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LDRD Final Report: Capabilities for Uncertainty in Predictive Science

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Abstract

Predictive simulation of systems comprised of numerous interconnected, tightly coupled components promises to help solve many problems of scientific and national interest. However predictive simulation of such systems is extremely challenging due to the coupling of a diverse set of physical and biological length and time scales. This report investigates uncertainty quantification methods for such systems that attempt to exploit their structure to gain computational efficiency. The traditional layering of uncertainty quantification around nonlinear solution processes is inverted to allow for heterogeneous uncertainty quantification methods to be applied to each component in a coupled system. Moreover this approach allows stochastic dimension reduction techniques to be applied at each coupling interface. The mathematical feasibility of these ideas is investigated in this report, and mathematical formulations for the resulting stochastically coupled nonlinear systems are developed.

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Chapter 1

Introduction

This report encapsulates the results of an FY08 late-start LDRD investigating mathematical and computational methods for predictive simulation of coupled systems. Predictive simulation of systems comprised of numerous interconnected, tightly coupled components promises to help solve many problems of scientific and national interest. Examples include design and licensing of current and future nuclear energy reactors, development of renewable energy technologies, vulnerability analysis of water and power supplies, and understanding of complex biological networks. Often these systems strongly couple many different physical or biological processes exhibiting phenomena at a diverse set of length and/or time scales. Therefore simulating the entire coupled system at the level of fidelity to capture this phenomena is extremely difficult for many systems of interest. Moreover, *predictive simulation* of these systems requires significantly more computational effort than single-point high-fidelity simulations; rather simulation code verification, model validation, and uncertainty quantification (UQ) are indispensable processes required to justify a predictive capability in a mathematically and scientifically rigorous manner. However implementing these processes is very computationally challenging, making rigorous predictive simulation of many coupled systems extremely difficult.

While these problems are clearly very challenging, they also present tremendous opportunities for the development of new predictive simulation methods optimized for these types of systems. In this report we investigate uncertainty quantification methods for coupled systems that try to take advantage of the inherent structure in these systems with the goal of making the overall uncertainty computation more efficient. In particular, we show that it is feasible to apply well-known uncertainty quantification methods to each component in a coupled system independently to take advantage of UQ methods that may be optimized for those components. This approach inverts the traditional layering of a UQ method on top of a deterministic nonlinear solution method, and can be thought of as an intrusive UQ method for coupled systems (where the UQ method applied to each component may be intrusive or non-intrusive). In addition to allowing for specialized and heterogeneous UQ methods, it also allows stochastic dimension reduction techniques to be applied at the interface between each coupled component. Since, for most UQ methods, the cost of the uncertainty calculation grows exponentially with this dimension, this technique can drastically reduce the overall cost. The difficulty with this approach is that it translates what was a deterministic coupled system into what is now a stochastically coupled system, requiring extension of traditional deterministic coupled system nonlinear solution processes to the stochastic case.

The organization of this report is as follows. In the following section, three types of coupled systems that are commonly studied are discussed and mathematical representations are formulated. Then in Chapter 2, and overview of deterministic nonlinear coupling methods is provided, followed by a review of popular uncertainty quantification methods for single component applications in Chapter 3. Chapter 4 contains the main technical contribution of this report and describes several approaches for applying the UQ methods discussed in Chapter 3 on a component by component basis in a coupled system, using the nonlinear solution methods presented in Chapter 2 to solve the resulting stochastically-coupled nonlinear system. In this chapter we also discuss approaches for reducing the cost of the overall uncertainty calculation through stochastic dimension reduction at the coupling interfaces. Finally in Chapter 5 we summarize the conclusions of this work and provide recommendations for future efforts in exploiting this work to impact real-world coupled systems in science applications.

1.1 Mathematical Models of Coupled Systems

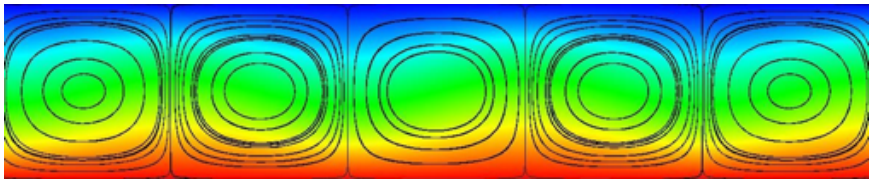
The work presented in this report is limited to three broad categories of coupled systems that are widely studied through the scientific community: multi-physics systems, interfacially coupled systems, and network systems. Moreover our work is limited to either steady-state problems or transient problems where a suitable implicit time discretization method has been chosen. In the latter case, the methods discussed here are then applicable to the implicit nonlinear equations for each time step. We realize the interplay between time discretization, nonlinear solution, and uncertainty quantification is very important and can be quite delicate in practice. However rigorous examination of this interplay was well beyond the scope of the LDRD and this report. We now discuss each of the three types of coupled systems studied in more detail.

The first class of coupled systems studied is multi-physics systems, which are systems consisting of multiple interacting physics in a single computational domain. A well-known example is coupled flow and heat transfer in a fluid body (see Figure 1.1(a)). Here the components of one physical process (fluid flow) interact with the components of another (heat transfer) at all points in the physical domain. Such systems are often modeled by a set of coupled, possibly nonlinear, partial differential equations over a given domain. After discretization in space, a generic two-component multi-physics system can be represented by the following coupled nonlinear equations:

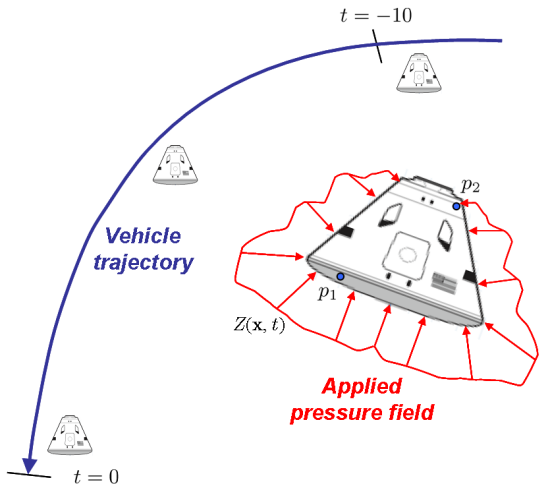
$$\begin{aligned} f_1(u_1, u_2) &= 0, \\ f_2(u_1, u_2) &= 0. \end{aligned} \tag{1.1}$$

Here $u_1 \in \mathbb{R}^{n_1}$ and $u_2 \in \mathbb{R}^{n_2}$ represent the discretized solution variables for each physical system, and $f_1 : \mathbb{R}^{n_1+n_2} \to \mathbb{R}^{n_1}$ and $f_2 : \mathbb{R}^{n_1+n_2} \to \mathbb{R}^{n_2}$ represent the corresponding discretized residuals.

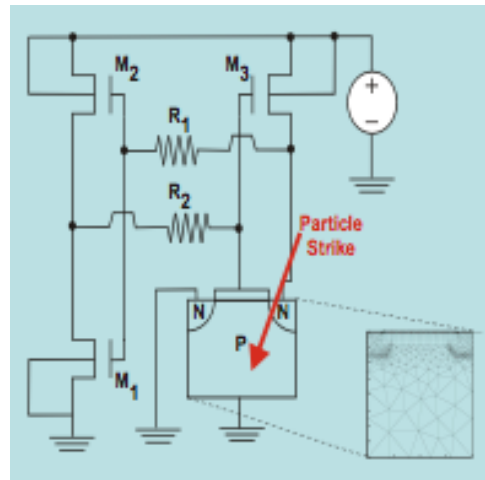
A second, more restricted type of coupling, is interfacial coupling. Here we have two



(a) Multi-physics coupling



(b) Interfacial coupling



(c) Network coupling

Figure 1.1. Three types of coupled systems. (a) Multi-physics coupling of two-dimensional fluid flow (black streamlines) and temperature (color gradient). (b) Interfacial coupling between turbulent air flow and structural dynamics through the shell of the vehicle (reprinted with permission from [31]). (c) Network coupling of a high-fidelity electrical circuit device model to a low fidelity network, simulating radiation damage to the electrical circuit.

or more physical domains each containing separate physical processes, joined by a common interface. The physical processes are independent in each domain apart from the interaction at the interface. A relevant example within Sandia is the modeling of a reentry vehicle as it travels through the atmosphere (see Figure 1.1(b)). The flight of the vehicle through the atmosphere creates a pressure load on the shell of the vehicle which in turn affects the structural dynamics of the interior of the vehicle. Here the two domains are the fluid exterior to the vehicle (compressible, turbulent fluid flow) and the interior of the vehicle (structural dynamics) coupled through the shell of the vehicle (interface). The physics in each domain is typically modeled as a set of partial differential equations that are coupled through boundary conditions. After spatial discretization, a generic two-component interfacially coupled system

can be represented as

$$\begin{aligned} f_1(u_1, g_2(u_2)) &= 0, \\ f_2(g_1(u_1), u_2) &= 0. \end{aligned} \tag{1.2}$$

Here $g_1 : \mathbb{R}^{n_1} \to \mathbb{R}^{m_1}$ and $g_2 : \mathbb{R}^{n_2} \to \mathbb{R}^{m_2}$ represent the interfaces between systems 1 and 2 and typically map their argument to a much lower dimensional space, i.e., $m_1 \ll n_1$ and $m_2 \ll n_2$. In this case the discrete residuals $f_1 : \mathbb{R}^{n_1+m_2} \to \mathbb{R}^{n_1}$ and $f_2 : \mathbb{R}^{m_1+n_2} \to \mathbb{R}^{n_2}$ only depend on the other solution variables through the interfaces g_1 and g_2.

The third type of coupling considered is that of network systems. Here, a possibly large number of separate domains are coupled together through a series of low-fidelity interactions. A well studied example is an electronic circuit (see Figure 1.1(c)) where many electrical components are coupled together through a series of electrical connections. The electrical properties of each device evolve according to their physics, and the voltages and currents at their connections. These connections in turn are assumed to satisfy some low-fidelity relationship, such as Kirchhoff's laws. The fidelity of the components in a network system often vary, from high-fidelity single and multi-physics models to low fidelity compact models. Thus the overall mathematical structure of such systems can take many forms, but have the unifying feature that the network model must be discrete in space, i.e., either a system of ordinary or differential-algebraic equations (for time-dependent problems) or a system of algebraic equations (for steady problems). The models for each system component could be a single or multi-physics system of partial differential equations or a set of algebraic/ordinary-differential/differential-algebraic equations. To mathematically represent such a system, consider the simple network schematic described by Figure 1.2, consisting of three vertices (or nodes) connected by two components. A set of scalar unknowns x_1, x_2

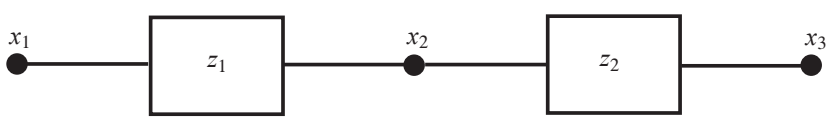


Figure 1.2. A simple two component network example.

and x_3 is associated with each vertex. In an electrical circuit, these would represent voltages. Assume each device connecting vertices 1 to 2 and 2 to 3 has a scalar output z_1 and z_2 respectively, that is a function of the unknowns associated with each vertex connected to the device. In a circuit, these outputs correspond to the current through the device as determined by the voltages. Moreover assume these outputs are determined by solving an auxiliary set of implicit algebraic equations, i.e.,

$$\begin{aligned} z_1 &= g_1(u_1, x_1, x_2) \ \text{ s.t. } \ f_1(u_1, x_1, x_2) = 0, \\ z_2 &= g_2(u_2, x_2, x_3) \ \text{ s.t. } \ f_2(u_2, x_2, x_3) = 0. \end{aligned} \tag{1.3}$$

These equations could, for example, represent high-fidelity PDE models of electrical devices which determine electrical currents as a function of supplied voltage boundary conditions.

Finally, the unknown nodal values $x = (x_1, x_2, x_3)$ are determined by solving an implicit set of nonlinear equations $F(z, x) = 0$ for x, where $z = (z_1, z_2)$. The complete specification of the network nonlinear problem is then

$$\begin{aligned} z_1 &= g_1(u_1, x_1, x_2) \;\text{ s.t. }\; f_1(u_1, x_1, x_2) = 0, \\ z_2 &= g_2(u_2, x_2, x_3) \;\text{ s.t. }\; f_2(u_2, x_2, x_3) = 0, \\ 0 &= F(z, x). \end{aligned} \tag{1.4}$$

Often in computational settings, all three types of coupled systems may occur in a given system simulation. Therefore it is important to leverage nonlinear solution algorithms that are optimized for each type of coupled system and strength of coupling. An overview of available approaches is provided in the next chapter.

Chapter 2

Solution Strategies for Nonlinear Coupled Systems

When discussing solution strategies for the types of coupled systems presented in the previous chapter, one must distinguish between coupled physics and coupled simulation codes. In principle, any single simulation code can be written to simulate any of these types of coupled systems. Typically in this case, a fully coupled Newton method (possibly with a globalization strategy) is employed to approximate the solution to the coupled nonlinear equations. An equally important case is when multiple simulation codes are coupled in some fashion to simulate a coupled system, where each simulation code separately approximates the solution to one or more sets of physics in the coupled system. The advantage of this approach is it leverages existing simulation code technology when transitioning to coupled systems. This advantage is non-trivial given that in many cases domain-specific knowledge is built into simulation codes for specialized physics that may be difficult or impossible to generalize when incorporating new physics. The difficulty with this approach is that it can be difficult to extract the relevant derivative information in order to implement robust and efficient simulation strategies. For that reason, numerous nonlinear solution strategies that try to obtain Newton-like efficiency and robustness while minimizing the amount of derivative information necessary have been studied [50]. In this chapter we provide a brief overview of some of these methods that are more strongly suited to the types of coupled systems discussed previously in order to provide a setting to generalize them for uncertainty quantification in Chapter 4.

2.1 Forward Coupling

A significant simplification occurs for all three types of coupled systems when the system is only forwardly coupled, i.e., the two-component multi-physics system (1.1) becomes

$$\begin{aligned} f_1(u_1) &= 0, \\ f_2(u_1, u_2) &= 0, \end{aligned} \tag{2.1}$$

while the two-component interfacially coupled system (1.2) becomes

$$\begin{aligned} f_1(u_1) &= 0, \\ f_2(g_1(u_1), u_2) &= 0, \end{aligned} \tag{2.2}$$

and finally the two-component network coupled system (1.4) becomes

$$\begin{aligned} z_1 &= g_1(u_1, x_1) \;\text{ s.t. }\; f_1(u_1, x_1) = 0, \\ z_2 &= g_2(u_2, x_2, x_3) \;\text{ s.t. }\; f_2(u_2, x_2, x_3) = 0, \\ 0 &= F(z, x). \end{aligned} \tag{2.3}$$

In all three cases, the solution to the first system u_1 can be solved for independently and substituted into the remaining equations. This allows any nonlinear solver method to be separately applied to the first and remaining systems with no solver communication between them. Of course, this setting is clearly not generic, but forms the basis of the Picard method when treating the fully coupled system.

2.2 Picard Iteration

Picard iteration, also known as successive substitution, is a simple numerical method for approximating the solution to a fully coupled system (1.1), (1.2) or (1.4). It works by solving each component in the coupled system for its solution variables, treating the other variables as fixed quantities. This is repeated in a round-robin fashion until some measure of convergence is achieved (typically the size of the change of the solution variables from iteration to iteration, and/or the size of the residual of each component evaluated at the most current solution values). For example, an algorithm for applying this technique to the two-component interfacially coupled system (1.2) is displayed in Algorithm 1. As with

Algorithm 1 Picard iteration for the two-component interfacially coupled system(1.2).

Require: Initial guesses $u_1^{(0)}$ and $u_2^{(0)}$ for u_1 and u_2:
  k = 0
  while not converged **do**
    k = k+1
    Solve $f_1(u_1^{(k)}, g_2(u_2^{(k-1)})) = 0$ for $u_1^{(k)}$
    Solve $f_2(g_1(u_1^{(k)}), u_2^{(k)}) = 0$ for $u_2^{(k)}$
  end while

forward coupling, any solver method can be used for each of the solves above. The problem with this approach is that convergence is slow (linear), and needs additional requirements on f_1 and f_2 to converge [50].

2.3 Newton's Method

Due to the slow convergence and lack of robustness of Picard iteration, Newton's method is often preferred for simulating coupled systems. However its implementation is significantly

more complicated in that at each iteration, it requires solving the following Newton systems:

$$\begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{bmatrix} \begin{bmatrix} \Delta u_1^{(k)} \\ \Delta u_2^{(k)} \end{bmatrix} = - \begin{bmatrix} f_1(u_1^{(k-1)}, u_2^{(k-1)}) \\ f_2(u_1^{(k-1)}, u_2^{(k-1)}) \end{bmatrix} \tag{2.4}$$

for multi-physics coupling,

$$\begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial g_2}\frac{\partial g_2}{\partial u_2} \\ \frac{\partial f_2}{\partial g_1}\frac{\partial g_1}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{bmatrix} \begin{bmatrix} \Delta u_1^{(k)} \\ \Delta u_2^{(k)} \end{bmatrix} = - \begin{bmatrix} f_1(u_1^{(k-1)}, g_2(u_2^{(k-1)})) \\ f_2(g_1(u_1^{(k-1)}), u_2^{(k-1)}) \end{bmatrix} \tag{2.5}$$

for interfacial coupling, and

$$\begin{bmatrix} \frac{\partial f_1}{\partial u_1} & 0 & \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & 0 \\ 0 & \frac{\partial f_2}{\partial u_2} & 0 & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial F}{\partial z_1}\frac{\partial g_1}{\partial u_1} & \frac{\partial F}{\partial z_2}\frac{\partial g_2}{\partial u_2} & \frac{\partial F}{\partial z_1}\frac{\partial g_1}{\partial x_1} + \frac{\partial F}{\partial x_1} & \frac{\partial F}{\partial z_1}\frac{\partial g_1}{\partial x_2} + \frac{\partial F}{\partial z_2}\frac{\partial g_2}{\partial x_2} + \frac{\partial F}{\partial x_2} & \frac{\partial F}{\partial z_2}\frac{\partial g_2}{\partial x_3} + \frac{\partial F}{\partial x_3} \end{bmatrix} \begin{bmatrix} \Delta u_1^{(k)} \\ \Delta u_2^{(k)} \\ \Delta x_1^{(k)} \\ \Delta x_2^{(k)} \\ \Delta x_3^{(k)} \end{bmatrix} = - \begin{bmatrix} f_1(u_1^{(k-1)}, x_1^{(k-1)}, x_2^{(k-1)}) \\ f_2(u_2^{(k-1)}, x_2^{(k-1)}, x_3^{(k-1)}) \\ F(z^{(k-1)}, x^{(k-1)}) \end{bmatrix} \tag{2.6}$$

for network coupling, where $u_1^{(k)} = u_1^{(k-1)} + \Delta u_1^{(k)}$, and so on. Numerous methods are available for estimating the cross-physics derivatives appearing in these systems [50].

2.4 Nonlinear Elimination

The disadvantage of the full Newton approach is it requires forming and solving the fully-coupled Newton systems (2.4), (2.5), and (2.6), making it very difficult to use nonlinear solvers, linear solvers, and preconditioners that are specialized to each system component. An alternative approach that maintains the quadratic convergence of Newton's method, but allows for greater flexibility in the choice of solver for each system component is nonlinear elimination. This approach works by eliminating solution variables from each system component, relying on the Implicit Function Theorem. For example, the equation $f_1(u_1, g_2(u_2)) = 0$ for an interfacially coupled system can thought of as an implicit equation defining u_1 as a function of u_2, which can be numerically evaluated using any appropriate nonlinear solver method. We then apply a nonlinear solver method to the reduced system

$$f_2(g_1(u_1(u_2)), u_2) = 0. \tag{2.7}$$

Applying Newton's method to this system requires computation of the sensitivity $\partial u_1/\partial u_2$, which by the Implicit Function Theorem is

$$\frac{\partial u_1}{\partial u_2} = - \left(\frac{\partial f_1}{\partial u_1}\right)^{-1} \frac{\partial f_1}{\partial g_2}\frac{\partial g_2}{\partial u_2}. \tag{2.8}$$

Note this linear system involves the same matrix as Newton's method applied to the system $f_1(u_1, g_2(u_2)) = 0$ with u_2 held fixed, with m_2 right-hand-sides. Clearly this approach is only effective when m_2 is reasonably small, and therefore is typically not appropriate for shared-domain multi-physics problems such as (1.1). The Newton system required for Newton's method applied to the reduced system (2.7) is

$$\left(\frac{\partial f_2}{\partial g_1}\frac{\partial g_1}{\partial u_1}\frac{\partial u_1}{\partial u_2} + \frac{\partial f_2}{\partial u_2}\right)\Delta u_2^{(k)} = -f_2(g_1(u_1^{(k)}), u_2^{(k-1)}). \tag{2.9}$$

The complete algorithm for a Newton-based nonlinear elimination method for interfacial coupling is displayed in Algorithm 2.

Algorithm 2 Newton-based nonlinear elimination for two-component interfacial coupling.

Require: Initial guesses $u_1^{(0)}$ and $u_2^{(0)}$ for u_1 and u_2
  k = 0
  while not converged **do**
    k = k+1
    Solve $f_1(u_1^{(k)}, g_2(u_2^{(k-1)})) = 0$ for $u_1^{(k)}$
    Compute $\frac{\partial u_1^{(k)}}{\partial u_2^{(k-1)}} = -\frac{\partial f_1}{\partial u_1}^{-1}\frac{\partial f_1}{\partial g_2}\frac{\partial g_2}{\partial u_2^{(k-1)}}$
    Solve $\left(\frac{\partial f_2}{\partial g_1}\frac{\partial g_1}{\partial u_1^{(k)}}\frac{\partial u_1^{(k)}}{\partial u_2^{(k-1)}} + \frac{\partial f_2}{\partial u_2^{(k-1)}}\right)\Delta u_2^{(k)} = -f_2(g_1(u_1^{(k)}), u_2^{(k-1)})$
    $u_2^{(k)} = u_2^{(k-1)} + \Delta u_2^{(k)}$
  end while

Nonlinear elimination is also effective for network problems such as (1.4). In this case however, both u_1 and u_2 are eliminated, leaving just the network solve $F(z, x) = 0$. More precisely, the equations $f_1(u_1, x_1, x_2) = 0$ and $f_2(u_2, x_2, x_3) = 0$ implicitly define u_1 and u_2 as functions of x_1, x_2 and x_2, x_3 respectively. Through the relations $z_1 = g_1(u_1, x_1, x_2)$ and $z_2 = g_2(u_2, x_2, x_3)$, z_1 and z_2 are then implicit functions of x with derivatives

$$\begin{aligned}
\frac{\partial z_1}{\partial x_1} &= -\frac{\partial g_1}{\partial u_1}\left(\frac{\partial f_1}{\partial u_1}\right)^{-1}\frac{\partial f_1}{\partial x_1} + \frac{\partial g_1}{\partial x_1},\\
\frac{\partial z_1}{\partial x_2} &= -\frac{\partial g_1}{\partial u_1}\left(\frac{\partial f_1}{\partial u_1}\right)^{-1}\frac{\partial f_1}{\partial x_2} + \frac{\partial g_1}{\partial x_2},\\
\frac{\partial z_2}{\partial x_2} &= -\frac{\partial g_2}{\partial u_2}\left(\frac{\partial f_2}{\partial u_2}\right)^{-1}\frac{\partial f_2}{\partial x_2} + \frac{\partial g_2}{\partial x_2},\\
\frac{\partial z_2}{\partial x_3} &= -\frac{\partial g_2}{\partial u_2}\left(\frac{\partial f_2}{\partial u_2}\right)^{-1}\frac{\partial f_2}{\partial x_3} + \frac{\partial g_2}{\partial x_3}.
\end{aligned} \tag{2.10}$$

Newton's method applied to the network equation $F(z, x) = 0$ then yields the linear system

$$\left(\frac{\partial F}{\partial z}\frac{\partial z}{\partial x} + \frac{\partial F}{\partial x}\right)\Delta x^{(k)} = -F(y^{(k-1)}, x^{(k-1)}). \tag{2.11}$$

Algorithm 3 Newton-based nonlinear elimination for two-component network coupling.

Require: Initial guesses $u_1^{(0)}$, $u_2^{(0)}$, and $x^{(0)}$ for u_1, u_2, and x.
  k = 0
  while not converged **do**
    k = k+1
    Solve $f_1(u_1^{(k)}, x_1^{(k-1)}, x_2^{(k-1)}) = 0$ for $u_1^{(k)}$
    Solve $f_2(u_2^{(k)}, x_2^{(k-1)}, x_3^{(k-1)}) = 0$ for $u_2^{(k)}$
    Evaluate $z_1^{(k)} = g_1(u_1^{(k)}, x_1^{(k-1)}, x_2^{(k-1)})$
    Evaluate $z_2^{(k)} = g_2(u_2^{(k)}, x_2^{(k-1)}, x_3^{(k-1)})$
    Compute $\partial z^{(k)}/\partial x^{(k-1)}$ via (2.10)
    Solve $\left(\frac{\partial F}{\partial z^{(k)}}\frac{\partial z^{(k)}}{\partial x^{(k-1)}} + \frac{\partial F}{\partial x^{(k-1)}}\right)\Delta x^{(k)} = -F(z^{(k)}, x^{(k-1)})$
    $x^{(k)} = x^{(k-1)} + \Delta x^{(k)}$
  end while

The complete algorithm for a Newton-based nonlinear elimination method for network coupling is displayed in Algorithm 3.

The three nonlinear solution methods discussed here provide the necessary algorithmic foundation for simulation of nonlinear coupled systems from a nonlinear solver perspective. We now turn to a discussion of popular uncertainty quantification methods for propagating uncertainties through individual components in a coupled system.

Chapter 3

Uncertainty Representation and Propagation Methods

Most applications in engineering and science are affected by uncertainty in the input data [5, 6]. For example, highly heterogeneous materials may have properties that vary over small length scales so that these properties have to be often determined from measurements at a few locations. These types of uncertainties are known as epistemic since they are related to incomplete knowledge. In other situations, uncertainty can be due to an intrinsic variability in the system as, for instance, in turbulent fluctuations of a flow field around an airplane wing. When sufficient data does exist, probability distributions can be utilized to fully characterize these uncertainties in a statistical manner, and are referred to as being aleatory. In practice, it is necessary to address both types of uncertainties. Discussions about sources of uncertainties are given, in a general setting, in [22] and for some applications to solid mechanics, in [16, 28, 29, 67, 68].

Because it is essential for dealing with realistic experimental data and assessing the reliability of predictions based on numerical simulations, the development of UQ methodologies is a very active area of research. There are, in fact, several approaches being followed for quantifying uncertainties: *worst-case-scenario* (or anti-optimization) methods [13, 49] that are useful in cases where one knows only a little information about the uncertainty in the input data, *probabilistic* methods that characterize uncertainties using stochastic differential equations [2, 3, 9, 10, 17, 18, 34, 40–42, 54, 55, 57, 58, 62–66, 75–83, 89, 99, 100, 102, 104], and *knowledge-based* methods that characterize uncertainties using fuzzy sets [19, 27], evidence theory (Dempster-Shafer theory) [30, 56, 73], subjective probability [48, 90], Bayesian inference [14, 15, 20, 59, 93, 103], and other means of including expert opinions. All three approaches can be applied directly or indirectly to partial differential equations (PDEs) with uncertain input data. Despite the large effort these citations represent, it is widely recognized that new, more effective methods for treating uncertainty are still needed and will become increasingly important in virtually all branches of engineering and science [7, 74].

A crucial, yet often complicated, ingredient that all approaches to UQ must incorporate is a proper description of the uncertainty in the system parameters and the external environment. All such uncertainties can be included in mathematical models adopting the probabilistic approach, provided enough information is available for an accurate statistical characterization of the data. Moreover, the mathematical model may depend on a set of

distinct uncertain parameters, which may be represented as random variables with a given joint probability distribution. In other situations, the input data may vary randomly from one point of the physical domain to another and from one time instant to another. In these cases, the uncertainty in the inputs should rather be described in terms of random fields. Approaches to describe *correlated* random fields consist of the Karhunen-Loève expansion (KL) [61] (or Fourier-Karhunen-Loève expansion [60]), or expansions in terms of global orthogonal polynomials [41, 95, 101]. Both expansions represent the field via an infinite number of random variables, and exist provided that the random field has a bounded second moment. Other nonlinear expansions [44] and transformations [66, 96] have been considered. While these expansions are infinite, often realizations slowly vary in space and time, and thus only a few terms are typically needed to accurately approximate the random field [8, 33]. In the following section, more detail is provided on the representation of random fields, and in particular on the Karhunen-Loève expansion which will be useful in Chapter 4 for dimension reduction between coupled components. For a more thorough treatment of random fields and their representations, see [31].

3.1 Representation of Random Fields

Let d be a positive integer, $D \subset \mathbb{R}^d$ be compact, and $(\Omega, \mathcal{B}, \mu)$ be a complete probability space. For any $x \in D$ let $u_x : \Omega \to \mathbb{R}^m$ be an m-valued random vector. If $d = 1$, the collection $\{u_x : x \in D\}$ is called a stochastic process, and if $d > 1$ it is referred to as a random field. For given $x \in D$ and $\omega \in \Omega$, we will equivalently use the notation $u_x(\omega) = u(x, \omega)$. Assume for each $x \in D$ that $u_x \in L^2_\mu(\Omega)$. Define the expectation operator

$$Eu_x = \int_\Omega u_x d\mu \tag{3.1}$$

and the covariance operator

$$\mathrm{cov}_u(x, x') = E\left((u_x - Eu_x)(u_{x'} - Eu_{x'})^T\right). \tag{3.2}$$

Treated as a linear operator on $\mathbb{R}^m$, the covariance operator is clearly symmetric. Moreover, if we assume it is bounded in the sense

$$\int_D \int_D ||\mathrm{cov}_u(x, x')||_F^2 dx dx' < \infty \tag{3.3}$$

(e.g., if it is jointly continuous in x and x') where $||\cdot||_F$ denotes the Frobenius norm, then it has an infinite set of decreasing, non-negative eigenvalues λ_k and eigenfunctions $b_k(x)$ which satisfy

$$\int_D \mathrm{cov}_u(x, x') b_k(x') dx' = \lambda_k b_k(x), \quad k = 1, \ldots, \infty. \tag{3.4}$$

The eigenfunctions are orthonormal in that

$$\int_D b_i^T(x) b_j(x) dx = \delta_{ij}, \quad i, j = 1, \ldots, \infty. \tag{3.5}$$

Moreover u_x admits the representation

$$u_x(\omega) = Eu_x + \sum_{k=0}^{\infty} \sqrt{\lambda_k} b_k(x) \xi_k(\omega) \tag{3.6}$$

where each $\xi_k : \Omega \to \mathbb{R}$ is a random variable satisfying

$$\eta_k(\omega) = \frac{1}{\sqrt{\lambda_k}} \int_D b_k^T(x)(u(x,\omega) - Eu_x)dx. \tag{3.7}$$

Equation (3.6) is called the Karhunen-Loève expansion [61] of the random field u. The random variables $\{\xi_k\}$ have zero mean and unit covariance, i.e., $E(\xi_i \xi_j) = \delta_{ij}$ for $i, j = 1, \ldots, \infty$. By truncating Equation (3.6) at some finite number of terms N, a finite dimensional approximation of the random field u is obtained.

3.2 An Overview of Numerical Uncertainty Quantification Methods

We now provide a brief overview of several popular numerical uncertainty quantification methods for estimating uncertainties in simulation code outputs. Monte Carlo methods (see, e.g., [32]) are the most popular approaches for approximating expected values and other statistical moments of quantities of interest based on the solution of stochastic problems. They are based on independent realizations of the input random variables ξ; approximations of the expectation or other quantities of interest are obtained by a simply averaging over the corresponding realizations of that quantity. Thus, the method requires a deterministic simulation for each realization. The resulting numerical error is proportional to $1/\sqrt{M}$, where M is the number of realizations, thus requiring a very large number of samples to achieve small errors. In particular cases, convergence can be improved [52, 72, 86]. Other ensemble-based methods such as quasi-Monte Carlo, Latin hypercube sampling, lattice rules and orthogonal arrays (e.g., see [47, 69] and the references therein), have been devised to produce "faster" convergence rates, e.g., proportional to $(\log(M)^{r(N)}/M)$, where $r(N) > 0$ grows with the number N of random variables.

Recently, other approaches have been proposed that often feature much faster convergence rates. These include stochastic Galerkin methods [9, 10, 23, 24, 33, 40, 41, 57, 66, 76, 99], stochastic collocation methods [11, 65, 70, 71, 84, 98], and perturbation, Neumann and Taylor expansion methods [4, 36, 53, 55, 62, 85, 96, 97]. These approaches transform the original stochastic problem into a deterministic one with a large number of parameters and differ in the choice of the approximating spaces. We refer to these as stochastic Galerkin methods by generalizing the traditional definition in Section 3.3 to include most, if not all, of these methods. For more details please refer to the recent work [45, 46]. They employ standard approximations in physical space, e.g., a finite element method, and polynomial approximation in the probability domain, either by full polynomial spaces [39, 66, 99], tensor product polynomial spaces [9, 33, 76], or piecewise polynomial spaces [9, 57]. The efforts

[40, 41] use a formal Wiener chaos, or polynomial chaos, expansion in terms of Hermite polynomials. A similar approach using general orthogonal polynomials is described by [99]. Generally, these techniques are intrusive in the sense that they are non-ensemble-based methods, requiring the solution of discrete systems that couple all spatial and probabilistic degrees of freedom. Recently, non-intrusive polynomial chaos methods [1, 21, 51] have been developed that, through the use of quadrature rules, decouple the stochastic and spatial degrees of freedom.

More recently, stochastic collocation methods that are based on either full or sparse tensor product approximation spaces [11, 12, 35, 65, 70, 71, 94, 98] have gained considerable attention. As shown in [11], stochastic collocation methods can essentially match the fast convergence of intrusive polynomial chaos methods, even coinciding with them in particular cases. The major difference between them is that stochastic collocation methods are ensemble-based, non-intrusive approaches that achieve fast convergence rates by exploiting the inherent regularity of PDE and ODE solutions with respect to parameters [87, 88]. Compared to non-intrusive polynomial chaos methods, they also require fewer assumption on the underlying stochastic problem. Finally, they can also viewed as a stochastic Galerkin method (see the next section) in which one uses Lagrange interpolatory polynomials built from the zeros of orthogonal polynomials with respect to the joint PDF of the input random variables. For more details about the relations between these methods see [45].

3.3 The Stochastic Galerkin UQ Framework

Many of the numerical methods discussed above can be developed within a single stochastic Galerkin framework. This framework translates the underlying stochastic problem to a deterministic-parametric problem over a finite-dimensional parameter space. This translation forms the basis for the coupled-system uncertainty quantification approach discussed in the next chapter. We now summarize the stochastic Galerkin framework, showing how the Monte Carlo, stochastic collocation, and polynomial chaos methods derive from it based on the choice of approximating basis over the parameter space. We assume the physical system of interest is finite dimensional (e.g., system of ordinary differential equations), or has been discretized in space to yield a finite dimensional approximation. Consistent with the assumption throughout this report, we assume the system is steady, or a suitable implicit time discretization scheme has already been applied, and therefore the system is represented by a finite-dimensional system of algebraic equations (for either the steady-state approximation or a time-step in a temporal discretization)

$$f(u) = 0, \quad f : \mathbb{R}^n \to \mathbb{R}^n. \tag{3.8}$$

We assume the physical system represented by (3.8) is subject to a finite set of random parameters $\xi = (\xi_1, \ldots, \xi_N) : \Omega \to \mathbb{R}^N$ defined on a probability space $(\Omega, \mathcal{B}, \mu)$, either because the problem itself can be described by a finite number of random variables or because the input coefficients are modeled as truncated random fields. We wish to approximate a random

function $u : \Omega \to \mathbb{R}^n$ such that the following equation is satisfied μ-almost everywhere:

$$f(u(\xi), \xi) = 0. \tag{3.9}$$

Denote by $\Gamma = \xi(\Omega)$ the image of ξ in $\mathbb{R}^N$ and assume the components $\xi = (\xi_1, \ldots, \xi_N)$ have a joint probability density function (PDF) $\rho : \Gamma \to \mathbb{R}_+$ with $\rho \in L^\infty(\Gamma)$. We assume each component of u belongs to $L^2_\rho(\Gamma)$.

For a given P, let V_P be a finite-dimensional subspace of $L^2_\rho(\Gamma)$ with dimension $P+1$. Let $\{\psi_k : k = 0, \ldots, P\}$ be a basis for V_P, and given a set of coefficients $\{u_k \in \mathbb{R}^n : k = 0, \ldots, P\}$, define

$$\hat{u}(y) = \sum_{k=0}^{P} u_k \psi_k(y), \quad y \in \Gamma. \tag{3.10}$$

The stochastic Galerkin approximation to the solution of (3.9) is a representation of the form (3.10) such that

$$\int_\Gamma f(\hat{u}(y), y)\psi_k(y)\rho(y)dy = 0, \quad k = 0, \ldots, P. \tag{3.11}$$

In general, Equation (3.11) defines an implicit set of nonlinear equations for all of the expansion coefficients $\{u_k : k = 0, \ldots, P\}$. Thus it induces a new deterministic nonlinear problem

$$\bar{f}(\bar{u}) = 0, \quad \bar{f} = (\bar{f}_0, \ldots, \bar{f}_P) : \mathbb{R}^{(P+1)n} \to \mathbb{R}^{(P+1)n} \tag{3.12}$$

for the unknown expansion coefficients $\bar{u} = (u_0, \ldots, u_P)$. The form of this set of equations, and the resulting solution techniques required to approximate solutions, depend greatly on the choice of basis $\{\psi_k\}$. Three choices of basis will be described below, yielding the Monte Carlo, stochastic collocation, and polynomial chaos methods. In each case, the form of the nonlinear equations $\bar{f}(\bar{u}) = 0$ will be indicated, as well as its Jacobian derivative $\partial\bar{f}/\partial\bar{u}$, which will be useful in the following chapter on applying these methods to each component in a coupled system.

3.3.1 Monte Carlo

The Monte Carlo method approximates an integral quantity of interest $g(u(\xi))$ of the solution to (3.9) by simply averaging that quantity of interest over a suitably chosen set of deterministic realizations $\{y_j : j = 0, \ldots, P\}$ of the random parameters ξ. Given this set of realizations, let $\cup_{k=0}^{P}\Gamma_k$ denote a partitioning of Γ into disjoint subsets where each $y_k \in \Gamma_k$ for $k = 0, \ldots, P$. For each k, define $\psi_k(y) = 1$ if $y \in \Gamma_k$ and zero otherwise, and let u_k satisfy $f(u_k, y_k) = 0$. Define $\hat{u}$ as above, then for $k = 0, \ldots, P$,

$$\int_\Gamma f(\hat{u}(y), y)\psi_k(y)\rho(y)dy = \int_{\Gamma_k} f(u_k, y)\rho(y)dy \approx 0. \tag{3.13}$$

Thus Monte Carlo is a stochastic Galerkin method using a piecewise constant basis. As expected, the nonlinear problem (3.12) defining the coefficients $\bar{u}$ is given by the following

set of uncoupled nonlinear problems:

$$\bar{f}_k(\bar{u}) = f(u_k, y_k), \quad k = 0, \ldots, P \tag{3.14}$$

which are solved separately for each u_k. Moreover its Jacobian is block-diagonal:

$$\frac{\partial \bar{f}_i}{\partial \bar{u}_j} = \frac{\partial f}{\partial u}(u_j, y_j)\delta_{ij}, \quad i, j = 0, \ldots, P. \tag{3.15}$$

3.3.2 Stochastic Collocation

The stochastic collocation method approximates the solution to (3.9) through interpolation at a suitably chosen set of interpolation points $\{y_k : k = 0, \ldots, P\}$:

$$\hat{u}(y) = \sum_{k=0}^{P} u_k \psi_k(y), \quad f(u_k, y_k) = 0, \quad k = 0, \ldots, P, \tag{3.16}$$

where $\{\psi_k\}$ are Lagrange interpolatory polynomials:

$$\psi_k(y_j) = \delta_{kj}, \quad k, j = 0, \ldots, P. \tag{3.17}$$

If the integrals in the defining stochastic Galerkin equations (3.11) are approximated via a quadrature method with weights $\{w_k\}$ using the interpolation points $\{y_k\}$ as the quadrature points, then we have for $k = 0, \ldots, P$,

$$\int_\Gamma f(\hat{u}(y), y)\psi_k(y)\rho(y)dy \approx \sum_{j=0}^{P} w_j f(\hat{u}(y_j), y_j)\psi_k(y_j)\rho(y_j) = w_k f(u_k, y_k)\rho(y_k) = 0. \tag{3.18}$$

Thus stochastic collocation is a stochastic Galerkin method using a Lagrange interpolatory basis. As with the Monte Carlo method above, the equations (3.12) defining the coefficients $\bar{u}$ are uncoupled

$$\bar{f}_k(\bar{u}) = f(u_k, y_k), \quad k = 0, \ldots, P \tag{3.19}$$

with a block-diagonal Jacobian

$$\frac{\partial \bar{f}_i}{\partial \bar{u}_j} = \frac{\partial f}{\partial u}(u_j, y_j)\delta_{ij}, \quad i, j = 0, \ldots, P. \tag{3.20}$$

3.3.3 Polynomial Chaos

The polynomial chaos method computes a representation (3.10) where the basis $\{\psi_k : k = 0, \ldots, P\}$ is chosen as a set of multi-dimensional polynomials that are orthogonal with respect to the density ρ:

$$\int_\Gamma \psi_i(y)\psi_j(y)\rho(y)dy = \delta_{ij}, \quad i, j = 0, \ldots, P. \tag{3.21}$$

In most settings, the polynomials ψ_k are tensor products of one-dimensional polynomials where the total polynomial degree is restricted to be less than or equal to a given degree M (the so-called complete polynomial basis). In this case the density ρ must factor, $\rho(y) = \rho_1(y_1)\dots\rho_N(y_N)$, which is in general only true if the input random variables ξ are independent. For a given dimension N and degree M, the size of this basis P is given by

$$P = \frac{(N+M)!}{N!M!}. \tag{3.22}$$

Note this is considerably smaller than the full tensor product size of M^N. When ρ is the Gaussian density and the $\{\psi_k\}$ are Hermite polynomials, the method is referred to as polynomial chaos. For other labeled densities (e.g., uniform) with corresponding polynomials (e.g., Legendre), it is referred to as generalized polynomial chaos.

Generally this approach creates a fully-coupled nonlinear system

$$\bar{f}_k(\bar{u}) = \int_\Gamma f(\hat{u}(y), y)\psi_k(y)\rho(y)dy = 0, \quad k = 0, \dots, P. \tag{3.23}$$

for the unknown expansion coefficients $\bar{u}$ that must be formulated and solved. For general nonlinear problems, the integral appearing in (3.23) can only be approximated. For linear problems, or problems that only contain multiplicative nonlinearities, they can be evaluated exactly using the orthogonality relationships (3.21) (e.g., see [41]). However this requires rewriting a simulation code that evaluates f to one that evaluates $\bar{f}$. This can be automated somewhat, and extended to general nonlinear problems, using the ideas of automatic differentiation [43] along with formulas to approximate polynomial chaos expansions of more general nonlinearities such as transcendental functions [25]. Moreover, applying this technique to nonlinear problems requires solving (3.23) using an appropriate nonlinear solver, typically Newton's method, which requires evaluating the Jacobian

$$\begin{aligned} \frac{\partial \bar{f}_i}{\partial \bar{u}_j} &= \int_\Gamma \frac{\partial f}{\partial u}(\hat{u}(y), y)\psi_i(y)\psi_j(y)\rho(y)dy \\ &\approx \sum_{k=0}^{P} J_k \langle \psi_i \psi_j \psi_k \rangle \quad i, j = 0, \dots, P \end{aligned} \tag{3.24}$$

where

$$\langle h(y) \rangle \equiv \int_\Gamma h(y)\rho(y)dy \tag{3.25}$$

for any integrable function h and

$$\sum_{k=0}^{P} J_k \psi_k(y) \approx \frac{\partial f}{\partial u}(\hat{u}(y), y) \tag{3.26}$$

is the polynomial chaos expansion of the system Jacobian, with

$$J_k \equiv \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma \frac{\partial f}{\partial u}(\hat{u}(y), y)\psi_k(y)\rho(y)dy, \quad k = 0, \dots, P. \tag{3.27}$$

A discussion of methods for solving the resulting set of linear equations for the Newton updates is beyond the scope of this report.

3.3.4 Non-Intrusive Polynomial Chaos

A variant of the polynomial chaos method has been developed that eliminates the need to solve a fully coupled system for the expansion coefficients $\bar{u}$. This approach, dubbed non-intrusive polynomial chaos, approximates the solution in the same basis, but has coefficients defined by

$$u_k = \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma u(y)\psi_k(y)\rho(y)dy, \quad k = 0, \ldots, P. \tag{3.28}$$

In practice, the integrals appearing in (3.28) are approximated via a quadrature method

$$\frac{1}{\langle \psi_k^2 \rangle} \int_\Omega u(\xi)\psi_k(\xi)d\mu \approx \frac{1}{\langle \psi_k^2 \rangle} \sum_{j=0}^{Q} w_j \tilde{u}_j \psi_k(y_j), \quad f(\tilde{u}_j, y_j) = 0, \quad j = 0, \ldots Q, \tag{3.29}$$

given suitably chosen quadrature points $\{y_j\}$ and weights $\{w_j\}$. This method is different from all of the previous methods in that it is not directly a Galerkin method, however it still can be viewed as inducing a nonlinear problem $\bar{f} = 0$, if we use the quadrature values $\tilde{u}_j$, $j = 0, \ldots, Q$ as the unknown coefficients, instead of the expansion coefficients u_k, $k = 0, \ldots, P$. In this case,

$$\bar{f}_j(\tilde{u}) = f(\tilde{u}_j, y_j) \tag{3.30}$$

where $\tilde{u} = (\tilde{u}_0, \ldots, \tilde{u}_Q)$. This appears to be quite similar to stochastic collocation, and if the quadrature points $\{y_j\}$ are chosen to be the same, then the determined values $\{\tilde{u}_j\}$ are the stochastic collocation coefficients. The polynomial chaos coefficients are then given by a simple linear transformation

$$u_k = \frac{1}{\langle \psi_k^2 \rangle} \sum_{j=0}^{Q} w_j \tilde{u}_j \psi_k(y_j), \quad k = 0, \ldots, P. \tag{3.31}$$

Thus we see that the non-intrusive polynomial chaos method is a linear transformation of the stochastic collocation method, which amounts to a change of basis (from Lagrange to an orthogonal basis).

Chapter 4

Uncertainty Quantification of Coupled Systems

We now turn to the primary technical focus of this report, investigating uncertainty quantification methods for coupled systems. We consider the three families of coupled systems described in Section 1.1 using the two component multi-physics (1.1), interfacial (1.2), and network (1.4) prototypical examples to develop our ideas. As described in Section 3.3, we assume each component in the coupled system is subject to a finite set of random parameters $\xi_i = (\xi_{i_1}, \ldots, \xi_{i_{N_i}}) : \Omega \to \mathbb{R}^{N_i}$, $i = 1, 2$ defined on a probability space $(\Omega, \mathcal{B}, \mu)$. For a multi-physics problem, we wish to approximate random functions u_1 and u_2 such that the following equations are satisfied μ-almost everywhere:

$$\begin{aligned} f_1(u_1(\xi), u_2(\xi), \xi_1) &= 0, \\ f_2(u_1(\xi), u_2(\xi), \xi_2) &= 0, \end{aligned} \tag{4.1}$$

where $\xi = (\xi_1, \xi_2)$. Notice that even though each component f_i is only subject to the random parameters ξ_i, the solution (u_1, u_2) must be approximated over the product space $\xi = (\xi_1, \xi_2)$ because the equations are coupled. We have a similar formulation for the interfacially coupled system

$$\begin{aligned} f_1(u_1(\xi), g_2(u_2(\xi)), \xi_1) &= 0, \\ f_2(g_1(u_1(\xi)), u_2(\xi), \xi_2) &= 0, \end{aligned} \tag{4.2}$$

where we have assumed for simplicity the random appears directly within each component f_i, not within the interface g_i. For the network coupled system, we wish to solve for random functions u_1, u_2, x and y such that μ-almost everywhere

$$\begin{aligned} z_1(\xi) &= g_1(u_1(\xi), x_1(\xi), x_2(\xi)) \ \text{ s.t. } \ f_1(u_1(\xi), x_1(\xi), x_2(\xi), \xi_1) = 0, \\ z_2(\xi) &= g_2(u_2(\xi), x_2(\xi), x_3(\xi)) \ \text{ s.t. } \ f_2(u_2(\xi), x_2(\xi), x_3(\xi), \xi_2) = 0, \\ 0 &= F(z(\xi), x(\xi)). \end{aligned} \tag{4.3}$$

Again, we have assumed uncertainty does not directly enter into the component interfaces g_i or into the network F itself.

In principle, any of the uncertainty propagation methods discussed in Chapter 3 can be applied directly to any of these three types of coupled system uncertainty quantification

problems, treating it as a larger implicit system for all of the unknowns. This is the typical approach for estimating uncertainties in these types of problems. While convenient, such an approach disregards all structure inherent in the coupled system itself. The aim of this work is to leverage this structure with the hopes of making the overall uncertainty computation more efficient. The approach is to instead apply the stochastic Galerkin methods from Chapter 3 to each component f_i of the coupled system separately while applying the nonlinear solution strategies from Chapter 2 to solve the stochastic coupled problem. The rationale behind this is it would first allow different UQ methods to be applied to each component, and second allow stochastic dimension reduction ideas to be applied at the interface of each component. With this in mind, we describe in the next section how to formulate and solve a stochastic coupled system using this approach, building on the ideas from Chapters 2 and 3. We also examine the implications of applying different UQ methods to separate coupled system components. This is then followed by a discussion of dimension reduction ideas in Section 4.2.

4.1 Intrusive Coupled System Uncertainty Quantification

As described in Section 3.3, application of a stochastic Galerkin method to compute an approximate solution $\hat{u}(\xi) = \sum_{k=0}^{P} u_k \psi_k(\xi)$ to a nonlinear system $f(u(\xi), \xi) = 0$ induces a new, deterministic nonlinear problem $\bar{f}(\bar{u}) = 0$ for the expansion coefficients $\bar{u} = (u_0, \ldots, u_P)$, with the form of this system determined by the choice of stochastic Galerkin method. This property allows us to easily translate a stochastic coupled system into a similar deterministic nonlinear problem. As before, let ρ be the joint PDF of ξ, $\Gamma_1 = \xi_1(\Omega)$, $\Gamma_2 = \xi_2(\Omega)$ and $\Gamma = \xi(\Omega) = \Gamma_1 \times \Gamma_2$. Consider first the multi-physics problem (4.1). Let P_1 and P_2 be given, $V_{P_1}^1$ and $V_{P_2}^2$ be finite-dimensional subspaces of $L_\rho^2(\Gamma)$ with dimension $P_1 + 1$ and $P_2 + 1$ and with bases $\{\psi_k : k = 0, \ldots, P_1\}$ and $\{\phi_k : k = 0, \ldots, P_2\}$ respectively. Given coefficients $\{u_1^k : k = 0, \ldots, P_1\}$, $\{u_2^k : k = 0, \ldots, P_2\}$ define for $y \in \Gamma$

$$\begin{aligned} \hat{u}_1(y) &= \sum_{k=0}^{P_1} u_1^k \psi_k(y), \\ \hat{u}_2(y) &= \sum_{k=0}^{P_2} u_2^k \phi_k(y). \end{aligned} \tag{4.4}$$

Let $\bar{u}_1 = (u_1^0, \ldots, u_1^{P_1})$ and $\bar{u}_2 = (u_2^0, \ldots, u_2^{P_2})$, then (4.1) induces the deterministic nonlinear problem

$$\begin{aligned} \bar{f}_1(\bar{u}_1, \bar{u}_2) &= 0, \\ \bar{f}_2(\bar{u}_1, \bar{u}_2) &= 0, \end{aligned} \tag{4.5}$$

where

$$\begin{aligned}\bar{f}_1^k(\bar{u}_1,\bar{u}_2) &= \int_\Gamma f_1(\hat{u}_1(y),\hat{u}_2(y),\pi_1(y))\psi_k(y)\rho(y)dy, \quad k=0,\dots,P_1,\\ \bar{f}_2^k(\bar{u}_1,\bar{u}_2) &= \int_\Gamma f_2(\hat{u}_1(y),\hat{u}_2(y),\pi_2(y))\phi_k(y)\rho(y)dy, \quad k=0,\dots,P_2.\end{aligned} \tag{4.6}$$

Here $\pi_1 : \Gamma \to \Gamma_1$ and $\pi_2 : \Gamma \to \Gamma_2$ are projection operators defined by $\pi_i(y_1, y_2) = y_i$, $i = 1, 2$, for any $(y_1, y_2) \in \Gamma$. Equation (4.5) defines a deterministic nonlinear system for the unknown coefficients $\bar{u}_1$ and $\bar{u}_2$, whose solution then can be approximated by any suitable nonlinear solution strategy discussed in Chapter 2. A similar construction yields a corresponding nonlinear problem for the interfacially coupled system

$$\begin{aligned}\bar{f}_1(\bar{u}_1,\bar{g}_2(\bar{u}_2)) &= 0,\\ \bar{f}_2(\bar{g}_1(\bar{u}_1),\bar{u}_2) &= 0,\end{aligned} \tag{4.7}$$

where ($\bar{g}_1(\bar{u}_1)$ and $\bar{g}_2(\bar{u}_2)$ are merely notational conveniences)

$$\begin{aligned}\bar{f}_1^k(\bar{u}_1,\bar{g}_2(\bar{u}_2)) &= \int_\Gamma f_1(\hat{u}_1(y),g_2(\hat{u}_2(y)),\pi_1(y))\psi_k(y)\rho(y)dy, \quad k=0,\dots,P_1,\\ \bar{f}_2^k(\bar{g}_1(\bar{u}_1),\bar{u}_2) &= \int_\Gamma f_2(g_1(\hat{u}_1(y)),\hat{u}_2(y),\pi_2(y))\phi_k(y)\rho(y)dy, \quad k=0,\dots,P_2.\end{aligned} \tag{4.8}$$

For the network system we must define expansions for the network variables $x = (x_1, x_2, x_3)$ and $z = (z_1, z_2)$ in a given basis $\{\eta_k : k = 0, \dots, P_3\}$:

$$\hat{x}(y) = \sum_{k=0}^{P_3} x^k \eta_k(y), \quad y \in \Gamma, \tag{4.9}$$

$$\hat{z}(y) = \sum_{k=0}^{P_3} z^k \eta_k(y), \quad y \in \Gamma. \tag{4.10}$$

Defining $\bar{x} = (x^0, \dots, x^{P_3})$ and $\bar{z} = (z^0, \dots, z^{P_3})$ (with similar definitions for the components of x and z), we then have the stochastic Galerkin network system

$$\begin{aligned}\bar{z}_1 &= \bar{g}_1(\bar{u}_1,\bar{x}_1,\bar{x}_2) \ \text{ s.t. } \ \bar{f}_1(\bar{u}_1,\bar{x}_1,\bar{x}_2) = 0,\\ \bar{z}_2 &= \bar{g}_2(\bar{u}_2,\bar{x}_2,\bar{x}_3) \ \text{ s.t. } \ \bar{f}_2(\bar{u}_2,\bar{x}_2,\bar{x}_3) = 0,\\ 0 &= \bar{F}(\bar{z},\bar{x})\end{aligned} \tag{4.11}$$

with

$$\begin{aligned}\bar{f}_1^k(\bar{u}_1,\bar{x}_1,\bar{x}_2) &= \int_\Gamma f_1(\hat{u}_1(y),\hat{x}_1(y),\hat{x}_2(y),\pi_1(y))\psi_k(y)\rho(y)dy, \quad k=0,\dots,P_1,\\ \bar{f}_2^k(\bar{u}_2,\bar{x}_2,\bar{x}_3) &= \int_\Gamma f_2(\hat{u}_2(y),\hat{x}_2(y),\hat{x}_3(y),\pi_2(y))\phi_k(y)\rho(y)dy, \quad k=0,\dots,P_2,\\ \hat{z}_1(y) &= g_1(\hat{u}_1(y),\hat{x}_1(y),\hat{x}_2(y)),\\ \hat{z}_2(y) &= g_2(\hat{u}_2(y),\hat{x}_2(y),\hat{x}_3(y)),\\ \bar{F}^k(\bar{z},\bar{x}) &= \int_\Gamma F(\hat{z}(y),\hat{x}(y))\eta_k(y)\rho(y)dy, \quad k=0,\dots,P_1.\end{aligned} \tag{4.12}$$

For all three types of coupled system problems, the nonlinear solution strategies discussed in Chapter 2 can then be applied to (4.1), (4.2) and (4.3), as they are merely deterministic nonlinear problems for the unknown expansion coefficients introduced by the chosen stochastic Galerkin method. Formulas from Chapter 3 show how to evaluate the residuals appearing in these equations for each choice of method, as well as derivatives needed for Newton-based approaches. Moreover, different bases (and thus stochastic Galerkin methods) can be applied for each system, i.e., $\psi_k \neq \phi_k$ for each k. Of course, the devil here is really in the details. Therefore more details on how the systems are formulated, as well as the implications of choosing different bases for each component, are discussed in the following subsections for each of the nonlinear solver methods presented in Chapter 2.

4.1.1 Forwardly Coupled Systems

Before moving on to the fully coupled case, we first discuss the simpler forwardly coupled scenario. Consider, for example, the forwardly coupled version of the multi-physics problem (4.1):

$$\begin{aligned} f_1(u_1(\xi_1), \xi_1) &= 0, \\ f_2(u_1(\xi_1), u_2(\xi_1, \xi_2), \xi_2) &= 0, \end{aligned} \tag{4.13}$$

which after applying a stochastic Galerkin method with

$$\begin{aligned} \hat{u}_1(y) &= \sum_{k=0}^{P_1} u_1^k \psi_k(y), \quad y \in \Gamma_1 \\ \hat{u}_2(y) &= \sum_{k=0}^{P_2} u_2^k \phi_k(y), \quad y \in \Gamma \end{aligned} \tag{4.14}$$

yields the forwardly coupled problem

$$\begin{aligned} \bar{f}_1(\bar{u}_1) &= 0, \\ \bar{f}_2(\bar{u}_1, \bar{u}_2) &= 0. \end{aligned} \tag{4.15}$$

As usual, the first system of (4.15) can be solved for $\bar{u}_1$ (which only requires a solution over the space Γ_1), and then substituted into the second system. This requires evaluating the stochastic Galerkin residual for the second system in a potentially different basis than the input $\hat{u}_1$:

$$\bar{f}_2^k(\bar{u}_1, \bar{u}_2) = \int_\Gamma f_2(\hat{u}_1(\pi_1(y)), \hat{u}_2(y), \pi_2(y))\phi_k(y)\rho(y)dy, \quad k = 0, \ldots, P_2. \tag{4.16}$$

For any of the sampling type methods (Monte Carlo, stochastic collocation and non-intrusive polynomial chaos) applied to the second step, all that is required is to be able to evaluate $\hat{u}_1$ at an arbitrary point y if the bases are different. This in turn requires forming the basis $\{\psi_k\}$, which is never done for Monte Carlo (because of the very large number of samples)

and is often not done for stochastic collocation (forming the interpolating polynomials in high-dimensions with unstructured collocation grids is difficult). However for intrusive and non-intrusive polynomial chaos, forming the basis is an inherent part of the method, and therefore is not an issue. Conversely, some implementations of intrusive polynomial chaos require converting all input expansions to the chosen orthogonal polynomial basis. Thus applying this method to the second solve requires converting $\hat{u}_1$ to the same $\{\phi_k\}$ basis if it is not represented in the same basis. Such a conversion is not difficult to compute if the basis for $\hat{u}_1$ is at hand:

$$\tilde{u}_1(y) = \sum_{k=0}^{\tilde{P}_1} \tilde{u}_1^k \phi_k(y), \quad \tilde{u}_1^k = \frac{1}{\langle \phi_k^2 \rangle} \int_{\Gamma_1} \hat{u}_1(y)\phi_k(y)\rho(y)dy, \quad k = 0, \ldots, \tilde{P}_1. \tag{4.17}$$

Thus we see that, in general, heterogeneous UQ methods are only practical if the basis can actually be formed, i.e., stochastic collocation with structured grids and intrusive/non-intrusive polynomial chaos. This holds true for fully-coupled systems as well, since Picard iteration is essentially a series of forward coupling problems, and the Newton approaches incorporate derivative approximations to speed up Picard's method.

4.1.2 Picard Iteration

The Picard iteration method presented in Section 2.2 naturally generalizes to the stochastic Galerkin nonlinear problems (4.5) and (4.7) to compute the unknown coefficients $\bar{u}_1$ $\bar{u}_2$. As with forward coupling, the UQ methods evaluating $\bar{u}_1$ and $\bar{u}_2$ are essentially independent at each stage of the iteration, and different UQ methods can be used for each system (with the same caveats as described above).

4.1.3 Newton's Method

We now move to Newton-based methods, starting with the full Newton method from Section 2.3. For simplicity, we only examine Newton's method applied to the multi-physics problem (4.5). In this case we are required to solve the following linear system

$$\begin{bmatrix} \frac{\partial \bar{f}_1}{\partial \bar{u}_1} & \frac{\partial \bar{f}_1}{\partial \bar{u}_2} \\ \frac{\partial \bar{f}_2}{\partial \bar{u}_1} & \frac{\partial \bar{f}_2}{\partial \bar{u}_2} \end{bmatrix} \begin{bmatrix} \Delta \bar{u}_1 \\ \Delta \bar{u}_2 \end{bmatrix} = - \begin{bmatrix} \bar{f}_1(\bar{u}_1, \bar{u}_2) \\ \bar{f}_2(\bar{u}_1, \bar{u}_2) \end{bmatrix} \tag{4.18}$$

for the updates $\Delta \bar{u}_1$ and $\Delta \bar{u}_2$. For a sampling method applied to the first system, we have for the residual

$$\bar{f}_1^i = f_1(u_1^i, \hat{u}_2(y_i), \pi_1(y_i)), \quad i = 0, \ldots, P_1, \tag{4.19}$$

and therefore the first system derivatives are given by

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_1^j} = \frac{\partial f_1}{\partial u_1}(u_1^i, \hat{u}_2(y_i), \pi_1(y_i))\delta_{ij}, \quad i,j = 0,\ldots,P_1 \tag{4.20}$$

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_2^j} = \frac{\partial f_1}{\partial u_2}(u_1^i, \hat{u}_2(y_i), \pi_1(y_i))\phi_j(y_i), \quad i = 0,\ldots,P_1,\ j = 0,\ldots,P_2. \tag{4.21}$$

Notice that $\partial \bar{f}_1/\partial \bar{u}_1$ is block diagonal, whereas $\partial \bar{f}_1/\partial \bar{u}_2$ is not unless $\phi_j(y_i) = \delta_{ij}$, i.e., if $\phi_j = \psi_j$. Similar formulas can derived for a sampling method applied to system 2, and therefore we see that the Newton system can be reordered to a block 2-by-2 diagonal system only when the same sampling-based UQ method is applied to both systems. In this case, this is then equivalent to applying the same sampling-based method to the original coupled deterministic system.

For polynomial chaos applied to system 1, the residual $\bar{f}_1$ is given by (4.6), and its derivatives are

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_1^j} = \int_\Gamma \frac{\partial f_1}{\partial u_1}(\hat{u}_1(y), \hat{u}_2(y), \pi_1(y))\psi_i(y)\psi_j(y)\rho(y)dy \tag{4.22}$$

$$\approx \sum_{k=0}^{P_1} J_{11}^k \langle \psi_i \psi_j \psi_k \rangle \quad i,j = 0,\ldots,P_1, \tag{4.23}$$

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_2^j} = \int_\Gamma \frac{\partial f_1}{\partial u_2}(\hat{u}_1(y), \hat{u}_2(y), \pi_1(y))\psi_i(y)\phi_j(y)\rho(y)dy \tag{4.24}$$

$$\approx \sum_{k=0}^{P_1} J_{12}^k \langle \psi_i \phi_j \psi_k \rangle \quad i = 0,\ldots,P_1,\ j = 0,\ldots,P_2, \tag{4.25}$$

where

$$J_{11}^k = \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma \frac{\partial f_1}{\partial u_1}(\hat{u}_1(y), \hat{u}_2(y), \pi_1(y))\psi_k(y)\rho(y)dy, \quad k = 0,\ldots,P_1, \tag{4.26}$$

$$J_{12}^k = \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma \frac{\partial f_1}{\partial u_2}(\hat{u}_1(y), \hat{u}_2(y), \pi_1(y))\psi_k(y)\rho(y)dy, \quad k = 0,\ldots,P_1. \tag{4.27}$$

Again, similar formulas can be derived for polynomial chaos applied to system 2, and it is straightforward to show that if polynomial chaos is applied to both systems, this is equivalent to applying polynomial chaos to the original coupled system.

These derivations show that when a heterogeneous UQ method is applied between systems 1 and 2, we do not obtain a block diagonal system, or even a portion of a block diagonal system, even when one is a sampling method. This is a serious drawback when using sampling-only methods, however one is already accustomed to this when using polynomial chaos type methods. Therefore the combination of say, stochastic collocation and polynomial chaos is quite feasible, as long as the stochastic collocation Lagrange basis can be formed. The efficiency of this is strongly dependent on cost of solving the resulting coupled Newton system.

4.1.4 Nonlinear Elimination for Interfacial Coupling

We next consider the nonlinear elimination method for interfacial-type coupling described in 2. As shown in Algorithm 2, there are three stages for each iteration of the nonlinear elimination algorithm. The first is to solve $\bar{f}_1(\bar{u}_1, \bar{g}_2(\bar{u}_2)) = 0$ for $\bar{u}_1$, treating $\bar{u}_2$ as fixed, using an appropriate nonlinear solver method. The next step is to compute the sensitivities

$$\frac{\partial \bar{u}_1}{\partial \bar{u}_2} = -\left(\frac{\partial \bar{f}_1}{\partial \bar{u}_1}\right)^{-1} \frac{\partial \bar{f}_1}{\partial \bar{u}_2}. \tag{4.28}$$

If a sampling-type method is applied for the first system, we have

$$\bar{f}_1^i = f_1(u_1^i, g_2(\hat{u}_2(y_i)), \pi_1(y_i)), \quad i = 0, \ldots, P_1, \tag{4.29}$$

and therefore

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_1^j} = \frac{\partial f_1}{\partial u_1}(u_1^i, g_2(\hat{u}_2(y_i)), \pi_1(y_i))\delta_{ij}, \quad i, j = 0, \ldots, P_1 \tag{4.30}$$

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_2^j} = \frac{\partial f_1}{\partial g_2}(u_1^i, g_2(\hat{u}_2(y_i)), \pi_1(y_i))\frac{\partial g_2}{\partial u_2}(\hat{u}_2(y_i))\phi_j(y_i), \quad i = 0, \ldots, P_1,\ j = 0, \ldots, P_2. \tag{4.31}$$

Since $\partial \bar{f}_1 / \partial \bar{u}_1$ is block diagonal, we then have

$$\left(\frac{\partial \bar{u}_1}{\partial \bar{u}_2}\right)_{ij} = \phi_j(y_i)\left(\frac{\partial f_1}{\partial u_1}(u_1^i, g_2(\hat{u}_2(y_i)), \pi_1(y_i))\right)^{-1} \frac{\partial f_1}{\partial g_2}(u_1^i, g_2(\hat{u}_2(y_i)), \pi_1(y_i))\frac{\partial g_2}{\partial u_2}(\hat{u}_2(y_i)) \tag{4.32}$$

for $i = 0, \ldots, P_1$ and $j = 0, \ldots, P_2$. This is exactly collocation on the standard deterministic sensitivity solve taking into account the additional functional dependence of $\hat{u}_2$ on its coefficients $\bar{u}_2$. Notice that the resulting sensitivity matrix is block diagonal only if a heterogeneous UQ method is applied so that $\phi_i(y_j) = \delta_{ij}$.

For a polynomial chaos applied to the first system, we have $\bar{f}_1(\bar{u}_1, \bar{g}_2(\bar{u}_2))$ given by (4.8) and therefore

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_1^j} = \int_\Gamma \frac{\partial f_1}{\partial u_1}(\hat{u}_1(y), g_2(\hat{u}_2(y)), \pi_1(y))\psi_i(y)\psi_j(y)\rho(y)dy \tag{4.33}$$

$$\approx \sum_{k=0}^{P_1} J_{11}^k \langle \psi_i \psi_j \psi_k \rangle \quad i, j = 0, \ldots, P_1, \tag{4.34}$$

$$\frac{\partial \bar{f}_1^i}{\partial \bar{u}_2^j} = \int_\Gamma \frac{\partial f_1}{\partial g_2}(\hat{u}_1(y), g_2(\hat{u}_2(y)), \pi_1(y))\frac{\partial g_2}{\partial u_2}(\hat{u}_2(y))\psi_i(y)\phi_j(y)\rho(y)dy \tag{4.35}$$

$$\approx \sum_{k=0}^{P_1} J_{12}^k \langle \psi_i \phi_j \psi_k \rangle \quad i = 0, \ldots, P_1,\ j = 0, \ldots, P_2, \tag{4.36}$$

where

$$J_{11}^k = \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma \frac{\partial f_1}{\partial u_1}(\hat{u}_1(y), g_2(\hat{u}_2(y)), \pi_1(y))\psi_k(y)\rho(y)dy, \quad k = 0, \ldots, P_1, \tag{4.37}$$

$$J_{12}^k = \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma \frac{\partial f_1}{\partial u_2}(\hat{u}_1(y), g_2(\hat{u}_2(y)), \pi_1(y))\frac{\partial g_2}{\partial u_2}(\hat{u}_2(y))\psi_k(y)\rho(y)dy, \quad k = 0, \ldots, P_1. \tag{4.38}$$

Notice that here we have defined $\{J_{12}^k\}$ to be the coefficients of the polynomial chaos expansion of $(\partial f_1/\partial g_2)(\partial g_2/\partial u_2)$, not $\partial f_1/\partial g_2$. From these formulas $\partial \bar{u}_1/\partial \bar{u}_2$ can then be computed via (4.28).

The final step in the nonlinear elimination procedure is to formulate and solve the Newton equation for the second system:

$$\left(\frac{\partial \bar{f}_2}{\partial \bar{u}_1}\frac{\partial \bar{u}_1}{\partial \bar{u}_2} + \frac{\partial \bar{f}_2}{\partial \bar{u}_2}\right)\Delta \bar{u}_2 = -\bar{f}_2(\bar{g}_1(\bar{u}_1), \bar{u}_2). \tag{4.39}$$

As with the first system, we have the defining equations for the coefficients $\bar{u}_2$ when using a sampling method

$$\bar{f}_2^i = f_2(g_1(\hat{u}_1(y_i)), u_2^i, \pi_2(y_i)), \quad i = 0, \ldots, P_2. \tag{4.40}$$

and thus

$$\frac{\partial \bar{f}_2^i}{\partial \bar{u}_2^j} = \frac{\partial f_2}{\partial u_2}(g_1(\hat{u}_1(y_i)), u_2^i, \pi_2(y_i))\delta_{ij}, \tag{4.41}$$

$$\frac{\partial \bar{f}_2^i}{\partial \bar{u}_1^j} = \frac{\partial f_2}{\partial g_1}(g_1(\hat{u}_1(y_i)), u_2^i, \pi_2(y_i))\frac{\partial g_1}{\partial u_1}(\hat{u}_1(y_i))\psi_j(y_i). \tag{4.42}$$

The (i, j) block entry for $i, j = 0, \ldots, P_2$ of the matrix in (4.39) is then given by

$$\begin{aligned}\left(\frac{\partial \bar{f}_2}{\partial \bar{u}_1}\frac{\partial \bar{u}_1}{\partial \bar{u}_2} + \frac{\partial \bar{f}_2}{\partial \bar{u}_2}\right)_{ij} &= \sum_{l=0}^{P_1} \frac{\partial \bar{f}_2^i}{\partial \bar{u}_1^l}\frac{\partial \bar{u}_1^l}{\partial \bar{u}_1^j} + \frac{\partial \bar{f}_2^i}{\partial \bar{u}_2^j} \\ &= \frac{\partial f_2}{\partial g_1}(g_1(\hat{u}_1(y_i)), u_2^i, \pi_2(y_i))\frac{\partial g_1}{\partial u_1}(\hat{u}_1(y_i))\sum_{l=0}^{P_1}\psi_l(y_i)\frac{\partial \bar{u}_1^l}{\partial \bar{u}_1^j} + \delta_{ij}\frac{\partial f_2}{\partial u_2}(g_1(\hat{u}_1(y_i)), u_2^i, \pi_2(y_i)).\end{aligned} \tag{4.43}$$

As with Newton's method we do not obtain a block-diagonal system in general. However, if the same sampling method is applied to the first system, then $P_1 = P_2$, $\psi_l(y_i) = \delta_{li}$, $\phi_j(y_i) = \delta_{ij}$, and (4.43) reduces to the block diagonal nonlinear elimination system

$$\left(\frac{\partial \bar{f}_2}{\partial \bar{u}_1}\frac{\partial \bar{u}_1}{\partial \bar{u}_2} + \frac{\partial \bar{f}_2}{\partial \bar{u}_2}\right)_{ij} = \delta_{ij}\left(\frac{\partial f_2}{\partial g_1}(g_1(u_1^i), u_2^i, \pi_2(y_i))\frac{\partial g_1}{\partial u_1}(u_1^i)\frac{\partial \bar{u}_1^i}{\partial \bar{u}_2^i} + \frac{\partial f_2}{\partial u_2}(g_1(u_1^i)), u_2^i, \pi_2(y_i))\right). \tag{4.44}$$

Similarly, for polynomial chaos applied to this system we have $\bar{f}_2(\bar{g}_1(\bar{u}_1), \bar{u}_2)$ given by (4.8) and

$$\frac{\partial \bar{f}_2^i}{\partial \bar{u}_2^j} = \int_\Gamma \frac{\partial f_2}{\partial u_2}(g_1(\hat{u}_1(y)), \hat{u}_2(y), \pi_2(y))\phi_i(y)\phi_j(y)\rho(y)dy \tag{4.45}$$

$$\approx \sum_{k=0}^{P_2} J_{22}^k \langle \phi_i \phi_j \phi_k \rangle \quad i, j = 0, \ldots, P_2, \tag{4.46}$$

$$\frac{\partial \bar{f}_2^i}{\partial \bar{u}_1^j} = \int_\Gamma \frac{\partial f_2}{\partial g_1}(g_1(\hat{u}_1(y)), \hat{u}_2(y), \pi_2(y))\frac{\partial g_1}{\partial u_1}(\hat{u}_1(y))\phi_i(y)\psi_j(y)\rho(y)dy \tag{4.47}$$

$$\approx \sum_{k=0}^{P_2} J_{21}^k \langle \phi_i \psi_j \phi_k \rangle \quad i = 0, \ldots, P_2,\ j = 0, \ldots, P_1, \tag{4.48}$$

where

$$J_{22}^k = \frac{1}{\langle \phi_k^2 \rangle} \int_\Gamma \frac{\partial f_2}{\partial u_2}(g_1(\hat{u}_1(y)), \hat{u}_2(y), \pi_2(y))\phi_k(y)\rho(y)dy, \quad k = 0, \ldots, P_2, \tag{4.49}$$

$$J_{21}^k = \frac{1}{\langle \phi_k^2 \rangle} \int_\Gamma \frac{\partial f_2}{\partial u_1}(g_1(\hat{u}_1(y)), \hat{u}_2(y), \pi_2(y))\frac{\partial g_1}{\partial u_1}(\hat{u}_1(y))\phi_k(y)\rho(y)dy, \quad k = 0, \ldots, P_2. \tag{4.50}$$

From these formulas, and the corresponding formulas for $\partial \bar{u}_1 / \partial \bar{u}_2$, the linear system (4.39) can then be constructed.

4.1.5 Nonlinear Elimination for Network Coupling

We finally consider the nonlinear elimination method for network-type coupling described in Chapter 2. Referring to Algorithm 3, there are four stages of the algorithm when applied to stochastic Galerkin system (4.11) that we must consider. First is the evaluation $\bar{u}_1$ and $\bar{u}_2$ from the equations $\bar{f}_1(\bar{u}_1, \bar{x}_1, \bar{x}_2) = 0$ and $\bar{f}_2(\bar{u}_2, \bar{x}_2, \bar{x}_3) = 0$. This just requires straightforward application of the appropriate nonlinear solution strategy given the choice of the stochastic Galerkin methods for each of these systems. Second is the evaluation of the coefficients $\bar{z}$ from the relationships $\hat{z}_1(y) = g_1(\hat{u}_1(y), \hat{x}_1(y), \hat{x}_2(y))$ and $\hat{z}_2(y) = g_2(\hat{u}_2(y), \hat{x}_2(y), \hat{x}_3(y))$. This is straightforward given the choice of the stochastic Galerkin method, e.g., for a sampling method

$$z_1^k = g_1(\hat{u}_1(y_k), x_1^k, x_2^k), \quad k = 0, \ldots, P_3 \tag{4.51}$$

and for polynomial chaos

$$z_1^k = \frac{1}{\langle \eta_k^2 \rangle} \int_\Gamma g_1(\hat{u}_1(y), \hat{x}_1(y), \hat{x}_2(y))\eta_k(y)\rho(y)dy, \quad k = 0, \ldots, P_3. \tag{4.52}$$

Third is the evaluation of the sensitivities $\partial \bar{z} / \partial \bar{x}$, corresponding to (2.10). The techniques for evaluating these sensitivities have already been discussed above in the nonlinear elimination

section for interfacial coupling. For example, with a sampling method applied to the network system we have

$$\frac{\partial \bar{z}_1^i}{\partial \bar{x}_1^j} = \sum_{l=0}^{P_1} \frac{\partial g_1}{\partial u_1}(\hat{u}_1(y_i), x_1^i, x_2^i)) \frac{\partial u_1^l}{\partial x_1^j} \psi_l(y_i) + \frac{\partial g_1}{\partial x_1}(\hat{u}_1(y_i), x_1^i, x_2^i))\delta_{ij}, \quad i,j = 0,\ldots,P_3 \quad (4.53)$$

where $\partial u_1^l / \partial x_1^j = (\partial \bar{u}_1 / \partial \bar{x}_1)_{lj}$ is determined from $\bar{f}_1(\bar{u}_1, \bar{x}_1, \bar{x}_2) = 0$, given the choice of stochastic Galerkin method for this system. As should be expected, this sensitivity matrix is only block diagonal if each network component and the network system use the same sampling method. Similarly for the polynomial chaos approach applied to the network system we have

$$\begin{aligned}\frac{\partial \bar{z}_1^i}{\partial \bar{x}_1^j} = \frac{1}{\langle \eta_i^2 \rangle} \sum_{l=0}^{P_1} \int_\Gamma \frac{\partial g_1}{\partial u_1}(\hat{u}_1(y), \hat{x}_1(y), \hat{x}_2(y)) \frac{\partial u_1^l}{\partial x_1^j} \psi_l(y) \eta_i(y) \rho(y) dy \\ + \frac{1}{\langle \eta_i^2 \rangle} \int_\Gamma \frac{\partial g_1}{\partial x_1}(\hat{u}_1(y), \hat{x}_1(y), \hat{x}_2(y)) \eta_j(y) \eta_i(y) \rho(y) dy, \quad i,j = 0,\ldots,P_3. \quad (4.54)\end{aligned}$$

The fourth step is the evaluation and solution of the network Newton system

$$\left(\frac{\partial \bar{F}}{\partial \bar{z}} \frac{\partial \bar{z}}{\partial \bar{x}} + \frac{\partial \bar{F}}{\partial \bar{x}} \right) \Delta \bar{x} = -\bar{F}(\bar{z}, \bar{x}). \quad (4.55)$$

The formation of this linear system is quite similar to that described in the nonlinear elimination for interfacial coupling section above, and therefore will not be repeated here. We emphasize that if a sampling method is applied to the network system, we do not obtain a block-diagonal Newton system, unless all components in the network employ the same sampling method.

4.1.6 Convergence Criteria

An important aspect of the previous nonlinear solution algorithms applied to the uncertainty quantification system is deciding convergence. The advantage of the approach discussed in this report is that it transforms the stochastic problem into a deterministic-parametric problem for the expansions coefficients $\bar{u}_1$ and $\bar{u}_2$. Thus standard, deterministic convergence criteria can be applied such as update norms (e.g., $||\Delta \bar{u}_1||_2$) and residual norms (e.g., $||\bar{f}_1||_2$) which can easily be computed in terms of their coefficients. Note that it would also be possible to use statistical moments as convergence criteria such as the mean or standard deviation of $\hat{u}_1$ and $\hat{u}_2$. This may make more sense if one is only interested in such moments since the convergence criteria would relate directly to the accuracy to which those moments have been approximated. However if the full expansion is needed, for example for probability or validation calculations, then basing convergence on the coefficients directly is likely more advisable.

4.2 Inter-System Stochastic Dimension Reduction

As we have seen in the previous section, an advantage of this intrusive uncertainty quantification approach for coupled systems is that it provides greater freedom to how uncertainty is estimated in each component of that system. In particular we have shown that each component can employ a different stochastic Galerkin method, representing its solution component in a different stochastic Galerkin basis. Throughout that section however, we have assumed each component is computing its approximation over the same stochastic space, with the same random vectors as coordinates, and with the same joint probability distribution function. We now relax that assumption, with an eye toward reducing the dimension of the stochastic space each component computes its approximate expansion over. Given that for most of these methods the cost grows exponentially with the dimension of this space, any reduction in the dimension can potentially dramatically reduce the overall computational cost. We first consider the more general case of multi-physics coupling, which requires employing random field modeling techniques from Section 3.1, and then move to the simpler case of interfacial and network coupling.

4.2.1 Dimension Reduction in Multi-Physics Systems

Consider the following scalar multi-physics coupled PDE system:

$$\begin{aligned} \mathcal{F}_1(u_1(x,\xi), u_2(x,\xi), x, \xi_1) = 0, \\ \mathcal{F}_2(u_1(x,\xi), u_2(x,\xi), x, \xi_2) = 0, \end{aligned} \tag{4.56}$$

defined on a bounded domain $x \subset D \subset \mathbb{R}^d$ with a given finite dimensional set of random parameters ξ, and u_1, u_2 belonging to a given Hilbert space H. The solutions u_1 and u_2 are approximated using some spatial discretization method (e.g., finite-elements) and a stochastic Galerkin discretization, yielding approximate solutions

$$\begin{aligned} \hat{u}_1(x,\xi(\omega)) &= \sum_{j=0}^{n_1} \sum_{k=0}^{P_1} u_1^{jk} \chi_j(x) \psi_k(\xi(\omega)) \\ \hat{u}_2(x,\xi(\omega)) &= \sum_{j=0}^{n_2} \sum_{k=0}^{P_2} u_2^{jk} \theta_j(x) \phi_k(\xi(\omega)) \end{aligned} \tag{4.57}$$

where $\{\chi_j\}$ and $\{\theta_j\}$ are basis functions for the spatial discretization. Then $\hat{u}_1$ is a random field, and so its Karhunen-Loève expansion from Section 3.1 can be computed

$$\hat{u}_1(x,\xi(\omega)) = E\hat{u}_1(x,\xi) + \sum_{k=0}^{\infty} \sqrt{\lambda_k} b_k(x) \zeta_k(\omega) \tag{4.58}$$

where

$$\langle \mathrm{cov}_{\hat{u}_1}(x,\cdot), b_k \rangle_H = \lambda_k b_k(x), \quad k = 1, \ldots, \infty, \tag{4.59}$$

and $\langle \cdot, \cdot \rangle_H$ denotes the Hilbert space inner product. The covariance function $\text{cov}_{\hat{u}_1}$ is given by

$$\begin{aligned} \text{cov}_{\hat{u}_1}(x, x') &= E\left((\hat{u}_1(x,\xi) - E\hat{u}_1(x,\xi))(\hat{u}_1(x',\xi) - E\hat{u}_1(x',\xi))\right) \\ &= \sum_{j,l=0}^{n_1} \sum_{k,s=0}^{P_1} u_1^{jk} u_1^{ls} \phi_j(x)\phi_l(x')(E(\psi_k\psi_s) - E\psi_k E\psi_s). \end{aligned} \tag{4.60}$$

By examining the decay of the eigenvalues λ_k, a dimension $\tilde{N}_1$ can be determined to truncate the expansion (4.58)

$$\hat{u}_1(x, \xi(\omega)) \approx E\hat{u}_1(x,\xi) + \sum_{k=0}^{\tilde{N}_1} \sqrt{\lambda_k} b_k(x)\zeta_k(\omega). \tag{4.61}$$

This defines a new set finite-dimensional set of random variables $\zeta = (\zeta_1, \ldots, \zeta_{\tilde{N}_1})$ given by

$$\zeta_k(\omega) = \frac{1}{\sqrt{\lambda_k}} \langle \hat{u}_1(\cdot, \xi(\omega)) - E\hat{u}_1(\cdot,\xi), b_k \rangle_H, \quad k = 1, \ldots, \tilde{N}_1. \tag{4.62}$$

for which $\hat{u}_1$ can be approximated by (4.61). The essential idea here is to compute this representation at intermediate stages of the nonlinear solution process used to compute the coefficients $\hat{u}_1$ and $\hat{u}_2$, basing the representation on approximations from previous nonlinear iterations. The hope is the new space spanned by ζ will have significantly smaller dimension $\tilde{N}_1$ than N, that of the original space ξ for the same level of accuracy, making the cost of calculating the subsequent approximations of $\tilde{u}_1$ and $\tilde{u}_2$ significantly cheaper. In particular, consider the discrete nonlinear problem induced by (4.56) and (4.57)

$$\begin{aligned} \bar{f}_1(\bar{u}_1, \bar{u}_2) &= 0, \\ \bar{f}_2(\bar{u}_1, \bar{u}_2) &= 0, \end{aligned} \tag{4.63}$$

where $\bar{u}_i = (u_i^0, \ldots, u_i^{P_i})$ and $u_i^k = (u_i^{0k}, \ldots, u_i^{nk})$ for $k = 0, \ldots, P_i$ and $i = 1, 2$. Consider applying Picard iteration to (4.63), assuming that at stage k, approximations $u_1^{(k-1)}$ and $u_2^{(k-1)}$ are known. Assume the first step in the Picard iteration for stage k has been completed, producing the next approximate solution $u_1^{(k)}$ satisfying

$$\bar{f}_1(\bar{u}_1^{(k)}, \bar{u}_2^{(k-1)}) = 0. \tag{4.64}$$

Using this approximation $\bar{u}_1^{(k)}$, assume the truncated Karhunen-Loève expansion (4.61) has been computed, yielding a new set of random variables ζ defined by (4.62). With these new random variables, $\hat{u}_1^{(k)}$ is given by simply a degree-1 polynomial in ζ and defines a new coefficient vector $\tilde{u}_1^{(k)}$. Given the particular stochastic Galerkin method for the second system, assume a new basis $\{\eta_j : j = 0, \ldots \tilde{P}_2\}$ can be generated to approximate u_2 over (ζ, ξ_2):

$$\hat{u}_2(\zeta, \xi_2) \approx \sum_{j=0}^{\tilde{P}_2} \tilde{u}_2^j \eta_j(\zeta, \xi_2). \tag{4.65}$$

Define, as usual, $\tilde{u}_2 = (\tilde{u}_2^0, \ldots, \tilde{u}_2^{\tilde{P}_2})$, then the chosen stochastic Galerkin method defines a new nonlinear problem for the second system

$$\tilde{f}_2(\tilde{u}_1^{(k)}, \tilde{u}_2) = 0 \tag{4.66}$$

to be solved for $\tilde{u}_2$. This idea can then be repeated for the next iteration of the Picard method, applying the Karhunen-Loève expansion to the just approximated $\hat{u}_2$, and so on.

To implement this idea in a practical algorithm, several issues must be addressed. The first is, given a stochastic Galerkin expansion such as (4.57), how to solve the integral eigenproblem (4.59) for the Karhunen-Loève eigenvalues $\{\lambda_k\}$ and eigenfunctions $\{b_k\}$. We describe one approach here, following the ideas presented in [26], transforming the integral eigenproblem to a discrete eigenvalue problem based on a Galerkin projection. In particular, for each k the eigenfunction $b_k(x)$ can be approximated by the spatial discretization

$$b_k(x) \approx \hat{b}_k(x) = \sum_{j=0}^{n_1} \beta_{jk} \chi_j(x). \tag{4.67}$$

Substituting this into (4.59) and requiring the resulting error to be orthogonal to each ϕ_i yields the following discrete eigenvalue problem

$$M^T C M \beta_k = \lambda_k M^T \beta_k \tag{4.68}$$

where M is the mass matrix induced by the Hilbert space H

$$M_{ij} = \langle \phi_i, \phi_j \rangle_H, \quad i, j = 0, \ldots, n_1, \tag{4.69}$$

C is the nodal covariance matrix

$$C_{ij} = \sum_{k,l=0}^{P_1} u_1^{ik} u_1^{jl} (E(\psi_k \psi_l) - E\psi_k E\psi_l), \quad i, j = 0, \ldots, P_1, \tag{4.70}$$

and $\beta_k = (\beta_{0k}, \ldots, \beta_{nk})$. Thus the eigenfunctions and eigenvalues can be approximated through a single discrete eigenproblem of a size given by the spatial discretization.

The second issue is, once the Karhunen-Loève expansion has been computed defining the new random variables ζ, how to generate the new basis $\{\eta_j : j = 0, \ldots, \tilde{P}_2\}$. For polynomial chaos, this requires forming a new basis that is orthogonal with respect to the probability measure defined ζ. Methods for this have been investigated in the literature [91, 92] using a Stieltjes procedure for a general three-term recurrence relation [37, 38]. A significant issue here is the numerical efficiency and stability of these procedures, given that the distribution of ζ can not be written down in closed form and must be approximated through (4.62). In principle, such a procedure is not required for stochastic collocation, since it is not based on an orthogonal polynomial basis. However determining optimal collocation points requires finding the zeros of these same orthogonal polynomials. These zeros can be found through an eigenvalue problem derived from the three-term recurrence [37, 38].

The third issue is how to decide convergence. When the basis is fixed throughout the nonlinear solution process, the stochastic Galerkin expansion coefficients and/or the stochastic Galerkin residuals can be used to measure convergence, just as with any deterministic problem. The expansion coefficients certainly can no longer be used, as their definition is changing each iteration. It should still be feasible to use stochastic Galerkin residuals for convergence however, even though the space upon which they are defined is changing. This is somewhat akin to residual scaling that is changed at each iteration of the nonlinear solver. It would also be possible to use statistical moments as well.

The final issue is how to extend these ideas to Newton-based approaches. Given satisfactory resolution of the other three issues above, extending from Picard's Method to Newton's Method applied to (4.63) is not difficult. Assume a full Newton method is applied to (4.63), and at a given stage k, approximate solutions $\hat{u}_1^{(k-1)}$ and $\hat{u}_2(k-1)$ are known. The dimension reduction techniques described above can then be applied to both $\hat{u}_1^{(k-1)}$ and $\hat{u}_2^{(k-1)}$, yielding two new sets of random variables ζ_1 and ζ_2. New bases $\{\eta_k^1 : k = 0, \ldots \tilde{P}_1\}$ and $\{\eta_k^2 : k = 0, \ldots \tilde{P}_2\}$ are constructed over (ζ_2, ξ_1) and (ζ_1, ξ_2) respectively, which define a new nonlinear problem

$$\begin{aligned} \tilde{f}_1(\tilde{u}_1, \tilde{u}_2) &= 0 \\ \tilde{f}_2(\tilde{u}_1, \tilde{u}_2) &= 0 \end{aligned} \tag{4.71}$$

for the next iteration of Newton's method. The Newton system can then be formed and solved (using the current approximations for u_1 and u_2 in the new basis) using the techniques discussed earlier in this report. Convergence is then determined as described above. Note this not only potentially reduces the stochastic dimension N, but may also reduce the order of expansions required since at each stage the solution is re-approximated in a degree one basis.

4.2.2 Dimension Reduction in Interfacial and Network Systems

These ideas can be applied to interfacial and network coupled systems as well, and in fact, these are simpler in that the Karhunen-Loève expansion is not needed to reduce the dimension of the solution at the system interface (essentially the form of the interfacial or network system already does this through their form of coupling). For an interfacially coupled system

$$\begin{aligned} f_1(\hat{u}_1(\xi), g_2(\hat{u}_2(\xi)), \xi_1) &= 0, \\ f_2(g_1(\hat{u}_1(\xi)), \hat{u}_2(\xi), \xi_2) &= 0, \end{aligned} \tag{4.72}$$

new random variables can be directly defined

$$\begin{aligned} \zeta_1 &= g_1(\hat{u}_1(\xi)), \\ \zeta_2 &= g_2(\hat{u}_2(\xi)). \end{aligned} \tag{4.73}$$

Such random variables can be defined at each stage of a nonlinear solution process for solving the stochastic Galerkin system, in the same manner as described above. As in the multiphysics case, the primary issue here is computing the new bases $\{\eta_k^1\}$ and $\{\eta_k^2\}$ over the spaces

(ζ_2, ξ_1) and (ζ_1, ξ_2) respectively. The advantage here is the stochastic Galerkin method for each system only need compute an approximation over the minimum space necessary, that defined by its own random variables (ξ_i) and its interface to the other system (ζ_j). Of course, the same idea can be applied to the network system

$$\begin{aligned} \hat{y}_1 &= g_1(\hat{u}_1, \hat{x}_1, \hat{x}_2) \;\text{ s.t. }\; f_1(\hat{u}_1, \hat{x}_1, \hat{x}_2, \xi_1) = 0, \\ \hat{y}_2 &= g_2(\hat{u}_2, \hat{x}_2, \hat{x}_3) \;\text{ s.t. }\; f_2(\hat{u}_2, \hat{x}_2, \hat{x}_3, \xi_2) = 0, \\ 0 &= F(\hat{y}, \hat{x}) \end{aligned} \tag{4.74}$$

by defining random variables

$$\begin{aligned} \zeta_1 &= \hat{x}_1(\xi), \\ \zeta_2 &= \hat{x}_2(\xi), \\ \zeta_3 &= \hat{x}_3(\xi), \\ \zeta_4 &= \hat{y}_1(\xi), \\ \zeta_5 &= \hat{y}_2(\xi). \end{aligned} \tag{4.75}$$

As above, each system component is only required to compute an approximation over its own random variables plus its connections to the rest of the network, and the network system must only compute an approximation over the number of random variables equal to the number of network components.

Chapter 5

Summary and Conclusions

In this report we have described mathematical approaches for uncertainty quantification of coupled systems that attempt to exploit their inherent structure in order to reduce computational cost. Three basic forms of coupled systems were considered, shared-domain multi-physics, interfacially coupled, and network coupled systems. Several deterministic nonlinear solution strategies appropriate for these types of coupled systems were reviewed, including Picard iteration, Newton's method, and two forms of nonlinear elimination. Several uncertainty quantification methods were described as well, including Monte Carlo, stochastic collocation, polynomial chaos, and non-intrusive polynomial chaos, and cast in the unifying form of general stochastic Galerkin methods. It was shown how these methods translate a nonlinear stochastic system into a deterministic parametric nonlinear system, inducing a new nonlinear system of equations for the stochastic Galerkin expansion coefficients. This property was exploited to apply a potentially different stochastic Galerkin method to each component in a coupled system, yielding a new coupled system for the expansion coefficients. Solutions to this coupled system could then be approximated through the standard coupled-system nonlinear solution processes discussed earlier. Two potential benefits for this approach were discussed: heterogeneous uncertainty quantification where separate methods are applied to each component, and stochastic dimension reduction at the coupled system interface. Two approaches for the latter were presented, the first for multi-physics coupling based on Karhunen-Loève expansions of random fields, and the second for interfacial and network coupling based on stochastic Galerkin methods for random variables with general probability distributions. We now highlight important challenges in reaping these benefits in computational settings.

The first advantage of this intrusive coupled systems UQ approach is that it enables heterogeneous uncertainty quantification methods to be applied throughout the coupled system, and the feasibility of this idea was demonstrated in this report. As was shown in Section 4.1 however, this always results in a fully coupled nonlinear system for the expansion coefficients, even when normally uncoupled sampling methods are applied. This is true unless the same sampling method in the same basis is applied throughout the coupled system. Thus the potential benefits of reducing the cost of the uncertainty computation in each system component has to be weighed against the increased complexity and likely computational cost of needing to form and solve the fully coupled nonlinear system at the coupled system level. To address this issue, it is necessary to build simulation tools for coupled system components that support a variety of uncertainty quantification methods, and coupling tools that are

capable of both forming the fully coupled nonlinear systems arising from heterogeneous UQ, and can apply the strong solution strategies discussed in this report.

The second advantage of this approach is that it allows dimension reduction ideas to be applied at the interface between coupled system components, and again the feasibility of this was demonstrated in this report. Here the potential cost savings is quite dramatic, due to the exponential growth in computational cost with the dimension of the stochastic space for many of the stochastic Galerkin UQ methods. However this does not come without its costs as well. For multi-physics systems, the discrete Karhunen-Loève eigensystem (4.68) must be formed and solved for the eigenvectors and eigenvalues defining the new stochastic coordinates, then new basis functions must be generated based on the probability distribution of these new coordinates. For interfacial and network systems, only the latter step is required. Furthermore, these calculations must be performed at each iteration of the overall nonlinear solution process. It is unclear what effect, if any, this has on the convergence of the overall nonlinear solution process as well. Thus the benefit of reduced dimension must be weighed against the costs of these extra transformations, and possibly extra nonlinear iterations, to determine the overall benefit. Again, such comparisons can only be made with software tools implementing these ideas that can be applied to challenging coupled systems of interest.

In conclusion then, we see three fundamental research areas that must go forward for these ideas to have impact on challenging coupled systems:

1. Computational tools for random field modeling including Karhunen-Loève expansions of random fields defined by stochastic Galerkin expansions.
2. Computational tools for generating stochastic Galerkin expansions over stochastic spaces with general probability distributions.
3. Software tools for simulating coupled systems that support the intrusive UQ ideas presented here, including forming and solving heterogeneous UQ nonlinear systems, and applying dimesion reductions with corresponding stochastic coordinate/basis changes at each iteration.

We note that software tools for the first item are underway, through the PECOS library, which was partially supported through this LDRD. Initial software components in the direction of item three were also created through this LDRD, as part of the Albany rapid production project. However for these ideas to have any significant impact on real applications, a multi-year project dedicated to bringing these ideas together in a general computational and software framework will be necessary.

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