 0.3, \sigma = 0.5\Gamma$$

Next we consider the input noise with high strength corresponding to $\sigma = 0.9\Gamma$. The related results are plotted in Fig.(11.6) for three random samples. Although the parareal scheme still works for two samples in the top and middle panels, it fails for the third sample shown in the bottom panel as maximum number of iterations (which is set to 100) is reached without convergence. We conjecture such failure is partly attributed to the numerical scheme adopted for the coarse integrator which demands much finer integration time step and/or more iterations to converge.

(a) Time history

(b) Phase portrait

(c) Time history

(d) Phase portrait

(e) Time history

(f) Phase portrait

Figure 11.6: Samples of the response of the Duffing oscillator:

$$\Gamma = 0.3, \sigma = 0.9\Gamma$$

Case II: Noisy Period five subharmonic motion $\Gamma = 0.37$

In this section, we consider the case of $\Gamma = 0.37$. In the absence of random perturbation, the system displays a period-five subharmonic oscillation (period $T = \frac{10\pi}{\omega}$) leading to much slower dynamics compared to the case of $\Gamma = 0.3$. In contrast to the previous case, the response now periodically spans both the potential wells located at $u = \pm 1$. The performance of the parallel integrator is studied next with respect the strength of random noise as explained in the subsequent paragraphs.

The displacement response and the phase portrait for the noise free case are plotted in Fig(11.7a) and Fig(11.7b) respectively. Notwithstanding starting with grossly inaccurate initial condition, the parareal scheme again follows true solution trajectory after 59 iterations.

Figure 11.7: Performance of The Stochastic Parareal Integrator:

$$\Gamma = 0.37, \sigma = 0$$

The convergence of the parareal scheme with respect to the iteration number is shown in Fig.(11.8) for $k = 1$, $k = 3$, $k = 5$, $k = 6$, $k = 35$ and $k = 59$ iterations.

Figure 11.8: Convergence of the parareal algorithm ($k = 1, k = 3, k = 5, k = 6, k = 35$ and $k = 59$): $\Gamma = 0.37, \sigma = 0$

For a noise strength $\sigma = 0.1\Gamma$, the samples of noisy limit cycle motion are plotted in Fig.(11.9). Interestingly the presence of random noise occasionally entrains the dynamics in the potential wells at $u = \pm 1$. Such occasional entrainment phenomenon is absent for the harmonic perturbation alone ($\sigma = 0$). Recall that such behavior induced by random noise is in contrary to the previous case related to $\Gamma = 0.3$, whereby depending on the initial conditions, the dynamics is confined to a particular potential well located at either $u = 1$ or $u = -1$ for $\sigma = 0.1\Gamma$.

(a) Time history

(b) Phase portrait

(c) Time history

(d) Phase portrait

(e) Time history

(f) Phase portrait

Figure 11.9: Samples of the response of the Duffing oscillator:

$$\Gamma = 0.37, \sigma = 0.1\Gamma$$

The results for medium noise strength: $\sigma = 0.5\Gamma$ are presented in Fig.(11.10). As the noise strength increases, the presence of higher frequency oscillations become more apparent. This fact can be realized by comparing the phase portraits of those in Fig.(11.9) with Fig.(11.10). Evidently, the number of iterations required to converge depends on the random sample.

(a) Time history

(b) Phase portrait

(c) Time history

(d) Phase portrait

(e) Time history

(f) Phase portrait

Figure 11.10: Samples of the response of the Duffing oscillator:

$$\Gamma = 0.37, \sigma = 0.5\Gamma$$

Fig.(11.11) presents the results for sample trajectories for high strength of noise corresponding to $\sigma = 0.9\Gamma$, whereby the results obtained from parareal scheme become increasingly unwieldy. This phenomenon again can be attributed to the inadequacy of the coarse integrator as addressed in the previous case ($\Gamma = 0.3$).

(a) Time history

(b) Phase portrait

(c) Time history

(d) Phase portrait

(e) Time history

(f) Phase portrait

Figure 11.11: Samples of the response of the Duffing oscillator:

$$\Gamma = 0.37, \sigma = 0.9\Gamma$$

11.6 Parallel Performance

We measure the parallel performance of the adapted parareal algorithm by the strong scalability and speedup. The aim of the strong scalability test is to show the ability of the parallel algorithm to reduce the total execution time as we increase the number of processors [7]. The speedup measures the amount of the execution speed gained by increasing the number of processors [7]. The *total* speedup $S_t(np)$ of a parallel algorithm implemented on a parallel computer using np processors is defined as [7]

$$S_t(np) = \frac{T_s}{T(np)}, \quad (11.20)$$

where T_s refers to the total execution time of the sequential scheme using a single processor computer and $T(np)$ is the total execution time of the parallel scheme executed on a parallel computer using np processors. When the execution time of the sequential algorithm T_s is not available, the execution time of the parallel algorithm on a parallel computer using a single processor is used. In this case the speedup is called the *relative* speedup $S_r(np)$ and it is defined as [7]

$$S_r(np) = \frac{T(1)}{T(np)}, \quad (11.21)$$

where $T(1)$ and $T(np)$ denote the total execution time of the parallel algorithm executed on a parallel computer using a single and np processors respectively [7].

At this stage, it is worth emphasizing the fact that the time domain parallelism is beneficial only for relatively long time simulations. For short time simulations, the interprocessor

communication cost of the parallel algorithm cannot mask the computational cost. Indeed, when we use the previously used integration parameters ($T = [0, \frac{40\pi}{\omega}]$, $\Delta T = 0.63$ and $\Delta t = 0.003$) the sequential algorithm takes no time (almost zero) to execute. The parareal algorithm, on the other hand, demands relatively longer time to execute. Although the total execution time is about fraction of a second, increasing the number of processors up to a certain value leads to a reduction in the total execution time as illustrated in Table(11.1).

Table 11.1: Execution time in second for the parareal algorithm

No. of processors	Time: $\Gamma = 0.3$	Time: $\Gamma = 0.37$
1	8.489E-2	8.646E-2
2	4.694E-2	4.551E-2
4	2.217E-2	2.101E-2
8	2.834E-2	8.252E-2
16	12.178E-2	22.941E-2

For such short simulation time, the stochastic parareal algorithm is not a preferable alternative to the sequential method. To demonstrate the usefulness of the parallel scheme for fast simulation, we increase the total simulation time to $T = 500$. In addition, we take the coarse scale time step $\Delta T = 0.03$ and the fine scale time step $\Delta t = 1.5 \times 10^{-6}$. The parareal algorithm is implemented in a parallel environment using MPI libraries and executed on a Linux cluster consists of 1200 compute nodes with 6 cores and 36 GBytes of memory per node with InfiniBand interconnect [149]. A semi-implicit scheme is used for the serial algorithm and the results are generated using the above time integration grid (i.e. $T = 500$ and $\Delta t = 1.5 \times 10^{-6}$).

Next we study the parallel performance of the algorithm, for different strength of the random noise. In Fig.(11.12) and Fig.(11.13) we show the strong scalability and the corresponding total and relative speedup of the stochastic parareal algorithm for $\Gamma = 0.3$ and $\Gamma = 0.37$ respectively. Clearly, increasing the number of processors leads to a great reduction in the total execution time as demonstrated in the left panels of Fig.(11.12) and Fig.(11.13). For this specific example, the stochastic parareal method is only efficient when we use roughly more than 24 processors. In these cases, the execution time of the parareal scheme is lower than that of the sequential method. Increasing the number of processors beyond certain thresholds (96 for the case of $\Gamma = 0.3$ and 112 for the case of $\Gamma = 0.37$) does not reduce the execution time further as the communication overhead predominates over the computational cost.

Depending on the random sample and the strength of the noise, the total speedup $S_t(np)$ of the stochastic parareal scheme is between 2 and 3 as illustrated in the middle panels of Fig.(11.12) and Fig.(11.13). This means that the parallel method is faster than the sequential method by a factor between 2 to 3. On the other hand, the stochastic parareal scheme can achieve a relative speedup $S_r(np)$ up to 40 depending on the random sample and the strength of the noise as shown in the right panels of Fig.(11.12) and Fig.(11.13).

(a) Scalability: $\sigma = 0$ (b) Total speedup: $\sigma = 0$ (c) Relative speedup: $\sigma = 0$ (d) Scalability: $\sigma = 0.1\Gamma$ (e) Total speedup: $\sigma = 0.1\Gamma$ (f) Relative speedup: $\sigma = 0.1\Gamma$ (g) Scalability: $\sigma = 0.5\Gamma$ (h) Total speedup: $\sigma = 0.5\Gamma$ (i) Relative speedup: $\sigma = 0.5\Gamma$ Figure 11.12: Parallel scalability and speedup: $\Gamma = 0.3$

Figure 11.13: Parallel scalability and speedup: $\Gamma = 0.37$

Discussion

For the particular example considered here, the performance of the parareal scheme in terms of convergence rate and parallel scalability is dictated by the ratio $\frac{\Delta T}{\Delta t}$. For small Δt , relatively large amounts of computational work are performed independently by each processor. In other words, Δt determines the computational cost of the parareal algorithm. On the other hand, taking large ΔT not only affects the stability of the coarse integral, but also increases the iteration counts of the parareal algorithm to converge. Each iteration of the parareal scheme involves two communication events as shown in (steps 12 and 16) of Algorithm(21). Consequently, ΔT quantifies in some sense the communication cost of the parallel algorithm (the larger ΔT leads to the higher communication cost). Furthermore, recall that the coarse integral and the correction to the initial conditions (steps 14 and 15 respectively) in Algorithm(refPararealAlgorithm) are performed serially on the master processor ($rank = 0$). For small ΔT , the master processor may consume high CPU time, while the rest of the processors are idle. Therefore, the ratio $\frac{\Delta T}{\Delta t}$ can be used to qualitatively estimate the *granularity* of the parareal algorithm (i.e. computation/communication). For efficient parallel performance, one typically should maintain coarse granularity (e.g. relatively large ratio of $\frac{\Delta T}{\Delta t}$) while satisfying the convergence criteria of both the fine and coarse integration methods.

11.7 Summary

We made an initial attempt to study the efficiency and limitations of a stochastic parallel integration scheme for strongly nonlinear systems. At least for the Duffing oscillator considered here, the numerical results demonstrates the possible usefulness of the stochastic parareal scheme for efficient simulation of dynamical systems in parallel computers. For low to medium strength of noise, the parareal scheme tracks the response trajectories accurately. The failure of the scheme for high strength of input noise is also pointed out. The parallel implementation of the algorithm demonstrates that the parareal algorithm can accelerate the simulation time by a factor of 2 to 3 depending on the random sample and the strength of the noise.

In relation to some recent developments [68, 74–77, 79, 80], the parareal scheme may also be applied for efficient simulation of stochastic partial differential equation with random operator in conjunction with the spatial domain decomposition. On the other hand, the tracking sample path of randomly perturbed dynamical system subject to noisy observational data is most relevant to nonlinear filtering commonly used in data assimilation [162, 169–171]. This fact may offer the possibility of near real-time forecast (prediction) of the dynamics of engineering and natural systems (e.g. [169–171]) although more research is needed in this direction.

Chapter 12

Conclusions and Future Directions

12.1 Summary of Findings

Non-overlapping domain decomposition methods, namely iterative substructuring techniques are described for uncertainty quantification of large-scale computational models. The mathematical framework is based on non-overlapping domain decomposition in the geometric space and functional expansion along the stochastic dimension. For numerical illustrations, two-dimensional and three-dimensional SPDEs with spatially varying non-Gaussian random coefficients are considered. The numerical scalability of the algorithms are investigated with respect to the mesh size, subdomain size, fixed problem size per subdomain, level of uncertainty and order of the stochastic dimension. For a fixed mesh resolution, the total solution time cannot be reduced beyond a critical number of subdomains as the interprocessor communication overhead and memory bandwidth requirement predominate over floating point operations. In order to exploit the remaining idle processors in multi-processor computers, the investigation is directed towards achieving time domain

parallelism. To this end, a probabilistic version of a parallel time integration scheme is developed to simulate the trajectories of a noisy non-linear dynamical system described by SDEs. The primary contributions of this investigation are summarized as follows:

- Iterative substructuring techniques are developed to tackle the coupled large-scale linear systems arising in the context of the intrusive Spectral Stochastic Finite Element Method (SSFEM). The iterative algorithm circumvents the need of constructing both the local and global extended Schur complement matrices explicitly.
- A novel probabilistic one-level Neumann-Neumann domain decomposition preconditioner is introduced for the iterative solution of the coupled large-scale linear systems in the SSFEM. The performance of the algorithm is nearly independent of the level of uncertainty and the size of the stochastic dimension. The one-level domain decomposition algorithm demonstrates scalability for moderate range of processors/subdomains for the problem size considered in this investigation. The probabilistic Neumann-Neumann domain decomposition preconditioner is the essential ingredient to develop two-level domain decomposition algorithms for SPDEs.
- A novel two-level domain decomposition preconditioner is formulated for the iterative substructuring of SPDEs. Within the framework of the intrusive SSFEM, the two-level preconditioner is constructed by adding a probabilistic coarse problem to the one-level Neumann-Neumann preconditioner. The algorithm may be considered as a probabilistic version of the Balancing Domain Decomposition by Constraints (BDDC). The probabilistic two-level Neumann-Neumann preconditioner exhibits a scalable performance for problems in linear elasticity and flow through porous media

with spatially varying non-Gaussian random parameters.

- A novel primal-primal iterative substructuring technique is introduced to solve the large-scale linear system arising from the finite element discretization of stochastic PDEs. The algorithm offers a direct approach to formulate a two-level scalable preconditioner. The algorithm can be viewed as another probabilistic version of BDDC. The algorithm shows a scalable performance with respect to the order of the stochastic expansion, the spatial problem size, number of subdomains and fixed problem size per subdomain.
- A novel dual-primal iterative substructuring technique is formulated to tackle the coupled deterministic linear systems in the intrusive SSFEM of large-scale SPDEs. The proposed method may be viewed as the probabilistic version of the Dual-Primal Finite Element Tearing and Interconnecting (FETI-DP). The numerical results illustrate that the proposed algorithm is scalable with respect to the order of the stochastic expansion, the spatial problem size, number of subdomains and fixed problem size per subdomain. The probabilistic FETI-DP method demonstrates convergence properties similar to the probabilistic BDDC type two-level domain decomposition preconditioner for SPDEs.
- A parallel time integration algorithm for ODEs is adapted to tackle SDEs describing noise-driven dynamical systems. For the Duffing oscillator considered in this investigation, the numerical results demonstrate the possible usefulness of the stochastic parareal scheme for efficient simulation of dynamical systems in parallel computers. For low to medium strength of noise, the parareal scheme tracks the response trajec-

tories accurately. The parallel implementation of the algorithm demonstrates that the parareal algorithm can accelerate the simulation time by a factor of 2 to 3 depending on the random sample and the strength of the noise.

In the abstract form, the probabilistic two-level domain decomposition methods can be expressed as

$$\mathcal{M}^{-1} = \sum_{s=1}^{n_s} \mathcal{H}_f^{sT} [\mathcal{S}_f^s]^{-1} \mathcal{H}_f^s + \mathcal{H}_c^T [\mathcal{S}_c]^{-1} \mathcal{H}_c, \quad (12.1)$$

where $\mathcal{M}^{-1}$ denotes the preconditioner in the primal methods (and operator in the dual-primal method), $[\mathcal{S}_f^s]^{-1}$ is the local (fine) problem, $[\mathcal{S}_c]^{-1}$ is the (global) coarse problem, and $\mathcal{H}_f^s$ and $\mathcal{H}_c$ are the restriction operators. A summary of the two-level domain decomposition methods for the stochastic problems is shown in Table (12.1). Clearly, the fine $[\mathcal{S}_f^s]^{-1}$ and coarse $[\mathcal{S}_c]^{-1}$ level problems are the same in all the methods. The structure of the fine $\mathcal{H}_f^s$ and coarse $\mathcal{H}_c$ level restriction operators are the same in both the probabilistic primal-primal and dual-primal methods. Note that the two-level Neumann-Neumann preconditioner is employed to precondition the extended Schur complement system, whereas the primal-primal preconditioner is used to precondition the reduced system by excluding the variables associated with the corner nodes of the interface boundary. The primal-primal preconditioner has the same size and structure of the dual-primal operator.

Table 12.1: Connection among the two-level probabilistic Neumann-Neumann preconditioner, primal-primal preconditioner and dual-primal operator

Method	$\mathcal{H}_f^s$	$[\mathcal{S}_f^s]^{-1}$	$\mathcal{H}_c$	$[\mathcal{S}_c]^{-1}$
(a)	$\mathcal{R}_s^r \mathcal{D}_s \mathcal{R}_s$	$[\mathcal{S}_{rr}^s]^{-1}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{R}_s^c - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{R}_s^r) \mathcal{D}_s \mathcal{R}_s$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s$
(b)	$\mathcal{D}_r^s \mathcal{B}_r^s$	$[\mathcal{S}_{rr}^s]^{-1}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{D}_r^s \mathcal{B}_r^s$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s$
(c)	$\mathcal{B}_r^{sT}$	$[\mathcal{S}_{rr}^s]^{-1}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{B}_r^{sT}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s$

(a) : Two-Level Neumann-Neumann Preconditioner.

(b) : Primal-Primal Preconditioner.

(c) : Dual-Primal Operator.

12.2 Directions for Future Research

The computational framework of uncertainty analysis developed in this thesis demonstrates scalability for large range of processors. The rapid advances of high performance computing systems warrants further improvement of the aforementioned domain decomposition algorithms for SPDEs to exploit even larger (e.g. thousands) number of processors for uncertainty quantification of large-scale systems. To address this issue, the following future research directions are envisioned:

- The probabilistic coarse problem in the two-level domain decomposition methods for SPDEs plays the critical role to achieve a scalable performance. For large-scale three-dimensional problems, the size of the coarse problem increases rapidly with the number of subdomains. At each iteration of the two-level domain decomposition solver, the coarse problem have to be solved efficiently to spread information globally across the subdomains. The solution of the coarse problem becomes the performance bottleneck for large number of subdomains. For deterministic systems, this issue is addressed by the use of *inexact solvers* for the coarse problem [123, 131, 172]. For stochastic system, the Stochastic Reduced Basis Methods (SRBMs) [47–49] can be exploited to formulate a reduced-order probabilistic coarse problem which can be solved efficiently. This approach seems to be feasible as only a small number of basis vectors should be adequate to obtain a good approximate solution to the the coarse problem at much lower computational cost.
- To achieve better convergence properties for three-dimensional elasticity problems, additional primal constraints must be considered in constructing the probabilistic

coarse problem. These constraints may include averages over faces or averages and first-order moments over edges [81, 83, 135, 155, 156]. Optional Lagrange multipliers [81, 157] and transformation of basis [155, 156] approaches can be utilized to implement the additional constraints in the probabilistic FETI-DP and BDDC type preconditioner respectively.

- For a given problem size, the spatial domain decomposition techniques cannot reduce the total solution time beyond a certain number of processors. This limitation is due to hardware related issues such as latency and bandwidth of the communication network. To take the full advantage of the massively parallel computers, the concurrency should be exploited in both temporal and spatial dimension simultaneously. The parareal scheme for parallel time integration performs reasonably at least for the one degree of freedom system considered in the thesis. The performance study of the parareal scheme in conjunction with the spatial domain decomposition for time dependent SPDEs using SSFEM merits future investigation.
- Hybrid CPU/GPU clusters are becoming cost-effective high performance computing systems for computationally intensive applications. To effectively utilize this hybrid computing environment, further adaptations to the probabilistic domain decomposition solvers need to be considered. Such adaptations may include exploiting two-level concurrency, namely data and task parallelisms. Each subdomain can be assigned to a pair of CPU and GPU in each compute node. The data parallelism achieved by domain decomposition constitutes the global level of parallelization. This data parallel approach can be implemented using MPI on the CPU. Within each

compute node, the computational power of the GPU can be exploited to speedup the subdomain level computations. This local level of parallelization constitutes task parallelism to be delegated to the GPU.

- For deterministic PDEs, the scalability of a domain decomposition algorithm is estimated theoretically by the condition number bound of the preconditioned operator as [4, 5, 7]

$$\kappa(\mathbf{M}^{-1}\mathbf{S}) \leq C(1 + \log \frac{H}{h})^2, \quad (12.2)$$

where C is a positive constant (independent of the geometric parameters h and H) and h and H are the finite element mesh size and subdomain size respectively. When the condition number is independent of the subdomain size H (or number of subdomains $1/H$), the method is said to be scalable [4, 5, 7, 64]. For SPDEs, we conduct numerical experiments to demonstrate that the probabilistic two-level domain decomposition methods are scalable with respect to the number of subdomains [129]. A theoretical study to estimate the condition number bound for SPDEs is required. The condition number bound for SPDEs maybe cast in the following form

$$\kappa(\mathcal{M}^{-1}\mathcal{S}) \leq f(h, H, L, N), \quad (12.3)$$

where L and N denote the number of terms in KLE and PCE respectively.

Appendices

Appendix A

Uncertainty Representation by Stochastic Processes

The representation of uncertainty in the system parameters by PCE based on experimental data highly affects the accuracy of the response statistics [24, 173, 174]. Indeed, identification of the polynomial chaos coefficients from measurements is an active topic in the literature [24, 173–176]. Statistical estimation methods such as maximum likelihood estimation [175–177] and Bayesian inference [24, 174] are proposed to characterize the chaos coefficients from field observations. However, for cases when higher order of PCE is required to accurately represent random variables (e.g. multi-modal random variables), these approaches may be inefficient [24, 175] or become computationally intensive [173]. In order to reduce the computational complexity, an *empirical projection technique* is proposed in [173]. The methodology is based on representing a multi-modal random variable as a combination of uni-modal random variables [173]. Although the method may be compu-

tationally efficient, it requires very large number of samples as the dimension of the PCE increases [173].

For an elementary exposition of PCE, we consider a stochastic Poisson's problem defined on a square domain. We assume that the sufficient statistical data is available to represent the permeability coefficient as a random field. Consequently, we represent the permeability coefficient using PCE. Next, we propagate uncertainty in the model parameters through the system using both PCE and Monte Carlo simulation (MCS).

In Fig.(A.1), we show the discretized computational domain using 2093 nodes and 4028 elements. On this domain we consider Poisson's equation defined as

$$\nabla \cdot (\kappa(\mathbf{x}) \nabla u(\mathbf{x}, \theta)) = f(\mathbf{x}), \quad \mathbf{x} \in D, \quad (\text{A.1})$$

$$u(\mathbf{x}) = 0, \quad \mathbf{x} \in \partial D, \quad (\text{A.2})$$

where $f(\mathbf{x}) = 1.0$ and $\kappa(\mathbf{x}, \theta)$ is the permeability coefficient modelled as a stochastic process.

Figure A.1: The finite element mesh

Next we assume sufficient permeability tests are carried out which allow accurate representation of the permeability coefficient as a random field. As an ideal case, we assume the data is noise free and available at each point in the domain. In practice however, the available data is generally sparse and contains noise. For this case, maximum likelihood estimation [175–177] or Bayesian inference [24, 174] can be used to estimate the chaos coefficients of the permeability field. Samples of the permeability measurements are shown in Fig.(A.2). The samples are synthetically generated using a four dimensional third order PCE of a lognormal process (see Appendix B).

Figure A.2: Samples of the permeability measurements

The PCE of the permeability field $\kappa(\mathbf{x}, \theta)$ can be expressed as

$$\kappa(\mathbf{x}, \theta) = \sum_{j=0}^P \kappa_j(\mathbf{x}) \Psi_j(\boldsymbol{\xi}). \quad (\text{A.3})$$

For multi-modal random variables, very high-order PCE is needed to accurately represent the random field [173]. As an efficient alternative technique, multi-modal random variables can be represented as a mixture of uni-modal random variables [173]. The uni-modal random variables can be represented using low-order PCE and the expansion coefficients can be calculated using the empirical projection technique [173].

Assuming sufficient data is available and four dimensional third order PCE is sufficient to accurately represent the permeability field, the chaos coefficients $\kappa_j(\mathbf{x})$ can be obtained from the samples as

$$\hat{\kappa}_j(\mathbf{x}) = \frac{\langle \kappa(\mathbf{x}, \theta) \Psi_i(\boldsymbol{\xi}) \rangle}{\langle \Psi_i^2(\boldsymbol{\xi}) \rangle}. \quad (\text{A.4})$$

The estimates of the selected chaos coefficients $\hat{\kappa}_j(\mathbf{x})$ are shown in Fig.(A.3). Note that we use 1000 realizations to estimate the coefficients. The first coefficient $\hat{\kappa}_0(\mathbf{x})$ denotes the mean of the stochastic process. The higher order coefficients represent the non-Gaussian effect.

Figure A.3: Selected PC coefficients of the permeability random field

Firstly, we deterministically represent the permeability coefficient using the mean of the stochastic process. The corresponding deterministic solution field is shown in Fig.(A.4).

Secondly, we represent the permeability coefficient as a stochastic process using Eq.(A.3). The mean and standard deviation of the solution field obtained using PCE and MCS are plotted in Fig.(F.1). Acceptable agreement between PCE and MCS can be observed. The maximum CoV in the middle of the domain is about 25%. The mean and standard deviation have the same trend as the deterministic solution previously shown in Fig.(A.4).

Figure A.4: The deterministic solution field

Figure A.5: The mean and standard deviation of the solution process using PCE and MCS

Appendix B

Polynomial Chaos Expansion of Lognormal Stochastic Process

This section closely follows the references [96, 145]. Let $g(\mathbf{x}, \theta)$ be a Gaussian stochastic process and $C_{gg}(\mathbf{x}_1, \mathbf{x}_2)$ its covariance function. The KLE of the Gaussian process $g(\mathbf{x}, \theta)$ can be obtained as

$$g(\mathbf{x}, \theta) = g_0(\mathbf{x}) + \sum_{i=1}^L \sqrt{\lambda_i} \phi_i(\mathbf{x}) \xi_i(\theta). \quad (\text{B.1})$$

Eq.(B.1) can be rewritten in compact form as

$$g(\mathbf{x}, \theta) = \sum_{i=0}^L g_i(\mathbf{x}) \xi_i, \quad (\text{B.2})$$

where

$$\xi_0(\theta) = 1 \quad \text{and} \quad g_i(\mathbf{x}) = \sqrt{\lambda_i} \phi_i(\mathbf{x}). \quad (\text{B.3})$$

Let $l(\mathbf{x}, \theta)$ be a lognormal stochastic process obtained from the Gaussian stochastic process $g(\mathbf{x}, \theta)$ as

$$l(\mathbf{x}, \theta) = \exp [g(\mathbf{x}, \theta)]. \quad (\text{B.4})$$

Substituting the KLE of the Gaussian process given by Eq.(B.2) into Eq.(B.4) leads to

$$l(\mathbf{x}, \theta) = \exp \left[\sum_{i=0}^L g_i(\mathbf{x}) \xi_i \right]. \quad (\text{B.5})$$

The PCE of the lognormal process $l(\mathbf{x}, \theta)$ can be defined as

$$l(\mathbf{x}, \theta) = \sum_{i=0}^P l_i(\mathbf{x}) \Psi_i(\boldsymbol{\xi}), \quad (\text{B.6})$$

where

$$\langle \Psi_i(\boldsymbol{\xi}) \rangle = 0, \quad \langle \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) \rangle = \langle \Psi_i^2(\boldsymbol{\xi}) \rangle \delta_{ij}. \quad (\text{B.7})$$

Galerkin projection of Eq.(B.6) on the PC basis leads to

$$l_i(\mathbf{x}) = \frac{\langle l(\mathbf{x}, \theta) \Psi_i(\boldsymbol{\xi}) \rangle}{\langle \Psi_i^2(\boldsymbol{\xi}) \rangle}. \quad (\text{B.8})$$

The denominator in Eq.(B.8) can be evaluated analytically. The numerator is calculated as follows [145].

Using Eq.(B.5), the numerator in Eq.(B.8) can be expressed as [145]

$$\langle l(\mathbf{x}, \theta) \Psi_i(\boldsymbol{\xi}) \rangle = \exp[g_0(\mathbf{x})] \int_{-\infty}^{+\infty} \exp \left[\sum_{j=1}^L g_j(\mathbf{x}) \xi_j \right] \Psi_j(\boldsymbol{\xi}) \exp \left[-\frac{1}{2} \sum_{j=1}^L \xi_j \xi_j \right] d\boldsymbol{\xi}. \quad (\text{B.9})$$

The integration in Eq.(B.9) can be simplified to [145]

$$\langle l(\mathbf{x}, \theta) \Psi_i(\boldsymbol{\xi}) \rangle = \exp \left[g_0(\mathbf{x}) + \frac{1}{2} \sum_{j=1}^L g_j^2(\mathbf{x}) \right] \langle \Psi_j(\boldsymbol{\eta}) \rangle, \quad (\text{B.10})$$

where

$$\eta_j = \xi_j - g_j(\mathbf{x}). \quad (\text{B.11})$$

In a concise form, Eq.(B.10) can be expressed as

$$\langle l(\mathbf{x}, \theta) \Psi_i(\boldsymbol{\xi}) \rangle = l_0(\mathbf{x}) \langle \Psi_j(\boldsymbol{\eta}) \rangle, \quad (\text{B.12})$$

where $l_0(\mathbf{x})$ is the mean of the lognormal stochastic process defined as

$$l_0(\mathbf{x}) = \exp \left[g_0(\mathbf{x}) + \frac{1}{2} \sum_{j=1}^L g_j^2(\mathbf{x}) \right]. \quad (\text{B.13})$$

The quantity $\langle \Psi_j(\boldsymbol{\eta}) \rangle$ in Eq.(B.12) is the expectation of the PC basis centered around the Gaussian coefficients $g_i(\mathbf{x})$. This expectation can be evaluated analytically as shown in Table.(B.1) [145].

Table B.1: The expectation and variance of the PC basis

$\Psi_i(\xi)$	$\langle \Psi_i^2(\xi) \rangle$	$\langle \Psi_i(\eta) \rangle$
ξ_1	1	$g_1(\mathbf{x})$
ξ_2	1	$g_2(\mathbf{x})$
$\xi_1^2 - 1$	2	$g_1^2(\mathbf{x})$
$\xi_1 \xi_2$	1	$g_1(\mathbf{x}) g_2(\mathbf{x})$
$\xi_2^2 - 1$	2	$g_2^2(\mathbf{x})$
$\xi_1^3 - 3\xi_1$	6	$g_1^3(\mathbf{x})$
$\xi_1^2 \xi_2 - \xi_2$	2	$g_1^2(\mathbf{x}) g_2(\mathbf{x})$
$\xi_1 \xi_2^2 - \xi_1$	2	$g_1(\mathbf{x}) g_2^2(\mathbf{x})$
$\xi_2^3 - 3\xi_2$	6	$g_2^3(\mathbf{x})$

Using Eq.(B.12), the PC coefficients of the lognormal stochastic process in Eq.(B.8) can be rewritten as

$$l_i(\mathbf{x}) = l_0(\mathbf{x}) \frac{\langle \Psi_i(\eta) \rangle}{\langle \Psi_i^2(\xi) \rangle}. \quad (\text{B.14})$$

Finally, the PCE of the lognormal stochastic process can be expressed as

$$l(\mathbf{x}, \theta) = l_0(\mathbf{x}) \sum_{i=0}^L \frac{\langle \Psi_i(\eta) \rangle}{\langle \Psi_i^2(\xi) \rangle} \Psi_i(\xi). \quad (\text{B.15})$$

As a special case, let $g(\theta)$ be a Gaussian random variable defined as

$$g(\theta) = \mu_g + \sigma_g \xi, \quad (\text{B.16})$$

where μ_g is the mean and σ_g denotes the standard deviation. According to Eq.(B.15) the lognormal random variable can be represented as

$$l(\theta) = \mu_l \sum_{i=0}^{\infty} \frac{\sigma_g^i}{i!} \Psi_i(\xi) \quad (\text{B.17})$$

$$= \mu_l \left(1 + \sigma_g \xi + \frac{\sigma_g^2}{2} (\xi^2 - 1) + \frac{\sigma_g^3}{6} (\xi^3 - 3\xi) + \dots \right), \quad (\text{B.18})$$

where the mean of the lognormal random variable is defined as

$$\mu_l = \exp \left(\mu_g + \frac{1}{2} \sigma_g^2 \right). \quad (\text{B.19})$$

Appendix C

Spectral Stochastic Finite Element Method

This section closely follows the references [3, 11, 17, 37]. Consider a linear elliptic stochastic PDE defined on a domain Ω with a given data on the boundary $\partial\Omega$ as

$$\nabla \cdot (\kappa(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) = f(\mathbf{x}) \quad \mathbf{x} \in \Omega, \quad (\text{C.1})$$

$$u(\mathbf{x}, \theta) = 0 \quad \mathbf{x} \in \partial\Omega, \quad (\text{C.2})$$

where θ denotes the stochastic dimension, $\kappa(\mathbf{x}, \theta)$ is the random permeability coefficient, $u(\mathbf{x}, \theta)$ is the stochastic response and $f(\mathbf{x})$ represents the forcing term. The finite element discretization in the spatial domain leads to the following stochastic linear system [3, 11, 17, 37]

$$\mathbf{A}(\theta)\mathbf{u}(\theta) = \mathbf{f}, \quad (\text{C.3})$$

where $A(\theta)$ represents the global stiffness matrix with random coefficients. The global stiffness matrix can be expressed as a summation of the element stiffness matrices as

$$A(\theta) = \sum_{e=1}^{n_e} A^e(\theta), \quad (C.4)$$

where n_e denotes the total number of elements associated with the spatial discretization and $A^e(\theta)$ is the element stiffness matrix defined as [3, 11, 17, 37]

$$A^e(\theta) = \int_{\Omega^e} B^T D(\mathbf{x}, \theta) B \, d\Omega^e, \quad (C.5)$$

where B is strain matrix and $D(\mathbf{x}, \theta)$ represents the random constitutive matrix. Without loss of generality, the random properties is assumed to be isotropic field. Thus, $D(\mathbf{x}, \theta)$ can be expressed as [3, 11, 17, 37]

$$D(\mathbf{x}, \theta) = \kappa(\mathbf{x}, \theta) \mathbf{I}, \quad (C.6)$$

where $\mathbf{I}$ is the identity matrix. For general non-Gaussian material properties, the PCE can be used to represent the random permeability coefficient $\kappa(\mathbf{x}, \theta)$ as [3, 11, 17, 37]

$$\kappa(\mathbf{x}, \theta) = \sum_{i=0}^L \kappa_i(\mathbf{x}) \Psi_i, \quad (C.7)$$

where $\kappa_i(\mathbf{x})$ are the PCE coefficients and Ψ_i are a set of Hermite polynomials with the following properties

$$\langle \Psi_0 \rangle = 1, \quad \langle \Psi_i \rangle = 0 \quad \text{for } i \neq 0 \quad \text{and} \quad \langle \Psi_i \Psi_j \rangle = \delta_{ij} \langle \Psi_i^2 \rangle. \quad (C.8)$$

Substituting Eq.(C.6) and Eq.(C.7) into Eq.(C.5), we obtain

$$\mathbf{A}^e(\theta) = \sum_{i=0}^L \mathbf{A}_i^e \Psi_i(\theta), \quad (\text{C.9})$$

where

$$\mathbf{A}_i^e = \int_{\Omega^e} \mathbf{B}^T [\kappa_i(\mathbf{x}) \mathbf{I}] \mathbf{B} \, d\Omega^e. \quad (\text{C.10})$$

Substituting Eq.(C.9) into Eq.(C.4), we obtain

$$\mathbf{A}(\theta) = \sum_{i=0}^L \sum_{e=1}^{n_e} \mathbf{A}_i^e \Psi_i. \quad (\text{C.11})$$

Eq.(C.11) can be rearranged as

$$\mathbf{A}(\theta) = \sum_{i=0}^L \mathbf{A}_i \Psi_i, \quad (\text{C.12})$$

where

$$\mathbf{A}_i = \sum_{e=1}^{n_e} \mathbf{A}_i^e. \quad (\text{C.13})$$

The solution process can be expanded using the same PC basis as

$$\mathbf{u}(\theta) = \sum_{j=0}^N \mathbf{u}_j \Psi_j. \quad (\text{C.14})$$

Substituting Eq.(C.12) and Eq.(C.14) into Eq.(C.3), we obtain

$$\sum_{i=0}^L \sum_{j=0}^N \Psi_i \Psi_j \mathbf{A}_i \mathbf{u}_j = \mathbf{f}. \quad (\text{C.15})$$

Performing Galerkin projection over the space spanned by the polynomial chaoses Ψ_k , the following coupled deterministic system for the PC coefficients of the solution process is obtained [3, 11, 17, 37]

$$\sum_{j=0}^N \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_i \mathbf{u}_j = \langle \Psi_k \mathbf{f} \rangle, \quad k = 0, 1, \dots, N \quad (\text{C.16})$$

Equivalently, Eq.(C.16) can be reexpressed in a compact form as

$$\mathcal{AU} = \mathcal{F}, \quad (\text{C.17})$$

where

$$\mathcal{A}_{j,k} = \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_i, \quad \mathcal{U} = (\mathbf{u}_0, \dots, \mathbf{u}_N)^T \quad \text{and} \quad \mathcal{F}_k = \langle \Psi_k \mathbf{f} \rangle. \quad (\text{C.18})$$

Eq.(C.17) can be expanded as

$$\begin{bmatrix} \mathcal{A}_{0,0} & \mathcal{A}_{0,1} & \dots & \mathcal{A}_{0,N} \\ \mathcal{A}_{1,0} & \mathcal{A}_{1,1} & \dots & \mathcal{A}_{1,N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{A}_{N,0} & \mathcal{A}_{N,1} & \dots & \mathcal{A}_{N,N} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_0 \\ \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_N \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_0 \\ \mathcal{F}_1 \\ \vdots \\ \mathcal{F}_N \end{Bmatrix}. \quad (\text{C.19})$$

The solution of the coupled linear system defined in Eq.(C.19) provides the chaos coefficients of the solution process $(\mathbf{u}_0, \dots, \mathbf{u}_N)^T$. The mean and variance of the solution process can be obtained from Eq.(C.14) respectively as

$$\boldsymbol{\mu}_u = \sum_{j=0}^N \langle \Psi_j \rangle \mathbf{u}_j = \mathbf{u}_0, \quad (\text{C.20})$$

and

$$\sigma_u^2 = \langle (\mathbf{u}(\theta) - \boldsymbol{\mu}_u)^2 \rangle = \sum_{j=1}^N \langle \Psi_j^2 \rangle \mathbf{u}_j^2. \quad (\text{C.21})$$

Appendix D

Domain Decomposition Methods for SPDEs

This section closely follows the references [68, 74]. Consider a linear elliptic stochastic PDE defined on a domain Ω with a given data on the boundary $\partial\Omega$. The finite element approximation of the stochastic PDE leads to the following discrete linear system

$$\mathbf{A}(\theta)\mathbf{u}(\theta) = \mathbf{f}, \tag{D.1}$$

where $\mathbf{A}(\theta)$ is the stiffness matrix with random coefficients, $\mathbf{u}(\theta)$ is the stochastic process representing the response vector and $\mathbf{f}$ denotes the applied force. Let the spatial domain Ω be partitioned into two non-overlapping subdomains such that $\Omega = \Omega_1 \cup \Omega_2$, $\Omega_1 \cap \Omega_2 = \emptyset$ and $\Gamma = \partial\Omega_1 \cap \partial\Omega_2$ where Γ defines the interface of Ω_1 and Ω_2 [178]. Accordingly, the equilibrium system for a typical subdomain can be expressed as

$$\begin{bmatrix} \mathbf{A}_{II}^s(\theta) & \mathbf{A}_{I\Gamma}^s(\theta) \\ \mathbf{A}_{\Gamma I}^s(\theta) & \mathbf{A}_{\Gamma\Gamma}^s(\theta) \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s(\theta) \\ \mathbf{u}_\Gamma^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_\Gamma^s \end{Bmatrix}, \quad (\text{D.2})$$

where the partitions I and Γ relate to the interior and interface degrees of freedom, respectively. The uncertain system parameters can be expanded using PCE as

$$\sum_{i=0}^L \Psi_i \begin{bmatrix} \mathbf{A}_{II,i}^s & \mathbf{A}_{I\Gamma,i}^s \\ \mathbf{A}_{\Gamma I,i}^s & \mathbf{A}_{\Gamma\Gamma,i}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s(\theta) \\ \mathbf{u}_\Gamma^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_\Gamma^s \end{Bmatrix}. \quad (\text{D.3})$$

Enforcing the transmission conditions along the interface boundary, the equilibrium equation of the stochastic system defined by two subdomains can be represented as

$$\sum_{i=0}^L \Psi_i \begin{bmatrix} \mathbf{A}_{II,i}^1 & 0 & \mathbf{A}_{I\Gamma,i}^1 \\ 0 & \mathbf{A}_{II,i}^2 & \mathbf{A}_{I\Gamma,i}^2 \\ \mathbf{A}_{\Gamma I,i}^1 & \mathbf{A}_{\Gamma I,i}^2 & \mathbf{A}_{\Gamma\Gamma,i}^1 + \mathbf{A}_{\Gamma\Gamma,i}^2 \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^1(\theta) \\ \mathbf{u}_I^2(\theta) \\ \mathbf{u}_\Gamma(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^1 \\ \mathbf{f}_I^2 \\ \mathbf{f}_\Gamma^1 + \mathbf{f}_\Gamma^2 \end{Bmatrix}. \quad (\text{D.4})$$

The solution process can be expanding using the same PCE basis as

$$\begin{Bmatrix} \mathbf{u}_I^1(\theta) \\ \mathbf{u}_I^2(\theta) \\ \mathbf{u}_\Gamma(\theta) \end{Bmatrix} = \sum_{j=0}^N \Psi_j \begin{Bmatrix} \mathbf{u}_{I,j}^1 \\ \mathbf{u}_{I,j}^2 \\ \mathbf{u}_{\Gamma,j} \end{Bmatrix}. \quad (\text{D.5})$$

Substituting Eq.(D.5) in Eq.(D.4) leads to

$$\sum_{i=0}^L \sum_{j=0}^N \Psi_i \Psi_j \begin{bmatrix} \mathbf{A}_{II,i}^1 & 0 & \mathbf{A}_{I\Gamma,i}^1 \\ 0 & \mathbf{A}_{II,i}^2 & \mathbf{A}_{I\Gamma,i}^2 \\ \mathbf{A}_{\Gamma I,i}^1 & \mathbf{A}_{\Gamma I,i}^2 & \mathbf{A}_{\Gamma\Gamma,i}^1 + \mathbf{A}_{\Gamma\Gamma,i}^2 \end{bmatrix} \begin{Bmatrix} \mathbf{u}_{I,j}^1 \\ \mathbf{u}_{I,j}^2 \\ \mathbf{u}_{\Gamma,j} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^1 \\ \mathbf{f}_I^2 \\ \mathbf{f}_\Gamma^1 + \mathbf{f}_\Gamma^2 \end{Bmatrix}. \quad (\text{D.6})$$

Performing Galerkin projection on the space of the polynomial chaos $\{\Psi_i\}_{i=1}^N$ leads to

$$\begin{bmatrix} \mathcal{A}_{II}^1 & 0 & \mathcal{A}_{IR}^1 \\ 0 & \mathcal{A}_{II}^2 & \mathcal{A}_{IR}^2 \\ \mathcal{A}_{RI}^1 & \mathcal{A}_{RI}^2 & \mathcal{A}_{RR}^1 + \mathcal{A}_{RR}^2 \end{bmatrix} \begin{Bmatrix} \mathcal{U}_I^1 \\ \mathcal{U}_I^2 \\ \mathcal{U}_R \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_I^1 \\ \mathcal{F}_I^2 \\ \mathcal{F}_R^1 + \mathcal{F}_R^2 \end{Bmatrix}, \quad (\text{D.7})$$

where

$$[\mathcal{A}_{\alpha\beta}^s]_{jk} = \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_{\alpha\beta,i}^s \quad ; \quad \mathcal{F}_{\alpha,k}^s = \langle \Psi_k \mathbf{f}_{\alpha}^s \rangle, \quad (\text{D.8})$$

$$\mathcal{U}_I^m = (\mathbf{u}_{I,0}^m, \dots, \mathbf{u}_{I,N}^m)^T \quad ; \quad \mathcal{U}_R = (\mathbf{u}_{R,0}, \dots, \mathbf{u}_{R,N})^T.$$

The subscripts α and β can assume the index I and R . Block Gaussian elimination reduces Eq.(D.7) into the following system

$$\begin{bmatrix} \mathcal{A}_{II}^1 & 0 & \mathcal{A}_{IR}^1 \\ 0 & \mathcal{A}_{II}^2 & \mathcal{A}_{IR}^2 \\ 0 & 0 & \mathcal{S}^1 + \mathcal{S}^2 \end{bmatrix} \begin{Bmatrix} \mathcal{U}_I^1 \\ \mathcal{U}_I^2 \\ \mathcal{U}_R \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_I^1 \\ \mathcal{F}_I^2 \\ \mathcal{G}_R^1 + \mathcal{G}_R^2 \end{Bmatrix}. \quad (\text{D.9})$$

where

$$\mathcal{S}^s = \mathcal{A}_{RR}^s - \mathcal{A}_{RI}^s (\mathcal{A}_{II}^s)^{-1} \mathcal{A}_{IR}^s, \quad s = 1, 2 \quad (\text{D.10})$$

$$\mathcal{G}_R^s = \mathcal{F}_R^s - \mathcal{A}_{RI}^s (\mathcal{A}_{II}^s)^{-1} \mathcal{F}_I^s, \quad s = 1, 2 \quad (\text{D.11})$$

Eq.(D.9) can be rearranged as

$$\sum_{s=1}^2 \mathcal{S}^s \mathcal{U}_R = \sum_{s=1}^2 \mathcal{G}_R^s, \quad (\text{D.12})$$

$$\mathcal{A}_{II}^1 \mathcal{U}_I^1 = \mathcal{F}_I^1 - \mathcal{A}_{IR}^1 \mathcal{U}_R \quad (\text{D.13})$$

$$\mathcal{A}_{II}^2 \mathcal{U}_I^2 = \mathcal{F}_I^2 - \mathcal{A}_{IR}^2 \mathcal{U}_R \quad (\text{D.14})$$

Once the interface variables $\mathcal{U}_\Gamma$ obtained from Eq.(D.12), the interior variables $\mathcal{U}_I^1$ and $\mathcal{U}_I^2$ can be obtained in parallel from Eq.(D.13) and Eq.(D.14) respectively.

For the case of many subdomains, we define $\mathbf{R}_s$ as a restriction operator that maps the global interface unknown $\mathbf{u}_\Gamma$ to the local interface vector $\mathbf{u}_\Gamma^s$ as

$$\mathbf{u}_\Gamma^s = \mathbf{R}_s \mathbf{u}_\Gamma. \quad (\text{D.15})$$

In parallel implementation $\mathbf{R}_s$ acts as a *scatter* operator while $\mathbf{R}_s^T$ acts as a *gather* operator and is not constructed explicitly. Enforcing the transmission conditions (compatibility and equilibrium) along the interfaces, the global equilibrium equation of the stochastic system can be expressed in the following block linear systems of equations

$$\sum_{i=0}^L \Psi_i \begin{bmatrix} \mathbf{A}_{II,i}^1 & \cdots & 0 & \mathbf{A}_{I\Gamma,i}^1 \mathbf{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \mathbf{A}_{II,i}^{n_s} & \mathbf{A}_{I\Gamma,i}^{n_s} \mathbf{R}_{n_s} \\ \mathbf{R}_1^T \mathbf{A}_{I\Gamma,i}^1 & \cdots & \mathbf{R}_{n_s}^T \mathbf{A}_{I\Gamma,i}^{n_s} & \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{A}_{I\Gamma,i}^s \mathbf{R}_s \end{bmatrix} \begin{bmatrix} \mathbf{u}_I^1(\theta) \\ \vdots \\ \mathbf{u}_I^{n_s}(\theta) \\ \mathbf{u}_\Gamma(\theta) \end{bmatrix} = \begin{bmatrix} \mathbf{f}_I^1 \\ \vdots \\ \mathbf{f}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{f}_\Gamma^s \end{bmatrix}. \quad (\text{D.16})$$

The solution process can be expanded using the same polynomial chaos basis as

$$\begin{bmatrix} \mathbf{u}_I^1(\theta) \\ \vdots \\ \mathbf{u}_I^{n_s}(\theta) \\ \mathbf{u}_\Gamma(\theta) \end{bmatrix} = \sum_{j=0}^N \Psi_j \begin{bmatrix} \mathbf{u}_{I,j}^1 \\ \vdots \\ \mathbf{u}_{I,j}^{n_s} \\ \mathbf{u}_{\Gamma,j} \end{bmatrix}. \quad (\text{D.17})$$

Substituting Eq.(D.17) into Eq.(D.16) and performing the Galerkin projection to minimize the error over the space spanned by the chaos basis, the following coupled deterministic systems of equations is obtained

$$\begin{bmatrix} \mathcal{A}_{II}^1 & \dots & 0 & \mathcal{A}_{I\Gamma}^1 \mathcal{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathcal{A}_{II}^{n_s} & \mathcal{A}_{I\Gamma}^{n_s} \mathcal{R}_{n_s} \\ \mathcal{R}_1^T \mathcal{A}_{\Gamma I}^1 & \dots & \mathcal{R}_{n_s}^T \mathcal{A}_{\Gamma I}^{n_s} & \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{A}_{\Gamma\Gamma}^s \mathcal{R}_s \end{bmatrix} \begin{bmatrix} \mathcal{U}_I^1 \\ \vdots \\ \mathcal{U}_I^{n_s} \\ \mathcal{U}_\Gamma \end{bmatrix} = \begin{bmatrix} \mathcal{F}_I^1 \\ \vdots \\ \mathcal{F}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{F}_\Gamma^s \end{bmatrix}. \quad (\text{D.18})$$

The coefficient matrix in Eq.(D.18) is of order $n(N+1) \times n(N+1)$ where n and $(N+1)$ denote the number of the physical degrees of freedom for a typical subdomain and chaos coefficients, respectively. The stochastic counterpart of the restriction operator in Eq.(D.18) takes the following form

$$\mathcal{R}_s = \text{blockdiag}(\mathbf{R}_s^0, \dots, \mathbf{R}_s^N), \quad (\text{D.19})$$

where $(\mathbf{R}_s^0, \dots, \mathbf{R}_s^N)$ are the deterministic restriction operators given by Eq.(D.15). Block Gaussian elimination reduces the system in Eq.(D.18) to the following Schur complement system for the interface variable $\mathcal{U}_\Gamma$ as

$$\mathcal{S} \mathcal{U}_\Gamma = \mathcal{G}_\Gamma, \quad (\text{D.20})$$

where the global Schur complement matrix $\mathcal{S}$ is given by

$$\mathcal{S} = \sum_{s=1}^{n_s} \mathcal{R}_s^T [\mathcal{A}_{\Gamma\Gamma}^s - \mathcal{A}_{\Gamma I}^s (\mathcal{A}_{II}^s)^{-1} \mathcal{A}_{I\Gamma}^s] \mathcal{R}_s, \quad (\text{D.21})$$

and the corresponding right hand side vector $\mathcal{G}_\Gamma$ is

$$\mathcal{G}_\Gamma = \sum_{s=1}^{n_s} \mathcal{R}_s^T [\mathcal{F}_\Gamma^s - \mathcal{A}_{\Gamma I}^s (\mathcal{A}_{II}^s)^{-1} \mathcal{F}_I^s]. \quad (\text{D.22})$$

Once the interface unknowns $\mathcal{U}_\Gamma$ is available, the interior unknowns can be obtained concurrently by solving the interior problem on each subdomain as

$$\mathcal{A}_{II}^s \mathcal{U}_I^s = \mathcal{F}_I^s - \mathcal{A}_{\Gamma I}^s \mathcal{R}_s \mathcal{U}_\Gamma. \quad (\text{D.23})$$

Appendix E

Numerical Validation

We present numerical validations of the parallel code developed in this study in this section. Firstly, we validate the results of the KLE and domain decomposition method for SPDEs using those obtained by serial codes in Ref. [179]. Secondly, we contrast the performance of the domain decomposition method of SPDEs and MC simulation using the domain decomposition solver. Two- and three-dimensional elliptic SPDEs are considered.

Comparison of the Parallel and Serial Results

Using the parallel code of domain decomposition for SPDEs developed in this study, we reproduced the results reported in Ref. [179]. In particular, we consider a linear elliptic SPDE defined on L-shaped domain Ω with a given data on the boundary $\partial\Omega$ as

$$\begin{aligned}\nabla \cdot (\kappa(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) &= f(\mathbf{x}) \quad \mathbf{x} \in \Omega, \\ u(\mathbf{x}, \theta) &= 0 \quad \mathbf{x} \in \partial\Omega,\end{aligned}\tag{E.1}$$

where the coefficient $\kappa(\mathbf{x}, \theta)$ is modeled as a Gaussian process with an exponential covariance function defined as [179]

$$C_{\kappa\kappa}(\mathbf{x}, \mathbf{y}) = \exp \left(\frac{-4|x_1 - y_1|^2}{b} + \frac{-4|x_2 - y_2|^2}{b} \right). \tag{E.2}$$

For the numerical implementation, the correlation length is assumed to be $b = 0.5$.

Fig.(E.1) shows the monotonic decay of the eigenvalues of the exponential covariance function. Selected eigenfunctions of the covariance function are plotted in Fig.(E.2). The mean and standard deviation of the solution process are shown in Fig.(E.3). In this graphical scale, these results identically match with the corresponding results reported in Ref. [179].

Figure E.1: The decay of the eigenvalues of the covariance function

Figure E.2: Selected eigenfunctions of the covariance function

Figure E.3: The mean and standard deviation of the solution process

Comparison of PCE and MCS

Two-dimensional case:

In this section, we contrast the results obtained from the domain decomposition method of SPDEs and MC simulation using domain decomposition solver. Firstly, we consider the elliptic SPDE defined in Eq.(E.1) where the permeability coefficient $\kappa(\mathbf{x}, \theta)$ is modeled as a lognormal random variable. The Gaussian image of the random variable has a mean $\mu = 1.0$ and standard deviation $\sigma = 0.25$. Spatial discretization with linear triangular elements leads to 606,089 nodes. The decomposed computational domain is shown in Fig.(E.4).

Figure E.4: The decomposed domain

The mean response and standard deviation are plotted in Fig.(E.5). The results obtained from the domain decomposition method of SPDEs and MC simulation are identical in the scale of the graph. Latin Hypercube Sampling (LHS) [20] is used for efficient random sampling.

Figure E.5: The mean and standard deviation of the solution process

The convergence behavior of MC simulation with deterministic domain decomposition method and domain decomposition of SPDEs are shown in Fig.(E.6). The L_2 norm of the standard deviation vector is considered as the metric for convergence. The difference between the norms of the third order and fourth order PC expansions is indistinguishable in the plot meaning that PC expansion converges at the third order. The total execution time of MCS and PCE are shown in Fig.(E.7). As the order of PC expansion increases, the execution time increases almost linearly.

(a) MCS

(b) PCE

Figure E.6: The convergence of MCS and PCE

(a) MCS

(b) PCE

Figure E.7: The total execution time of MCS and PCE

Three-dimensional case:

Next, we consider a three-dimensional steady-state heat transfer problem where the thermal diffusivity coefficient $\kappa(\mathbf{x}, \theta)$ is modeled as a lognormal stochastic process obtained from

the underlying Gaussian process with an exponential covariance function. The volumetric heat source is assumed to be spatially invariant deterministic quantity $f(\mathbf{x}, \theta) = 1.0$. The mean and standard deviation of the solution process are plotted in Fig.(E.8). Once again, the MCS and PCE results match identically in the scale of the graph. Fig.(E.9) shows the convergence of the MCS and PCE. The associated total execution times are plotted in Fig.(E.10). Evidently, the PCE approach is about 10 times faster than MCS.

Figure E.8: The mean and standard deviation of the solution process

(a) MCS

(b) PCE

Figure E.9: The convergence of MCS and PCE

(a) MCS

(b) PCE

Figure E.10: The total execution time of MCS and PCE

Appendix F

Comparison among Jacobi, Block-Jacobi and Lumped Preconditioners

In this section, we compare the performance of the PCGM equipped with Jacobi, Block-Jacobi and Lumped preconditioners to tackle the extended Schur complement system. In particular, we tackle the extended Schur complement system defined as

$$\mathcal{M}^{-1}S \mathcal{U}_r = \mathcal{M}^{-1}\mathcal{G}_r, \tag{F.1}$$

where $\mathcal{M}^{-1}$ is the preconditioning matrix. For Jacobi, Block-Jacobi and Lumped preconditioners $\mathcal{M}^{-1}$ is defined respectively as

$$\mathcal{M}_J^{-1} = \text{diag}(\mathcal{S}^{-1}), \quad (\text{F.2})$$

$$\mathcal{M}_{BJ}^{-1} = \text{blockdiag}(\mathcal{S}_0^{-1}, \dots, \mathcal{S}_0^{-1}), \quad (\text{F.3})$$

$$\mathcal{M}_L^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T [\mathcal{A}_{rr}^s]^{-1} \mathcal{R}_s, \quad (\text{F.4})$$

where $\mathcal{S}_0$ is the deterministic Schur complement matrix corresponding to the mean material properties.

For the numerical experiment, we again consider a two-dimensional steady-state flow through random media (with stochastic permeability coefficient) defined as

$$\nabla \cdot (\kappa(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) = f(\mathbf{x}, \theta), \quad \mathbf{x} \in \Omega \quad (\text{F.5})$$

$$u(\mathbf{x}, \theta) = 0, \quad \mathbf{x} \in \partial\Omega, \quad (\text{F.6})$$

For simplicity, we represent the coefficient $\kappa(\mathbf{x}, \theta)$ as a longnormal random variable. Its polynomial chaos representation is given by [96, 145]

$$\kappa(\theta) = \mu_\kappa \sum_{i=0}^L \frac{\sigma_g^i}{i!} \Psi_i,$$

where

$$\mu_\kappa = \exp \left(\mu_g + \frac{1}{2} \sigma_g^2 \right),$$

where μ_g and σ_g are the mean and standard deviation of the underlying Gaussian random variable, respectively (see Appendix B).

The mean and standard deviation of the solution process for $\mu_g = 0.0$ and $\sigma_g = 0.25$ are shown in Fig.(F.1).

(a) Mean

(b) Standard deviation

Figure F.1: The mean and standard deviation of the solution process

In Fig.(F.2), we show the performance of the Jacobi, Block-Jacobi and Lumped preconditioners for a fixed value of the CoV while increasing the order of PCE. For two sub-domains, the iteration counts for both the Jacobi and Block-Jacobi preconditioners grow linearly as the order of PCE increases. For the lumped preconditioner, the iteration counts remain constant as we increase the order of PCE.

Figure F.2: Iteration counts for fixed CoV while increasing the order of
PCE

The performances of the Jacobi, Block-Jacobi and Lumped preconditioners for a fixed order of PCE while increasing the value of the CoV of the permeability coefficient are shown in Fig.(F.3). Clearly, increasing the level of uncertainty of the input parameter does not affect the performance of the Block-Jacobi and Lumped preconditioners. Although Block-Jacobi requires less number of iterations than the Lumped preconditioner, the explicit construction of Block-Jacobi preconditioner is computationally intensive.

Figure F.3: Iteration counts for fixed order of PCE while increasing the value of the CoV

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