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Experiment-Based Validation and Uncertainty Quantification of Partitioned Models: Improving Predictive Capability of Multi-Scale Plasticity Models

Garrison N. Stevens
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EXPERIMENT-BASED VALIDATION AND UNCERTAINTY QUANTIFICATION OF PARTITIONED MODELS: IMPROVING PREDICTIVE CAPABILITY OF MULTI-SCALE PLASTICITY MODELS

A Dissertation
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Civil Engineering

by
Garrison N. Stevens
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Presented to:
Dr. Sez Atamurktur, Committee Chair
Dr. Andrew Brown
Dr. Qiushi Chen
Dr. Hsein Juang
ABSTRACT

Partitioned analysis involves coupling of constituent models that resolve their own scales or physics by exchanging inputs and outputs in an iterative manner. Through partitioning, simulations of complex physical systems are becoming evermore present in scientific modeling, making Verification and Validation of partitioned models for the purpose of quantifying the predictive capability of their simulations increasingly important. Parameterization of the constituent models as well as the coupling interface requires a significant amount of information about the system, which is often imprecisely known. Consequently, uncertainties as well as biases in constituent models and their interface lead to concerns about the accumulation and compensation of these uncertainties and errors during the iterative procedures of partitioned analysis. Furthermore, partitioned analysis relies on the availability of reliable constituent models for each component of a system. When a constituent is unavailable, assumptions must be made to represent the coupling relationship, often through uncertain parameters that are then calibrated.

This dissertation contributes to the field of computational modeling by presenting novel methods that take advantage of the transparency of partitioned analysis to compare constituent models with separate-effect experiments (measurements contained to the constituent domain) and coupled models with integral-effect experiments (measurements capturing behavior of the full system). The methods developed herein focus on these two types of experiments seeking to maximize the information that can be gained from each, thus progressing our capability to assess and improve the predictive capability of
partitioned models through inverse analysis. The importance of this study stems from the need to make coupled models available for widespread use for predicting the behavior of complex systems with confidence to support decision-making in high-risk scenarios.

Methods proposed herein address the challenges currently limiting the predictive capability of coupled models through a focused analysis with available experiments. **Bias-corrected partitioned analysis** takes advantage of *separate-effect experiments* to reduce parametric uncertainty and quantify systematic bias at the constituent level followed by an integration of bias-correction to the coupling framework, thus ‘correcting’ the constituent model during coupling iterations and preventing the accumulation of errors due to the final predictions. Model bias is the result of assumptions made in the modeling process, often due to lack of understanding of the underlying physics. Such is the case when a constituent model of a system component is entirely unavailable and cannot be developed due to lack of knowledge. However, if this constituent model were to be available and coupled to existing models of the other system components, bias in the coupled system would be reduced. This dissertation proposes a novel statistical inference method for **developing empirical constituent models** where *integral-effect experiments* are used to infer relationships missing from system models. Thus, the proposed inverse analysis may be implemented to infer underlying coupled relationships, not only improving the predictive capability of models by producing empirical constituents to allow for coupling, but also advancing our fundamental understanding of dependencies in the coupled system. Throughout this dissertation, the applicability and feasibility of the proposed methods are demonstrated with advanced multi-scale and
multi-physics material models simulating complex material behaviors under extreme loading conditions, thus specifically contributing advancements to the material modeling community.
DEDICATION

I dedicate this dissertation to my family for their constant love and support.
ACKNOWLEDGEMENTS

I would first and foremost like to thank my advisor and committee chair, Dr. Atamturktur, for her guidance and support during my graduate studies and research. I would also like to thank Dr. Ricardo Lebensohn and Dr. George Kaschner of Los Alamos National Laboratory with their assistance with the Viscoplastic Self Consistent Code and the zirconium data used in this dissertation. I am grateful to Dr. Cetin Unal and Dr. Brian Williams for their guidance and collaboration in the development of the methodologies presented. Many thanks also go out to my committee members Dr. Andrew Brown, Dr. Qiushi Chen, and Dr. Hsein Juang for their willingness to mentor and serve on my committee throughout my journey at Clemson. Finally, I would like to thank the Department of Education: Graduate Assistance in Areas of National Need program as well as the Department of Energy: Nuclear Energy University Programs for providing funding in support of this research.
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CHAPTER ONE

INTRODUCTION

1. Motivation for the Dissertation

Physical phenomena in nature rarely act independently; rather, they interact with each other forming complex systems. In the past, these systems have been analyzed individually by either neglecting their mutual interactions or establishing unwarranted assumptions regarding the nature of the interactions. The evolution of partitioned analysis techniques over the last two decades, combined with advancements in high performance computing, have made it possible to develop coupled computer models for analyzing such interdependent systems by rigorously and realistically considering the exchange of inputs and outputs (Groen et al., 2012). Such advancements in modeling and simulations have been especially useful for the evaluation of high-consequence scenarios, such as failure analysis of nuclear reactors, performance of ballistic missile defense systems and blast damage to critical structures (Terejanu et al., 2011; Groen et al., 2012; Knezevic et al., 2012).

Partitioned analysis involves using iterative procedures to couple independently developed constituents. These coupled models may then be used to predict the behavior of the holistic system, more complex than the individual constituents themselves (Farajpour and Atamturktur, 2013). The focus of this dissertation on partitioned analysis methods is motivated by the distinct advantages of partitioned methods to utilize existing codes while bridging between disciplines. However, parameterization of the constituent models as well as the coupling interface requires a large amount of non-trivial
information about the system, which is often imprecisely known. Consequently, uncertainties inherent in the constituent and at the interface lead to concerns about accumulation of uncertainties in coupled model predictions (Bunya et al., 2010; Dietrich et al., 2010). In addition to uncertainties, the constituent models and the coupling interface may also have biases, which may compensate for each other or accumulate during iterative coupling operations (Avramova and Ivanov, 2010). It is therefore critical to establish the validity of the predictions derived from these coupled models to ensure their efficacy in decision-making. However, while there are well-established methods for validation for single-domain models, validation methods for coupled models have yet to be fully elucidated.

In this context, model validation is a means of instilling confidence in the predictive capability of numerical models through the systematic comparisons of model predictions against physical experiments (Schwer, 2007). Separation of constituent models into their relative domains through partitioned analysis creates a transparency within the system. This transparency, which has yet to be capitalized upon, results from the ability to gain information from both the constituent models, using separate-effect experiments in their respective constitutive domains, as well as the coupled model, using integral-effect experiments conducted in the coupled domain. The objective of this dissertation is to utilize the transparency partitioned analysis offers to develop useful, validated coupled models, be they multi-scale or multi-physics in nature. Development of a model validation framework amenable to benefit from distinct sets of experimental information will complement the recent widespread efforts on the development of
sophisticated coupled methods and accommodate the assessment of errors and uncertainties associated with coupled model predictions.

2. Main Contributions of the Dissertation

This dissertation contributes to the field of computational modeling by targeting separate-effect and integral-effect experiments in the development of methods to improve the assessment and mitigation of bias and uncertainties in strongly coupled models as well as develop constituents for unknown or uncertain coupling relationships. The importance of this study stems from the need to make coupled models available for widespread use for predicting the behavior of complex systems with confidence to support decision-making in high-risk scenarios.

Two unique methods are proposed in this dissertation to address the challenges currently limiting the predictive capability of coupled models, each focusing on a different type of experimental data. First, bias-corrected partitioned analysis is a method proposed to take advantage of separate-effect experiments to infer parameter values and systematic bias at the constituent level followed by an integration of this information into the coupling framework (Figure 1.1 top). In this figure, $\Psi$ represents the model bias of a constituent, which is quantified through comparison with separate-effect data. This approach has the benefit of ‘correcting’ the constituent model during coupling iterations and preventing the accumulation of errors due to model bias.
Bias-Corrected Partitioned Analysis

*Separate-effect* data is used to mitigate bias and uncertainty of coupled models at the constituent level.

*Chapter 3*

In numerical models of complex systems, systematic bias may be the result of neglected relationships, which could be represented by constituent models if they were attainable. Thus, the next contribution of this dissertation implicates integral-effect experiments to develop empirical constituent models, defining the nature of the missing engineering principles, through inverse analysis with existing physics-based constituents.

**Inference of Constituent Models**

*Integral-effect* data is used to improve predictive capability through development of coupled models in the absence of constituent knowledge or separate-effect experiments.

*Chapter 4*

Thermo-mechanical Coupling

*Chapter 5*

Elasto-plastic Multi-scale Coupling

Figure 1.1. Proposed methods for leveraging (top) separate-effect experiments and (bottom) integral-effect experiments for advancing coupled modeling capabilities.

In numerical models of complex systems, systematic bias may be the result of neglected relationships, which could be represented by constituent models if they were attainable. Thus, the next contribution of this dissertation implicates integral-effect experiments to develop empirical constituent models, defining the nature of the missing engineering principles, through inverse analysis with existing physics-based constituents.
(Figure 1.1 bottom). Herein, information related to these unknown constituent relationships is investigated through inverse analysis of integral-effect experiments. A novel statistical tool for inferring dependent relationships between parameters of a physics-based constituent model is presented. The functional form of this dependence inferred through the inverse methodology results in an empirical representation of the missing constituent model (indicated by grey boxes in Figure 1.1 bottom). Once an empirical constituent is available, a model developer may then couple this new constituent model to existing physics-based models with partitioned procedures to produce a new coupled model representing the dependencies that were previously neglected. Inference of such underlying constituent relationships not only stands to improve the predictive capability of the models, but also holds the potential to advance scientists’ fundamental understanding of the coupled system.

Each of the approaches and methods proposed in this dissertation may relate to the improvement of multi-scale or multi-physics models. Throughout this dissertation, the applicability and feasibility of the proposed methods are demonstrated with multi-scale or multi-physics material models. Multi-scale simulations involve a strongly coupled Finite Element – Viscoplastic-Self Consistent model that predicts elastic behavior at the macro-scale and viscoplastic behavior and texture development at the meso-scale for representing anisotropic zirconium exposed to creep loading. Multi-physics simulations involve a weakly coupled thermo-mechanical simulation of 5182 aluminum alloy operating under a set of various high temperature loads. Hence, the focus on modeling of
advanced material behaviors throughout the dissertation makes a contribution specifically to the material modeling community.

3. Dissertation Organization

This dissertation is organized into six chapters described in the following paragraphs.

Chapter two presents a review of coupling techniques for strongly coupled partitioned analysis problems, evaluating current practices in model verification, calibration, validation, and resource allocation. This chapter covers a breadth and depth of literature in current partitioned procedures and identifies areas of future research in the field. This review is a peer-reviewed journal publication that has been accepted to Archives of Computational Methods in Engineering.

Chapter three discusses the propagation of bias and uncertainty in a strongly coupled multi-scale plasticity model for predicting creep of a highly anisotropic zirconium material. This chapter presents a new bias-corrected partitioned analysis paradigm for improving the predictive capability of coupled models through knowledge gained by separate-effect experiments. This paradigm is demonstrated with a multi-scale model coupling a macro-scale finite element model and meso-scale VPSC material model. The chapter is a peer-reviewed journal manuscript published in the Journal of Multidiscipline Modeling in Materials and Structures.

1 Chapters 2-5 in this dissertation serve as stand-alone journal publications, therefore, some level of conceptual overlap is necessary.
Chapter four proposes a novel statistical method for inverse analysis of existing physics-based constituent models and integral-effect experiments to infer neglected coupling relationships. This method takes advantage of the information stored in integral-effect experiments to introduce a means of developing coupled models in situations where all of the knowledge to develop a purely physics-based model was unavailable or too computationally demanding for implementation. Opportunities enabled by this inverse methodology are demonstrated through a thermo-mechanical application, where the existing physics-based VPSC model predicts texture evolution of an aluminum alloy. Integral-effect experimental data of alloy specimens tested under different temperature conditions demonstrate a dependence of material properties on temperature setting, a thermo-mechanical relationship that the VPSC model is not capable of predicting on its own. Through the proposed Bayesian inverse analysis an empirical constituent model representing the thermal behavior of the system is developed and coupled to the VPSC model, producing newly developed coupled simulations with quantified uncertainty. This chapter is submitted as a technical manuscript to *Structural and Multidisciplinary Optimization*.

Chapter five extends the inverse methodology presented in chapter four for application to strongly coupled model development. These strongly coupled models used to represent systems that have a mutual dependence upon one another, communicate from one constituent to the next iteratively, posing a complex problem for inverse analysis. In this chapter the Bayesian inference method is applied to a multi-scale simulation of anisotropic elasto-plastic zirconium. Through this analysis the ability to infer the plastic
strain as a function of stress predicted by a finite element model by comparison with integral-effect strain measurements is demonstrated. The result of the proposed procedure is an empirical plasticity model that is then coupled to the finite element model for full system predictions. This chapter is in preparation for submission as a technical manuscript to the *International Journal of Numerical Methods in Engineering*.

Finally, chapter six summarizes the contributions of this dissertation. This overview includes the benefits, limitations, and future work associated with each new method presented.

**References**


CHAPTER TWO
MITIGATING ERROR AND UNCERTAINTY IN PARTITIONED ANALYSIS: A REVIEW OF VERIFICATION, CALIBRATION AND VALIDATION METHODS FOR COUPLED SIMULATIONS

1. Introduction

With advancements in parallel computing, computational models of physical and engineering systems that concurrently resolve multiple scales or physics have come to the forefront of scientific computing. Partitioned analysis represents complex systems by coupling constituent models (i.e. those focused on a single physics or scale without considering interactions), allowing them to interact and affect each other’s inputs in an iterative manner. In this process, both the constituent models and the coupling interface are contaminated with uncertainties and errors, which propagate during coupling iterations, degrading the predictive capability of the full system model. Verification and Validation is a field of study that addresses uncertainties and errors in numerical models and seeks to assess and improve the predictive capability of simulations (Schlesinger, 1979; Sargent, 1981; Roache, 1997; AIAA, 1998). It is only through verification and validation that the notion of predictive modeling becomes viable.

Model verification\(^2\) entails confirming numerical accuracy in a computational model (Thacker et al., 2004). Partitioned modeling provides the opportunity to evaluate

\(^2\) Verification procedures are further broken down into code verification (ensuring the computer code has been written correctly) and solution verification (quantifying numerical errors
the numerical errors in each of the constituents and trace the effect of such numerical errors through coupling operations, but comes with the requirement to evaluate numerical errors introduced by operations at the coupling interface. This is a particularly important issue for coupled models as the numerical errors may negatively influence the convergence of coupling iterations (Bejarano and Jin, 2008). Furthermore, if numerical errors are unduly large, convergence may not be achieved or worse, the coupled system may converge to an incorrect solution (Kim et al., 2009). Therefore, verification is a prerequisite step to validation to instill confidence that the model is indeed converging to the numerically correct solution (Atamturktur et al., 2012).

Model validation is the next step in preparing models for implementation in decision-making. It is important to differentiate between errors evaluated through verification and those evaluated through validation (Freitas, 2002): verification focuses on the numerical errors and uncertainties (i.e. mathematical aspects of the problem) while validation focuses on the representations of physics principles in the constituent models and their interface as well as the parameters that are part of these models (i.e. physical aspects of the problem) (Roache, 1997). As such, validation links the model to the physical world by assessing the agreement of model predictions with experimental measurements (Trucano et al., 2006). When necessary, the model’s predictive capability can be improved through calibration of parameter values and correction of systematic bias in model predictions. The modularity of partitioned analysis strengthens calibration introduced by factors such as round-off, iterations, and discretization) (Roy, 2005). Herein, we focus on solution verification.
and validation practices by making it possible to leverage separate-effect experiments, conducted at the constituent domains, as well as integral-effect experiments, conducted at the full system domain.

A distinct advantage of partitioned analysis, which has yet to be fully exploited, is the transparency it offers in the verification and validation process through the decomposition of a full system model into constituents. Highly complex systems have interconnected constituents and components where coupling takes place at multiple levels resulting in a hierarchy of model integration: constituents representing a functional unit are coupled to represent components that are in turn coupled to represent the full system (Oberkampf and Trucano, 2002). Figure 2.1 illustrates the transparency of partitioned analysis in that a model developer gains the ability to complete verification as well as calibration and validation against separate, intermediate, and integral-effect experimental data at every level as the models become progressively integrated.

3 “Constituent” is used to define a model representing an isolated physical phenomena or behavior within a scale. “Component” involves the coupling of some constituents, but does not resolve the full system.
Figure 2.1. Hierarchical scheme for multi-level coupling where separate-effect experiments relate to constituent models, intermediate-effect experiments relate to component models and integral-effect experiments relate to system models.

Improvements to a model’s predictive capability often require distribution of limited resources among code development and experimentation in a systematic manner (Atamturktur et al., 2015a). Thus, decisions must be made to select either further code development or extended experimental campaigns when the predictive capability of a model is not found to be satisfactory. Once again, partitioned analysis adds a new level of intricacy to this process from the established procedures for single-solver models, as the model developer is faced not only with decisions regarding settings for new tests or code development, but also selection of the constituent domains for which these tests and development should be completed. The complexity of these decisions warrants a systematic framework integrating verification and validation practices with allocation of available resources for the optimal improvement to predictive capability.
This article presents a thorough discussion on the realm of opportunities as well as new challenges partitioned analysis presents for development and improvement of coupled models, be they multi-scale or multi-physics in nature, through a review of the recent literature in this highly interdisciplinary field. Section 2 introduces partitioned analysis along with commonly implemented algorithms for iterative coupling. Section 3 reviews sources of numerical errors unique to partitioned models, which should be carefully considered during verification. Section 4 explores methods to take advantage of different levels of experiments in calibration and validation of partitioned models. Recommended procedures for resource allocation to carry out these verification, calibration, and validation activities are presented in Section 5. Finally, Section 6 concludes the review with a discussion of areas calling for future work.

2. Coupling Algorithms

2.1. Introduction to Coupled Modeling

In partitioned analysis, a complex science or engineering problem is decomposed into multiple domains based on functional, physical or scale-related differences. Partitioned analysis operates through execution of constituent models resolving each domain such that some of the input(s) of a constituent are defined by the output(s) of another. In contrast, the monolithic approach models the full system using one entity rather than several constituents (Felippa et al., 2001). Partitioned analysis is advantageous over monolithic modeling, as it allows the use of existing mature models, supplies flexibility in the solvers of constituents, maintains modularity, and takes full advantage of parallel computing (Michler et al., 2004; Matthies et al., 2006; Néron and Dureisseix,
2008). Also, partitioned analysis is often more practical due to its ability to carry out simulations of subsystems using solvers, integration schemes, boundary conditions and time steps appropriate to the specific domain, which are often already well-established by domain experts (Wüchner et al., 2007; Järvinen et al., 2008). Take, for example, the frequently encountered need to implement different boundary conditions for each domain in fluid-structure interaction simulations (Jahromi et al., 2007). Dirichlet-Neumann (also referred to as Dirichlet-Robin) coupling scheme allows for the fluid and structure to be separated into two domains, where the fluid constituent is solved with a Dirichlet (commonly referred to as strong) boundary condition and the structure constituent is solved with a Neumann (commonly referred to as weak) boundary condition (Badia et al., 2008). The flexibility to maintain separate boundary conditions with this approach allows for the deformation of the fluid to be easily accounted for while also easing the linking of fluid and structure domains, making the coupling more robust than methods requiring a strongly matched boundary condition on both domains as in monolithic models (Houzeaux and Codina, 2003). Through the flexibility to maintain domain-specific best practices, partitioned analysis has already opened the door for bridging traditionally isolated domains, such as fluid-structure interaction (Causin et al., 2005; Matthies et al., 2006), thermal-structure interaction (Felippa et al., 2001), soil-structure interaction (Jahromi et al., 2007), acoustic-structure interaction (Yoon et al., 2006), aerodynamics (Zhili and Jun, 2009), atmospheric and weather modeling (Harris et al., 2003; Lieber and Wolke, 2008), as well as multi-scale problems bridging atomistic, polycrystalline, and continuum scales (Knezevic et al., 2012; Abdulle and Jecker, 2014; Olson et al., 2014).
Coupling in partitioned analysis can be either weak, where the dependence between models is only one directional, or strong, where the compatibility and equilibrium equations are satisfied at the interface (Trčka et al., 2010). Schematics of such weak and strong coupling are shown in Figure 2.2 for two constituent models representing the behavior of a structural system with two domains. In both weakly and strongly coupled systems, the force output of the first constituent is transferred at the interface to the second constituent as an input. In the weakly coupled system (Figure 2.2a) there is no feedback from the second constituent back to the first, rather the displacement prediction of the second constituent simply progresses to the next time step. In the strongly coupled system (Figure 2.2b), however, there is communication across the interface in both directions, where the displacement predicted by the second constituent is entered into the first constituent for the recalculation of force. Therefore, the strong coupling requires iterations that continue until convergence is reached within reasonable tolerance limits at which point the model would progress to the next time step.

Strong coupling is referred to in the literature under a variety of names, including full (Farajpour and Atamturktur, 2012a), tight (Quaranta et al., 2004), onion (Hensen, 1999), and implicit (Valdés et al., 2012) coupling. For time dependent problems, strong coupling methods have been reported to provide better accuracy (Heil, 2004; Ahn and Kallinderis, 2006) and to be more stable when compared to weak coupling due to the sub-iterations within each time step compared to the once-per-time-step exchange of weak coupling (Wüchner et al., 2007). To improve the stability of a weakly coupled model,
small time steps are generally needed, whereas strong coupling is capable of remaining stable with large time steps (Ahn and Kallinderis, 2006).

![Diagram of weak and strong coupling]

(a) weak coupling

(b) strong coupling

Figure 2.2. Schematic representation of strong and weak partitioned analysis.

2.2. Partitioned Coupling Algorithms

In strong coupling, the fundamental purpose of coupling iterations is to determine the values for the shared inputs and outputs, without which neither constituent model can be executed. The simplest, and perhaps most intuitive, means for achieving strongly coupled models is the Block-Jacobi method (Fernández and Moubachir, 2005; Matthies et al., 2006), in which the outputs of each constituent are transferred all at once as the inputs to the other constituent(s) in the next iteration (Figure 2.3a). The Block-Jacobi scheme has the advantage of being highly parallelizable by allowing execution of all
constituents simultaneously (Hofman, 2003). Convergence of this coupling method, however, is not guaranteed even when starting values assigned to dependent parameters are arbitrarily close to the true values (Matthies and Steindorf, 2002).

Figure 2.3. Iterative coupling algorithms (a) Block-Jacobi method, (b) Block Gauss-Seidel method, (c) Block Jacobi and Block Gauss-Seidel Hybrid method (d) Optimization-Based Coupling method (e) Newton-like methods.

Figure 2.3b presents the Block Gauss-Seidel method, in which the transfer of outputs of each constituent is completed strictly in a predefined sequence (Joosten et al., 2009; Mahrenholz and Lumkes, 2010). This method has been reported to converge faster than the Block-Jacobi method (Cervera et al., 1996). This advantage however is countered by the fact that the Block Gauss-Seidel algorithm is a staggered procedure, where one constituent waits for the execution of the other, degrading computational
efficiency due to the lack of parallelizability. Furthermore, the convergence of Block Gauss-Seidel exhibits dependency on the order of operations (Menck, 2002; Adams et al., 2003; Yeckel et al., 2009). For simple problems, the order of constituents that guarantees convergence may be found mathematically by calculating the convergence factor and for more complex problems through trial and error. In either case, the dependence on the order of operations increases the computational demands. Especially for problems involving multiple constituents, the order that yields converged solutions becomes difficult to determine in a feasible manner (Farajpour and Atamturktur, 2013). To improve convergence characteristics and reduce the dependency on the ‘correct’ order of constituents, relaxation methods have been implemented (Joosten et al., 2009; von Scheven and Ramm, 2011). Relaxation improves convergence by manipulating constituent outputs before they are exchanged at the interface, improving upon the current solution using values from previous increments (Küttler and Wall, 2008; Joosten et al., 2009). Determination of optimal relaxation factors is reported to be influential in the success and acceleration of convergence (von Scheven and Ramm, 2011). Relaxation factors that are too large can lead to divergence, while factors that are too small can lead to unnecessary iterations (Küttler and Wall, 2009). There are several methods to compute the optimal relaxation parameter, the most commonly implemented being Aitken iteration and Gradient methods (Wall et al., 2007). It is important to note that although relaxation algorithms improve the possibility of convergence, they do not guarantee it (Derby et al., 2007).
In recognition of theses limitations, hybrid approaches (for instance, integrating Block Gauss-Seidel and Block Jacobi methods) have been developed to improve the computational efficiency and parallelizability of the Block Gauss-Seidel algorithm. An example of one such hybrid method is shown in Figure 2.3c. The hybrid approach exploits the parallelizability of Block Jacobi methods with the coupling scheme of Block Gauss-Seidel, where the constituents are divided into groups (Evans, 1984) such that one group runs in parallel using Block Jacobi (making these constituents entirely parallelizable), while the other group waits for outputs of these constituents to couple in a Block Gauss-Seidel approach (Zohdi, 2008). Once convergence of the values is achieved, the Block Gauss-Seidel method is once again applied to transfer the updated values between constituents (Wei’s s et al., 1999; Kowarschik et al., 2000; Zohdi, 2008). Hybrid methods have been shown to speed up convergence compared to the individual methods implemented independently (Harris et al., 2003). Hybrid methods, however, become difficult to implement for high dimensional problems dealing with many constituent models (Adams et al., 2003).

Another solution strategy for strong coupling is the optimization-based approach (Farajpour and Atamturktur, 2012b; Abdulle and Jecker, 2014; Olson et al., 2014). Optimization-based coupling has the advantage of solving constituents simultaneously through an objective function consisting of the coupling conditions. The objective function is minimized during coupling to determine the dependent parameter values (Figure 2.3d). Optimization-based methods are well suited for nonlinear problems since the nonlinearities in the coupling can be inherently addressed in the optimization function.
(Gunzburger and Lee, 2000). Solving constituents simultaneously in optimization-based coupling eliminates the dependence of convergence on predefined sequence faced in the Block Gauss-Seidel method. Additionally, the simultaneous solving of the constituents makes this method highly parallelizable. However, this improved computation from parallelization is typically compromised by the larger number of iterations needed as well as the computational burden of the optimization algorithm compared to other methods (Gunzburger and Lee, 2000; Farajpour and Atamturktur, 2012b).

Coupling of constituent models can also be achieved through Newton methods in which predictions of each constituent, computed by finding the roots of the governing equations, from the previous time step are used to update the functional form of the constituents for the next iteration (Figure 2.3e) (Abdulle and Jecker, 2014; Ben-Israel, 1966; Fernández and Moubachir, 2005; Heil, 2004; Matthies and Steindorf, 2002, 2003). Newton methods require a reduced number of iterations in comparison to Block Gauss-Seidel; however the demands of calculating the derivatives often increase computational expenses (Matthies and Steindorf, 2002; von Scheven and Ramm, 2011). For instance, the classic Newton-Raphson method, which calculates the exact Jacobian to find the roots of a governing equation, is known to have quadratic convergence (von Scheven and Ramm, 2011). However, the improved rate of convergence is countered by the high computational costs of calculating the exact Jacobian. Newton-Krylov methods improve upon the Newton-Raphson method by using a linear finite difference calculation to approximate the Jacobian, resulting in lower computational time than Newton-Raphson (Erban et al., 2006; Hammond et al., 2005; Michler et al., 2004; von Scheven and Ramm,
2011). Additionally, the Newton-Krylov requires significantly lower matrix storage, resulting in notably less memory requirements making the method desirable for large scale problems (Brown and Saad, 1990; Jones and Woodward, 2001). The computational benefits of linear Krylov estimation come with little sacrifice in accuracy compared to traditional Jacobian Newton methods, and even improved accuracy over other estimation methods such as the backward Euler (Rider et al., 1999). However, maintaining a high degree of accuracy in Krylov methods is dependent upon appropriate selection and application of pre-conditioners, which seek to reduce the number of iterations needed by informing the problem of suspected trends that would appear in the Jacobian (Brown and Saad, 1990; Knoll and Keyes, 2004).

3. Numerical Errors In Partitioned Analysis

Discrete modeling of any finite length, whether spatial or temporal, introduces discretization errors into a problem (Freitas, 2002). Further errors are introduced in partitioned models when the discretization of different domains does not match. Interpreting converged solutions of iterative procedures requires an understanding of these numerical errors inherent in predictions, which can be assessed through solution verification⁴ (Roy, 2005; Thacker et al., 2004). Assessment of these errors is particularly important in partitioned analysis because convergence of coupling iterations is dependent

⁴ The term “numerical error” is an umbrella term indicating three main sources of error: round-off, truncation, and discretization. We note that when one does not have a “truth” to compare to, the term numerical error can be referred to as “numerical uncertainty.” Herein the focus of the following sections is relative to discretization as this is the factor most influential in introducing errors in coupled models.
upon the numerical errors (Bejarano and Jin, 2008). In fact, convergence may not be achieved if the spatial discretization (i.e. mesh) and temporal discretization (i.e. time step) are not sufficiently refined (Roache, 1994). In addition, selected coupling algorithm also exhibits strong influence on the manner in which numerical errors propagate through the interface and ultimately on numerical errors of the fully coupled solutions (Larson, 2005).

3.1. Spatial Alignment

Maintaining discipline-specific best-practice for spatial discretization of each constituent model, which can help reduce numerical errors, is a benefit of partitioned analysis (Rangavajhala et al., 2011). Preserving these discipline-specific modeling strategies, however, may result in mesh mismatch, meaning that different mesh sizes and element types may be required for each domain (Jaiman et al., 2005) (illustrated in Figure 2.4). An additional source of numerical error results from the exchange of inputs from nodes having different spatial locations. Spatial alignment of coupling parameters is required when mesh mismatch causes the nodes of one domain to misalign with another, making it necessary to interpolate or extrapolate nodal values between the meshes. This issue is accentuated in strongly coupled models as opposed to weakly coupled models, due to the iterative nature of strong coupling passing parameters between domains multiple times (Rangavajhala et al., 2011). There are two scenarios common in coupled modeling where spatial alignment may be required, mismatched meshes (Figure 2.4a) and embedded meshes (Figure 2.4b).
Figure 2.4. Two constituent domains with mismatched meshes: (a) spatial meshes mismatched at the boundary (b) embedded meshes mismatched internally.

An intuitive option for reducing errors resulting from spatial synchronization is refining constituent meshes, which will in turn decrease the degree to which solutions are mismatched across the mesh. In partitioned analysis, there tend to be a number of possibilities for mesh refinement due to the many combinations of constituents paired with several refinement options for each. Computational demands become a concern, however, as computational time increases for running a refined model, limiting the number of refinement combinations that are feasible to test.

Mismatched meshes. When mapping outputs at the mesh interface, important conditions to consider include are conservation of energy, conservation of loads, order of convergence, and computational efficiency (de Boer et al., 2007). For mapping outputs between domains, nearest neighbor interpolation, projection methods, and interpolation by splines are widely-implemented options. Nearest-neighbor interpolation, in which data is transferred from the node in $\Omega_1$ to the closest node in $\Omega_2$ (Figure 2.4a) (Thévenaz et al., 2000), is the simplest method to implement but is only recommended for cases where the domains are close to matching, otherwise large errors may be introduced (de Boer et al.,
Projection methods, which transition solutions from one element type to another through specific schemes such as node-projection, quadrature-projection, and common-refinement, offer the benefit of improved accuracy (Jaiman et al., 2005). Node-projection scheme (Farhat et al., 1998), which projects an output of a fluid mesh node onto a surface solid element and then maps from the surface element to the solid nodes, has been found to have the highest error of available projection methods. Similarly, quadrature-projection scheme (Cebral and Lohner, 1997), which projects fluid quadrature points onto a solid surface element and then extrapolates to the solid boundary, has been shown to result in significant errors, though to a lesser degree than node-projection. Common-refinement scheme (Jiao and Heath, 2004), which defines sub-elements along the interface to average nodal outputs from both domains until convergence is achieved, has been found to be far superior to the other methods, reducing error in the coupled model orders of magnitude over node-projection and solid-projection in 2-dimensional simulations. However, the method comes with the restriction of being difficult to expand to 3-dimensional applications.

Embedded meshes. When the meshes are embedded, the domain of one constituent ($\Omega_2$ in Figure 2.4b) is completely immersed within another constituent ($\Omega_1$ in Figure 2.4b) (Tan et al., 2006). Computational fluid dynamics is the most common application of embedded meshes in the literature since fluid dynamics often incorporates a broad range of length scales, as demonstrated by applications with boundary layers or simulation of shock waves (Baker, 1997). Furthermore, in a fluid-structure interaction simulation, errors in the embedded model can fluctuate and be significantly higher than
other coupling methods that force a conformance of mesh boundaries between the domains (van Loon et al., 2007). Cartesian grid embedded boundary method is one approach for dealing with embedded meshes, favored for its simplified grid generation, data structures, and numerical methods. Johansen and Colella (Johansen and Colella, 1998) have tested the Cartesian grid embedded boundary method and proven the method to be second-order accurate without requiring unreasonable computational demands. An embedded mesh can also be aligned differently than the containing mesh. A coupled model with a misaligned embedded mesh, as opposed to a mesh where both domains are aligned, has been shown to result in higher errors in the final, full-system prediction (Tan et al., 2006).

3.2. Temporal Synchronization

Similar to spatial discretization, a common practice in the development of coupled models is maintaining independent time steps for each constituent domain. This practice arises from two key concerns: stability of the computations and computational demands. Stability of computations requires sufficiently small time steps in each computational domain, while computational demands make the implementation of a consistently small time step to match across all domains infeasible. Consideration of both of these factors often results in time steps that are either sub-stepped (Figure 2.5a) or misaligned (Figure 2.5b) to accommodate the domain requiring smaller time steps while maintaining computational efficiency in the other domain. Fluid-structure interaction problems provide an excellent example for the benefit of varied temporal discretization schemes as fluid flow models often require time steps orders of magnitude smaller than structural
models, however, each time step of a structural model is typically significantly greater in terms of computational demands (Fu et al., 2011). Thus, a serious conflict exists between the two objectives should the modeler try to match the time steps of both domains. Implementation of sub-stepping schemes, where the smaller time step is a fraction of the larger time step, has been found successful for computing stable solutions within reasonable computational demands for a multitude of fields, including fluid-structure interactions (Fu et al., 2011), electromagnetic interactions (Zhen et al., 2000), and plasticity modeling (Zhang et al., 2014, 2004).

(a) Sub-stepped time domains where the time step of $\Omega_2$ is $n$ times finer than that of $\Omega_1$.

(b) Unaligned time domains where the time step of $\Omega_2$ is three quarters that of $\Omega_1$ causing interpolation and extrapolation of outputs at the misaligned time step (dashed line).

**Figure 2.5. Constituent models with varied time steps.**

The concept of sub-stepping has been extended by Berrone (Berrone, 2009) by applying local sub-steps on an element to element basis. In this approach, the global time step remains the same for the entire model, but local time steps of elements in detailed
areas of the model are allowed to vary throughout the simulation. This approach maintains more accurate local solutions without significantly increasing computational demands of the complete model. Staggered approaches further address coupling of models with different time steps by having the model with a larger time step feed information backwards to the model with the smaller time step (Figure 2.6) (Pegon and Magonette, 2005; Bonelli et al., 2008). In this approach, one domain passes information forward two time steps ahead, then allowing the coupled parameters from the new time step to be shared with the second constituent, which may then update the first constituent. Following this procedure reduces the wait time between constituents, increasing the efficiency by allowing both constituents to compute simultaneously.

Figure 2.6. Parallelized staggered approach for coupling two constituent models.
4. Systematic Bias And Uncertainty In Partitioned Analysis

The coupling of constituent models in partitioned analysis allows systematic biases and uncertainties in model predictions to propagate from one constituent to the next. This propagation which occurs during iterative coupling operations makes partitioned analysis prone to not converging, or worse, converging to inaccurate solutions. Such *inaccurate convergence* is particularly worrisome, as it may make the solution appear plausible giving false confidence to the model developers about inaccurate scientific findings (Kim et al., 2009). Inaccurate convergence, observed in numerical simulations covering full spectrum of science and engineering fields, such as atmosphere-ocean interaction simulations (Döscher et al., 2002) and flow gasification models (Kumar and Ghoniem, 2012a), have been attributed to a variety of causes, including systematic bias and uncertainty in constituent model outputs and incomplete or simplified coupling of outputs at the coupling interface. The latter of these is referred to as interface systematic bias (Farajpour and Atamturktur, 2014) and is yet to be explored to the same degree as constituent model systematic bias.

Reducing systematic bias and uncertainty in coupled models is a highly important, non-trivial task. Model *calibration* leverages experimental measurements to infer both the likely values for poorly known model input parameters as well as the systematic bias inherent in predictions that cannot be remedied by manipulating input parameters, and is an area well-developed for single-solver models (i.e. those focused on single physics or scale without considering interactions) in nearly every field, ranging from economics to engineering (Hemez and Doebling, 2001; Werker and Brenner, 2004; Park and Qi, 2005;
Higdon et al., 2007; Hemez et al., 2010; Atamturktur et al., 2011; Roy and Oberkampf, 2011; Unal et al., 2011; Brown and Atamturktur, 2016). The literature on model calibration is just beginning to recognize distinct challenges and opportunities of calibration in partitioned analysis.

4.1. Systematic Bias and Uncertainty in Coupled Systems

Kim et al. (Kim et al., 2009) found the choice of coupling algorithm to be influential on the final converged solution, meaning that each of the algorithms shown in Figure 2.3 can result in a different degree of prediction inaccuracy and uncertainty due to the difference in how systematic biases and uncertainties are passed between models. Figure 2.7 provides a simplified illustration of such behavior, where systematic bias due to neglected, simplified, or misrepresented physics in one constituent causes convergence of the two-constituent strongly coupled system to incorrect values and parametric uncertainty due to imprecisely known input values results in convergence to a range of solutions. In Figure 2.7, the three different methods (i.e. Block-Jacobi, Newton-Raphson, and Optimization-based coupling) converge to different solutions. As seen, when systematic biases and uncertainties act simultaneously, either accumulating or compensating through the iterative process, matters become complicated and difficult to discern (Rizzi et al., 2012; Liang et al., 2015; Stevens et al., 2016).
Figure 2.7. Illustration of the changing convergence behavior considering systematic bias and uncertainty for Block-Jacobi, Newton-Raphson, and Optimization Based Coupling methods.

4.2. Calibration of Partitioned Models

The greatest advantage of partitioned analysis in the context of model calibration is arguably its ability to exploit separate-effect experiments, which are often more economical, less time-consuming and more feasible to conduct than integral-effect experiments. The use of separate-effect experiments during calibration also provides a
level of transparency in assessing the systematic biases and uncertainties in model predictions. These advantages, however, are accompanied by additional decisions, as a variety of experimental opportunities become available. With the introduction of this flexibility from partitioned analysis, model developers as well as experimentalist must select which experiments to conduct for calibration (discussed in more detail in Section 5.1).

A constituent model’s output (as well as the experimental measurements corresponding to that output) may be independent \( y^{ind} \), meaning it is not an input for another constituent, or dependent \( y^{dep} \), meaning it becomes an input parameter for another constituent thus forming a coupling interface. This distinction is important as it determines the nature of calibration that can take place and which experiments are necessary for comparing against during this calibration. Separate-effect experiments measuring \( y^{ind} \) enable the calibration of poorly known model parameters to reduce uncertainty in model predictions (see (Liu and Muraleetharan, 2012) for an example). Separate-effect experiments measuring \( y^{dep} \), on the other hand, enable the evaluation of not only uncertainties but also systematic biases in model predictions (Kumar and Ghoniem, 2012a).

Oliver et al. (Oliver et al., 2015) discussed the need to correct bias at the constituent level to reduce its effect on the coupled system predictions. However, published literature has paid little attention to bias correction, as previous studies using separate-effect experiments of dependent outputs were primarily focused on tracking the propagation of uncertainties through the coupling process (as demonstrated in (Kumar
and Ghoniem, 2012a)). A few studies have used separate-effect experiments to reduce systematic bias and uncertainty through model calibration that is closely integrated with the coupling algorithm (see Farajpour and Atamturktur, 2014; Stevens et al., 2016). The difference in these studies is that (Farajpour and Atamturktur, 2014) infer systematic bias in constituents only to avoid compensations during parameter calibration, whereas Stevens et al. (2016) apply bias-correction of constituent models within the coupling to mitigate the propagation of both systematic bias and uncertainty.

Aside from separate-effect experiments, previous studies have also implemented integral-effect experiments for the calibration of constituent model parameters (for example, see (Lin and Yim, 2006)) as well as calibration of parameters specifically related to the coupling interface, such as a coefficient of friction parameter between to two surfaces (Konyukhov et al., 2008) or hardening parameters representing hydro-mechanical coupling (Liu and Muraleetharan, 2012). Farajpour and Atamturktur (2014) expanded beyond parameter calibration to also bias-correct fully coupled predictions with respect to integral-effect experiment and also illustrated the way in which systematic bias present in constituent models can degrade predictions of the coupled model.

4.3. Model Validation in Partitioned Analysis

Calibration of models against experiments, be they separate-effect or integral-effect, is often a necessary step to improve the predictive capability of the full-system model. However, through calibration, models become conditioned upon this experimental data making a separate model validation step essential. Model validation is defined as the accumulation of evidence regarding model agreement with a unique set of suitable
physical evidence, with “unique” meaning that validation experiments are not used during calibration and “suitable” meaning that the validation experiments are relevant to the response of interest (i.e. the actual system response for which the model will be executed to predict).

Integral-effect experiments are highly valuable for validation of the coupled model as the coupled domain is where predictions critical for decision-making occur (Avramova and Ivanov, 2010; Kumar and Ghoniem, 2012b; Liu and Muraleetharan, 2012; Oliver et al., 2015). Korzekwa (2009) emphasizes that validation of strongly coupled models is important, as models of such complex systems often include components that cannot be accurately or completely modeled, despite efforts to reduce assumptions through coupling. While validation of the coupled model through integral-effect experiments is necessary, model developers are often faced with the challenge of validation data at the coupled level being limited or unavailable (Kumar and Ghoniem, 2012b; Tawhai and Bates, 2011).

5. Resource Allocation

The end goal of any model development is to implement the model for predictions that will guide decision makers. The predictive capability of coupled models may require improvement when the model does not meet satisfactory accuracy and precision criteria for implementation as a decision-making tool. Models can be refined in two ways (i) refining the physics representations in the models through further code development to reduce model bias and (ii) calibrating and validating the models with new experimental data to improve accuracy of calibration and inference of bias for correction. Refining
physics often requires adding parameters to a model, which may in turn increase the uncertainty in predictions. Thus, further code development and further experimentation in model predictions to reduce bias and uncertainty can become conflicting objectives (Thompson et al., 2010). The relative benefits of these two routes, further experimentation versus further code development, varies depending upon not only the available experimental measurements but also the existing predictive capability of the numerical model. Focussing specifically on the systematic bias can guide decision makers towards the selection of either new experimental efforts (if the discrepancy function, which is the functional form inferred to represent the systematic bias, has not yet converged) or further code development efforts (if the discrepancy is unduly large) (Atamturktur et al., 2015a). The problem of resource allocation is further exacerbated for strongly coupled numerical models with possibilities to evaluate not only each of the constituent models but also the coupled model and their relative separate-effect and integral-effect experiments.

5.1. Design of Calibration and Validation Experiments

The need for efficient design of experiments for single-solver models (as well as development of emulators) has been explored for decades (Kennard and Stone, 1969; Federov and Hackl, 1997; Li et al., 2010; Prabhu and Atamturktur, 2013). However, the design of experiments specifically geared towards the optimal coverage of a domain, and thus the best calibration of uncertain parameters and inference of model bias, is a newer topic more relevant to addressing the problem posed here (Williams et al., 2011; Atamturktur et al., 2013, 2015b).
Partitioned analysis requires not only selecting the constituent domain(s) within which the experiments should be conducted but also the experimental settings within each domain. This is because the maximum gain in predictive capability that can be obtained varies for different domains as well as different settings within a domain (Atamturktur et al., 2015a). Naturally, the need to consider multiple domains in partitioned analysis increases the importance of the selection of experiments so that each domain is adequately covered by the new design of experiments (see a discussion of coverage in (Atamturktur et al., 2015b; Hemez et al., 2010; Stull et al., 2011)). There are three options for designing experiments in these multiple-domain problems (i) focusing solely on separate-effect experiments to explore the constituent domains (Alvin and Reese, 2000; Vlachos et al., 2006; Sankararaman et al., 2013), (ii) focusing solely on integral-effect experiments to explore the coupled domain, and (iii) simultaneously considering separate-effect and integral-effect experiments. The second and third cases are, to our knowledge, yet to be studied and are therefore suggested paths for future research, as integral-effect experiments may be more costly but also more informative in calibration and also particularly useful for validation.

In partitioned models, sensitivity analysis may be used to identify the influence of constituent domains on the full system predictions (Alvin and Reese, 2000). Tomlin and Ziehn (Tomlin and Ziehn, 2011) emphasize the need for global sensitivity analysis, opposed to local sensitivity analysis, when exploring large, complex systems, such as those often represented by coupled models, due to the high variability that may occur in local sensitivity when evaluating a large solution space. Once sensitivity analysis has
reduced the number of calibration parameters to focus on, the domains and settings at which to conduct new experiments for improving our understanding of these parameters should be determined. Ideally, experiments would be designed so that they capture parameters in multiple domains, rather than confining the information gain to one parameter of a single domain (Oberkampf and Trucano, 2002).

Vlachos et al. (Vlachos et al., 2006) developed a global stochastic method tailored for coupled systems where settings for experiments in constituent model domains is selected considering the fact that certain parameters are more active at particular operational settings than others. Sensitivity of outputs being dependent on operational setting can be accounted for by considering (i) the number of parameters active at each setting and (ii) the value of sensitivity coefficients at these settings. An aspect of this framework that should be noted is its ability to consider parameters and settings in multiple domains simultaneously, rather than only designing experimental settings in one domain at a time. Sankararaman et al. (Sankararaman et al., 2013) selected not only constituent domains, but also the number of experiments to conduct within each domain through a Bayesian network. This process is completed through forward propagation of uncertainty to determine the reduction in variance of desired system level outputs followed by a backwards analysis to select experiments that give the highest reduction in variance given a set cost. It should be noted that the acyclic nature of the Bayesian network means that only forward propagation of uncertainty is possible and as such the method can only be applied to weakly coupled systems but does not hold for strongly coupled systems where there is an iterative feedback loop between the constituents.
Another important factor to also consider is cost as it too varies for different domains as well as settings within a domain. The limited amount of resources that can be dedicated for experiments often leads to a constrained optimization problem, which is commonly framed in one of two manners: given a set amount of resources minimize the error and variance in the model or given a standard or threshold for error and accuracy minimize the cost required to meet these standards (Sankararaman et al., 2013). The selection of the formulation is often determined by which constraint the decision-maker has knowledge of. However, in the case that neither or both of these constraints are known the optimization may be posed as a multi-objective problem (Liu et al., 2014).

5.2. Further Code Development

Further code development is called for when the discrepancy function of a model is either not converged even though the domain is sufficiently explored by the experiments, or when the discrepancy has converged but remains above desirable error threshold for the application. This model discrepancy is a result of insufficient modeling of the underlying physics and thus can be reduced by further code development. Code development to implement more detailed physics means increasing the model complexity (Salt, 1993). While simple models have lower development costs, faster run times, and require less data for calibrating, we ultimately need to determine the appropriate level of model detail with consideration of the application the model is meant to address (Law and McComas, 1991). Much like conducting new experiments, limitations to resources create a need for a systematic approach to prioritize code development. There are multiple options available for further code development of partitioned models: (i) the
physics in the constituent models can contain simplifying assumptions that may be eliminated by further code development and (ii) governing equations of the coupling interface may also lack enough detail and therefore require further development.

It should be intuitive that each constituent model would exercise a different influence on the predictive capability of the coupled model. Thus, when deciding which constituent model should be improved, both the prediction error associated with constituents and the respective sensitivity of the coupled system predictions to that constituent’s prediction error must be evaluated. Phenomenon Identification and Ranking Table is a commonly recommended method for addressing the latter part of this decision by evaluating the relative importance of constituents within a coupled process (Alvin and Reese, 2000). The two requirements of sensitivity analysis and analyses of error and uncertainty of predictions can be combined through comparison of fully coupled model predictions to integral-effect experiments, therefore providing a clever approach to prioritize constituent models and quantify the need for code development in each (Hegenderfer and Atamturktur, 2013). Expanding beyond integral-effect experiments, separate-effect experiments can also be used for uncertainty analysis, taking advantage of the transparency of partitioned models and the ready availability of these simpler experiments (Atamturktur and Farajpour, 2015). These preliminary efforts to prioritize the importance of further code development in constituents are moving the field forward, but incorporation of code development of the coupling interface has yet to be addressed and is a necessary step for future research.
Consideration of the resources that will be related to each code development effort are also important, including costs such as effort (people, time), project duration (time), and monetary requirements for supplies such as hardware (dollars). However, the cost associated with operating the model after the further code development has taken place (i.e. post-development resource consumption) is a significant detail not accounted for in current metrics (Brooks and Tobias, 1996). Cost of operating a model after further development is critical because if the model becomes too complex to operate for the intended application it may be rendered useless, thus wasting the resources that were used in developing it. As such, this is a logical inclusion in the next steps for developing a fully comprehensive metrics for efficient resource allocation in code development efforts of partitioned models.

6. Suggested Future Work And Conclusions

Strongly coupled models developed with partitioned analysis are providing new and exciting opportunities for modeling and simulation. Algorithms for iterative coupling of numerical models have been developed and well studied for years now, allowing partitioned analysis of complex systems to now be implemented in practice. This paper presented an overview of solutions that are being developed to address model Verification and Validation concerns as partitioned models are becoming commonly implemented for decision-making where satisfactory predictive capability is a key requirement.

With the benefits of partitioned analysis come challenges for ensuring the predictive ability of these models, as each constituent has its own domain, uncertainties,
and errors and the coupled model also has uncertainties and errors introduced at the interface. Coupling of independent domains having a unique spatial mesh and temporal discretization results in a new realm of numerical errors to be evaluated during verification procedures. A breadth of literature exists and has been reviewed in which these numerical errors that are exclusive to partitioned analysis are identified. Identification of these errors brings forth a call for solutions to reduce them, which research in relevant fields has begun exploring.

Furthermore, constituent models unavoidably have uncertainties and systematic biases that may propagate during coupling iterations, producing uncertainties and errors in the coupled solutions. Additionally, the coupling interface may introduce errors in the system. Demonstrations of specific applications using only separate- or integral-effect experiments to identify and remedy these inaccuracies are prominent. However, frameworks with clear plans for implementation of experiment-based validation of coupled models that exploit both separate-effect and integral-effect experiments in multi-scale, multi-physics modeling are currently lacking. A fully developed solution that considers all of the factors at play and is generalizable to many partitioned analysis applications is yet to be developed and is a clear path forward for future research to move the model validation and uncertainty quantification field forward.

Finally, literature contains preliminary efforts in developing methods to efficiently allocate resources for improving the predictive capability of partitioned models. Current research has determined specific elements of resource allocation and began developing methods to address the optimization of these individual elements.
Design of new experiments reduces uncertainty and better quantifies systematic bias of model predictions, but requires selection of both the constituent or coupled domain as well as number of experiments and settings within the domain. Currently, literature is available for selecting constituent domains and selecting settings, but no formal methods are available to address the two simultaneously or consider the selection of integral-effect experiments for comparing against the full system predictions. Code development improves the physical representation in the model and therefore reduces model bias to improve the accuracy and predictions. Existing methods suggest a priority for developing codes with consideration of development cost and potential improvements to the model, but neglect to consider implications of post-development operating costs. Ideal resource allocation, however, is not carried out on elements of the model’s predictive capability independently and must consider the increased consumption of resources for operating the model that can result from the improvements made to the model. Future research should explore paths that develop a full framework, including allocation of resources between both further code development and new experimental campaigns, as well as consideration of the different levels of the domains ranging from separate-effect experiments and constituent model predictions to integral-effect experiments and full system predictions, embracing the interfaces and component domains that may fall in between.

References


CHAPTER THREE

EXPERIMENT-BASED VALIDATION AND UNCERTAINTY
QUANTIFICATION OF COUPLED MULTI-SCALE PLASTICITY MODEL

1. Introduction

In partitioned analysis, independently developed constituent models are coupled together by exchanging inputs and outputs, typically through iterative procedures\(^5\) (Felippa et al. 2001, Rugonyi and Bathe 2001, Larson et al. 2005, Matthies et al. 2006, Leiva et al. 2010). Such coupling eliminates the need for strong (and occasionally unwarranted) assumptions about the interactions between multiple physical phenomena (Lieber and Wolke 2008) and results in representations of reality more accurate and complex than the individual constituents themselves (Farajpour and Atamturktur 2012). Coupled models developed with partitioned analysis are becoming prevalent in solving multi-physics (Kin et al. 2009) and multi-scale (Gawad et al. 2008) problems due to the many advantages partitioning provides, such as the ability to exploit existing codes reducing code development costs and demands (Sorti et al. 2009). Additionally, partitioned analysis renders a greater ability to solve high-complexity problems (Ibrahimbegovic et al. 2004) and the ability to run parallelized simulations (Park and Felippa 1983). Hence, strongly coupled multi-scale and multi-physics models are being increasingly used to support high consequence decision making, such as developing

\(^5\) Here, the term partitioned analysis (also commonly referred to as co-simulation) is used to define constituent models developed independent from each other regardless of whether their iterations advance in the same time step or not.
public policies, establishing safety procedures, and determining legal liabilities regarding not only regular system operations but also accident scenarios.

Partitioned analysis of multiple scales is especially useful for predicting time-dependent irreversible deformation in systems containing clear separation of scales, such as creep of Hexagonal Close Packed (HCP) zirconium (Wang et al. 2010). These models are necessary for understanding complex material behavior under high temperatures and stresses, such as those experienced by nuclear reactor cladding, large engine fan blades, etc. (Asayama and Hasebe 2000, Amodeo et al. 2011). Homogenization techniques such as the classic Taylor model are not suitable for modeling the constitutive behavior of these systems (Wang et al. 2010, Segurado et al. 2012), since obtaining accurate representations of the system response in extreme conditions is only possible when the high anisotropy and low symmetry of the crystals is accounted for through interactions between crystals. For this purpose, finite element (FE) methods are being implemented at the macro-scale to model the elastic response of the material, while single-crystal and polycrystal models are being used to represent the meso-scale viscoplasticity taking the microstructure texture evolution into account (Delannay et al. 2006, Roters et al. 2010, Knezevic et al. 2012).

These constituents, FE model in the macro scale and polycrystal models in the meso-scale, while elaborate, inevitably provide idealized representations of reality with inherent biases and uncertainties in each. If unaccounted for, these biases and uncertainties may propagate between constituent models via the coupling interface, compensating for each other or accumulating during iterations, ultimately resulting in
inferior predictive capability in the multi-scale coupled model. The effect of biases and uncertainties can be assessed by comparing (i) coupled model predictions to experiments of the complete system (referred to herein as integral-effect experiments) and (ii) constituent models to experiments within their respective domains (referred to herein as separate-effect experiments) (Figure 3.1). An important benefit of partitioned analysis is this transparency and the opportunity to exploit separate-effect experiments to improve the predictive ability of individual components of a more complex, coupled model. This improvement can be accomplished in two distinct, but interconnected manners: (i) inferring the bias in model predictions and (ii) mitigating the uncertainty in the model parameters (Kennedy and O’Hagan 2001, Higdon et al. 2008 and Farajpour and Atamturktur 2013). Herein, these two aspects are collectively referred to as “model calibration”.

Figure 3.1. Domain of separate-effect and integral-effect experiments demonstrated for a coupling problem consisting of two constituents.
In this manuscript, the authors present a framework for experiment-based model calibration and validation, taking advantage of both separate- and integral-effect experiments. The approach is demonstrated on the simulation of elasto-viscoplastic material behavior of metallic specimens achieved by coupling a FE model in the macro-scale and a self-consistent homogenization of polycrystalline behavior in the meso-scale. The macro-scale FE model is imbedded with a meso-scale viscoplastic self-consistent (VPSC) model at each integration point. The VPSC model updates material properties, such as crystal structure, at each time step as the macro-scale model is deformed (Knezevic et al. 2012). Error and uncertainty in the coupled model are mitigated through model calibration at the meso-scale, where parameter calibration and inference of model bias are completed using separate-effect experiments involving the loading curve of a sample of zirconium material from a uniaxial tension-compression test. Bias of the VPSC predictions is then corrected accordingly during each coupling iteration. Model validation is carried out at the macro-scale in that the predictions obtained through bias-corrected coupling process are compared against integral-effect experiments that involve the deformation of a highly anisotropic zirconium bar under a four-point bending load. This validation step demonstrates the capability of the proposed treatment of model calibration in partitioned models to yield improved accuracy in coupled model predictions.

This paper is organized as follows. In Section 2, the authors provide motivation for the management of bias and uncertainty in partitioned models accompanied by background discussion on the general framework of partitioned analysis. Next, an overview of state-of-the-art for calibration and validation of coupled models is presented
in Section 3. The framework for experiment-based calibration and validation of coupled models advocated herein, which utilizes both separate- and integral-effect experiments, is discussed in detail in Section 4. Section 5 introduces the meso- and macro-scale constituent models (VPSC and FE models) as well as the associated coupling process for the case study application. The experimental campaign and numerical model development for the zirconium case study are presented in Section 6. The methodology is implemented in Section 7 for calibration and bias-correction of strongly coupled VPSC-ABAQUS model for zirconium material. Finally, concluding remarks and key takeaways from the study are presented in Section 8.

2. Bias and Uncertainty in Coupled Models

During coupling iterations, not only the constituent model predictions but also their bias and uncertainty flow back and forth between the partitioned domains,\textsuperscript{6} as illustrated in Figure 3.2. Uncertainty in constituent model parameters ($\theta$ in Figure 3.2) causes variability in the coupled model predictions (Figure 3.2a), while bias in constituent model predictions ($\psi_A$ and $\psi_B$ in Figure 3.2) results in deviations from truth (Figure 3.2b). Occurring together, these biases and uncertainties may accumulate or compensate for each other quickly becoming highly complex and difficult to trace (Rizzi et al. 2012, Liang et al. 2015). The choice of coupling algorithm also influences the solutions as each algorithm passes biases and uncertainties in a different manner ultimately resulting in convergence to different solutions (Kim et al. 2009) all of which

\textsuperscript{6} Herein “domain” is defined as the boundaries within which each model is designed to operate (e.g. separate domains representing fluid and structure behaviors in a fluid-structure interaction problem).
may appear physically credible. Figure 3.2 demonstrates the effects of these biases and uncertainties on coupled model predictions in an isolated manner. Real systems, however, experience the degrading effects of both simultaneously.

The propagation of these biases and uncertainties between constituents can cause the coupling iterations to diverge or worse, converge to an incorrect solution as demonstrated in Figure 3.2. Such inaccurate convergence is particularly worrisome, as it may make the solution appear plausible, giving false confidence to the model developers about inaccurate scientific findings (Kim et al. 2009). Such inaccurate convergence has been observed in several applications in engineering and science (Döscher et al. 2002, Estep et al. 2008, Kim et al. 2009, Bunya et al. 2010, Dietrich et al. 2010, Kumar and Ghoniem 2011a). Döscher et al. (2002), for instance, noted the convergence of a coupled atmosphere-ocean model to incorrect sea ice area calculations. The authors attributed this inaccurate convergence to bias in heat fluxes originating from the atmospheric model, as the stand-alone ocean model with heat flux inputs from experimental data rather than the atmospheric model produced better agreement with sea ice area measurements. Kumar and Ghoniem (2011a) recognized bias in the predictions of a coupled flow gasification model not only due to bias in the constituent flow model, but also insufficient information being passed (i.e. missing parameters) from the flow solver to the particle dispersion model, referred to herein as interface bias ($\Psi_{A:B}$ and $\Psi_{B:A}$ in Figure 3.1).
Figure 3.2. Convergence of coupled model predictions to incorrect solutions due to (a) parametric uncertainty and (b) systematic bias.

Although biases and uncertainties inherent in constituent models are of a concern for partitioned models, partitioning provides a unique transparency for their assessment and mitigation. This transparency is due to the fact that variables shared to couple the constituent models can be evaluated as outputs at the constituent levels prior to coupling. Therefore, the transparency of partitioned models enables us to exploit separate-effect experiments conducted within each domain to calibrate the constituent models. The greatest advantage of partitioned analysis in the context of model calibration and validation is arguably its ability to exploit separate-effect experiments that are often more economical, less time-consuming and more feasible to conduct.
Figure 3.3 is a notional representation of the information flow as well as essential variables of a partitioned model. In this figure, control parameters, $x$, define the operational state of the system and are often known by both the experimentalist and model developer; calibration parameters, $\theta$, are those that are influential in model predictions but whose exact values are uncertain and thus require calibration; and remaining input parameters, $z$, are those that are necessary for operating the model but are neither control nor calibration parameters. As shown in this figure, constituents may have two basic types of inputs, dependent and independent. The dependent parameters ($dep$ in Figure 3.3) are the inputs to a constituent model that are dependent upon another constituent’s output. Without coupling, these dependent parameters are unknown to the model developer, thus requiring assumptions to be made regarding their values. In addition, each constituent model may have independent parameters ($ind$ in Figure 3.3), which are required for executing the constituent model but are not a function of another constituent’s output and thus, are simply specified by the model developer. Control parameter, $x$, may be independent (meaning it is known for a model) or dependent (meaning it is unknown and must be predicted by another model). Similarly, $z$, can be either independent or dependent parameters. If the dependent parameter becomes a control parameter, $x$, for another constituent model, the propagation of uncertainty tends to be of higher concern than if the dependent output is simply defining a system property, $z$ (Haydon and Deletic 2009). In our framework, calibration parameters are those which are poorly known but do not depend on another model’s output. Hence, according to our definition, calibration parameters are by default independent parameters.
In a similar manner, constituents may have two types of outputs, once again dependent and independent. Dependent outputs, $y_{dep}$, are those that become an input for another constituent, previously referred to as dependent parameters. Independent outputs, $y_{ind}$, are those that are not transferred to other constituents. Separate and integral-effect experiments can be conducted to observe either of these outputs, resulting in a variety of options for model calibration. For instance, one may focus on mitigating the uncertainty in calibration parameters, $\theta$, in any one of the constituent models using either separate- or integral-effect experiments that measure dependent or independent outputs. However, it is only when separate-effect experiments observing the dependent outputs are implemented, that one can quantify the propagation of uncertainty between models as well as determine the bias associated with constituent model predictions which will be passed during coupling iterations. If such separate-effect experiments are available, then correcting for said bias before it is transferred to the next constituent becomes possible.

Figure 3.3. Partitioned model with independent and dependent model parameters.
3. Background Perspectives

In calibrating constituent models against separate-effect experiments prior to coupling, the nature of calibration that can take place can be determined based on the types of experiments available (independent or dependent). Separate-effect experiments measuring $y^{ind}$ enable the calibration of poorly known parameters. One such example is discussed by Liu and Muraleetharan (2012) where several experimental techniques for capturing separate-effect behavior relative to several outputs of the system are implemented for calibrating constituent model parameters. Separate-effect experiments measuring dependent outputs, $y^{dep}$, on the other hand enables the evaluation of uncertainties as well as biases in the constituent model predictions that are passed to other constituents (Stevens and Atamturktur 2015). Kuman and Ghoniem (2011a) took advantage of separate-effect experiments of dependent outputs, but the information gained from these was limited to tracking the propagation of uncertainties through the coupling process rather than remedying the degrading effects of this propagation. Farajpour and Atamturktur (2014) proposed an integrated coupling-uncertainty quantification framework in which constituent model parameters were calibrated and bias was quantified using separate-effect experiments. However, their study only considered bias for the purpose of avoiding compensation for said bias by uncertain parameters during calibration. Oliver et al. (2015) discuss the importance of not only quantifying and tracking the propagation of bias and uncertainty in constituent models, but also correcting for these factors at the constituent level, as they will affect responses of the coupled system.
Partitioned models can also be calibrated against integral-effect experiments. Earlier studies have implemented integral-effect experiments for the calibration of independent parameters in constituent models (Lin and Yim 2006) as well as calibration of independent parameters specifically related to coupling, in that these parameters feed into both models (Liu and Muraleetharan 2012). Using integral-effect experiments, Farajpour and Atamturktur (2014) illustrated the importance of considering both bias and uncertainty in constituent model calibration by training a discrepancy model using integral-effect experiments to bias-correct the coupled predictions. Integral-effect experiments are also highly valuable for validation of the coupled model as the coupled domain is where predictions critical for decision-making will occur (Avramova and Ivanov 2010, Kumar and Ghoniem 2011b, Liu and Muraleetharan 2012). Korzekwa (2009) emphasizes the fact that validation of complex models is important, as models of such complex systems often include components that cannot be accurately modelled, despite efforts to reduce assumptions through coupling. While validation of the coupled model through integral-effect experiments is necessary, engineers are often faced with the challenge of validation data at the coupled level being limited or unavailable (Kumar and Ghoniem 2011b, Tawhai et al. 2011). However, bias correction of constituents throughout the coupling process using separate-effect experimental data combined with integral-effect experimental data for validation is to our knowledge yet to be explored.

**4. Methodological Approach**

This study presents a framework for bias-corrected partitioned analysis, which begins with model calibration of uncertain parameters and inference of model bias
completed within the constituent domain using separate-effect experiments. The application herein relies upon the Bayesian approach of Kennedy and O’Hagan (2001) and Higdon et al. (2008) for quantifying model bias. However, the framework for bias-corrected partitioned analysis is not constrained to the Bayesian approach. Rather, the method by which this bias is quantified is inconsequential to the way in which bias-corrected partitioned analysis of said bias is applied to the prediction, and as such the method selected for computer experiments. What is important, however, is the accuracy with which the method for quantifying bias is able to train the discrepancy function (Stevens and Atamturktur 2015) as well as assessing the calibration of parameters and inference of bias in a connected manner (Farajpour and Atamturktur 2014). A variety of methods are available for inferring bias in the constituents, starting with regression-based approaches directly relating bias to tested control settings, be they as simple linear functions (Derber and Wu 1998), high degree polynomials where coefficients are determined stochastically (Steinberg 1985), up to non-parametric fits such as a Gaussian Process Model (Sacks et al. 1989, Kennedy and O’Hagan 2001, Bayarri et al. 2007), and continuing away to methods for determining relationships between discrepancy and control settings such as a Maximum Likelihood Estimation of parameter distribution characteristics (Xiong et al. 2009, Atamturktur et al. 2015b) or a copula-based approach (Xi et al. 2014).

4.1. Constituent Model Calibration

Consider the forward operator of a real physical process given by $\zeta(x)$, where $x$ represents the control parameter settings that define the domain of applicability of the
problem. Experimental measurements, $y(x)$, conducted at a number of settings, $n$, are our primary means to observe reality, but are noisy representations of the true responses generated by the process $\zeta(x)$. Herein, we assume all observation errors are independent and identically distributed as Gaussian, i.e. $\epsilon \sim N(0, \sigma^2)$. Experimental measurements are related to the real process by:

$$y(x_i) = \zeta(x_i) + \epsilon(x_i), \quad i = 1, \ldots, n$$  \hspace{1cm} (Eq. 1)

In developing a numerical model, $\eta$, to mimic the process $\zeta(x)$ within the domain of applicability, two essential and intertwined aspects of the model must be defined. The first of these involves a series of assumptions representing the mechanistic principles invoked to establish a link between control parameters, $x$ and model output; and the second entails unknown (or poorly known) parameters, $\theta$, whose meanings are associated with the chosen mechanistic principles. The unknown parameter space is explored by sampling the numerical model with specified input values, $t$, thus generating a collection of simulations, where $m$ represents the number of simulations:

$$\eta(x^j, t^j), \quad j = 1, \ldots, m$$  \hspace{1cm} (Eq. 2)

Assessing the process in a Bayesian context requires sampling the parameter distributions by executing the model with different parameter sets $(x, t)$. Markov chain Monte Carlo (MCMC) is commonly used to explore the parameter domain as this sampling, especially implemented with Metropolis Hastings algorithm, is well suited for sampling an arbitrary distribution (Smith and Roberts 1993, Beck and Au 2002). However, MCMC sampling requires a large number of simulation runs, $m$, which may not be feasible for problems in which the numerical model, $\eta$, is computationally
demanding. Higdon et al. (2008) suggested the use of a Gaussian Process Model (GPM) when computational demands of the numerical model exceed reasonable means for MCMC sampling. A GPM is defined by a mean and covariance function, which relates all input settings throughout the model (Williams 1998, Rasmussen 2004, Williams and Rasmussen 2006, Santner et al. 2013). By controlling the form of this covariance, one can implement a representation of the model with desired smoothness throughout the domain of applicability. In this study, the model GPM is defined by a constant mean and a power exponential covariance as shown in Eq. 3, where $\lambda_\eta$ and $\rho_\eta$ are hyperparameters of the GPM to be trained.

$$\text{Cov}(\mathbf{x}, \mathbf{t}, (\mathbf{x}', \mathbf{t}')) = \frac{1}{\lambda_\eta} \prod_{k=1}^{p_x} \rho_{\eta_k}^{4(x_k-x'_k)^2} \times \prod_{k=1}^{p_t} (\rho_{\eta_k+p_x+k})^{4(t_k-t'_k)^2} \tag{Eq. 3}$$

Idealizations in the definition of the mechanistic principles causes biases in the model’s output. Bias can be considered to be a model’s fundamental inability to replicate reality due to incomplete representation of underlying physics or engineering principles and may originate from (i) missing input parameters (ii) missing or incorrectly defined relationships between control parameters and input parameters or (iii) missing or incorrectly defined relationships between input parameters. If biases are unaccounted for during calibration, the parameters may be adjusted to values that mask the presence of model error (Kennedy and O’Hagan 2001, Higdon et al. 2004, Higdon et al. 2008, Gaganis 2009, Atamturktur et al. 2012, Farajpour and Atamturktur 2013, Atamturktur et al. 2014). As suggested by Kennedy and O’Hagan (2001), we implement an additive
approach in which the real physical process $\zeta(x)$ is related to the numerical model with best estimate parameter values, $\theta$ by:

$$\zeta(x^i) = \eta(x^i, \theta) + \psi(x^i), \quad i = 1, \ldots, n$$  \hspace{1cm} (Eq. 4)

where $\eta(x^i, \theta)$ is the model outputs and $\psi(x^i)$ is the model bias at each tested setting, $i$ and $n$ is the number of experiments. Note that information regarding systematic bias is only available at control parameter settings where experiments have been conducted, $x^i$. Hence estimating the bias for all other control settings, $x$ requires that an independent model is trained. This independent model, $\delta(x)$ is henceforth referred to as “discrepancy”. There is likely to be limited information, if any, about the functional form of $\delta(x)$. Kennedy and O'Hagan (2001) suggested modeling the discrepancy using a nonparametric stationary Gaussian process in order to eliminate the need for potentially strong assumptions regarding its model form. We can represent the discrepancy over the domain of applicability (Higdon et al. 2008), once again using a zero mean GPM with a covariance function (shown in Eq. 5) which maintains a smooth, differentiable model fit throughout the domain. In this covariance function, $\lambda_\delta$ and $\rho_\delta$ are hyperparameters of the GPM to be calibrated.

$$\text{Cov}(x, x') = \frac{1}{\lambda_\delta} \prod_{k=1}^{p_x} \rho_\delta^{4(x_k - x'_k)^2} \quad \hspace{1cm} (Eq. 5)$$

Now that all sources of uncertainties have been defined, we can relate the numerical model predictions using best estimate parameters, $\eta(x, \theta)$, and the discrepancy function, $\delta(x)$, to experimental measurements at selected control settings, $i$, while also taking experimental error, $\epsilon(x)$, into consideration, as shown in Equation 6.
\[ y(x') = \eta(x', \theta) + \delta(x') + \epsilon(x') \quad i = 1, \ldots, n \quad (\text{Eq. 6}) \]

Missing physics in the constituent model is corrected for through the discrepancy function, \( \delta(x) \), which is trained to be an estimate of the model form error, \( \psi(x) \). This process of correcting for the inadequacy in the constituent model, referred to as “bias correction”, is implemented to ultimately improve predictions of the coupled model. Determination of the discrepancy function and calibration parameter values with relation to each other prevents unwarranted compensations between parameters, which may otherwise mask model bias (Kennedy and O’Hagan 2001, Higdon et al. 2008, Farajpour and Atamturktur 2014, Stevens and Atamturktur 2015). Approaching this problem in the Bayesian context allows for calibration of the uncertain parameters and discrepancy function simultaneously, while also providing a smooth incorporation of the experimental errors in the calibration. This is done by simultaneously inferring distributions for uncertain parameters, as well as the numerical model GPM hyperparameters and discrepancy model hyperparameters, conditioned upon a vector of sampled model outputs, \( \eta(x, t) \), and experimental data. Once the model is calibrated at the constituent level, conditioned upon separate-effect experiments, the discrepancy function can be implemented in an iterative manner to correct the constituent model through bias-corrected partitioned analysis.

4.2. Bias-Corrected Partitioned Analysis

In partitioned analysis, errors in constituents combine in a complex manner due to the iterative nature of the coupling iterations, making it difficult to trace the effects of constituent bias on the coupled model predictions. Partitioning allows for the calibration
and bias correction of constituent models using separate-effect experiments through two unique approaches. The first of these (Figure 3.4a) involves coupling constituent models followed by calibrating their output to separate-effect experiments (see Farajpour and Atamturktur 2014 for a demonstration of this approach). Herein, we propose a new framework referred to as “bias-corrected partitioned analysis”, which operates by first calibrating and bias correcting constituent models with respect to their respective separate-effect experiments following coupling the models in a second step (Figure 3.4b).

![Diagram of coupling and model calibration using separate-effect experiments.](image)

**Figure 3.4. Integration of coupling and model calibration using separate-effect experiments.**

This second framework has the advantage of reducing uncertainties and correcting for bias before they are allowed to spread throughout the coupling process and contaminate the coupled model predictions (which are typically what is used for decision-making). As a final step, validation is completed for the coupled domain using the integral-effect experiments. While this manuscript focuses on the correction of constituent models, the framework may also be expanded to correct for interface bias.
(recall $\Psi_{A-B}$ in Figure 3.1), should appropriate integral-effect experiments be available. Interface bias is introduced due to omitted or misrepresented relationships between constituents. These improperly defined relationships may be due to missing dependent parameters that should be transferred between models.

4.3. Conceptual Demonstration of Bias-corrected Partitioned Analysis

Consider two models representative of two domains ($\Omega_A$ and $\Omega_B$) coupled through the iterative exchange of outputs using a Newton-Raphson scheme (as shown in Figure 3.6). Let us take $\Omega_B$ as a biased model and $\Omega_A$ as a bias-free model. Figure 3.5a illustrates the biased predictions of $\Omega_B$ compared to a rich set of separate-effect experiments (our closest representation of truth). Here, we train a discrepancy function (dashed line shown in Figure 3.5b) using the bias inferred at tested settings (stars shown in Figure 3.5b).

![Figure 3.5](image)

**Figure 3.5.** (a) Stand-alone $\Omega_B$ model predictions compared and relative separate-effect experiments and (b) bias inferred at experimental measurement points and discrepancy trained throughout the model domain.
Note in Figure 3.5b that the discrepancy is defined for all values of $x_B$, control parameter for $\Omega_B$. This discrepancy function is used to correct the predictions of $\Omega_B$, which serves as a dependent input parameter for $\Omega_A$. In each iteration, the predictions of $\Omega_B$ are corrected by the value corresponding to the given $x_B$ in the discrepancy function (Figure 3.6). Once this bias correction is applied concurrently with the coupling scheme, predictions of the coupled model are improved. Here, the coupled predictions are made in the domain of $\Omega_A$, but require iterations between the models. A few important observations may be garnered from Figure 3.7. First, the coupled predictions shown for the domain of $\Omega_A$ are altered due to the bias in $\Omega_B$, even though $\Omega_A$ was an initially correct model. Hence, the degrading effect of bias is not limited to the domain in which it originates. Rather, much like an infectious disease, the constituent bias makes its way through the coupling interface to diminish predictive capabilities in the other domain. Second, in our academic example, bias correction of $\Omega_B$ at every iteration in the coupled model almost completely accounts for inaccuracies in the constituent and recovers a significant amount of error in the coupled model, bringing predictions of the coupled model to less than 1% error, in comparison to the 15% error prior to bias correction.

![Diagram](image)

**Figure 3.6. Illustration of bias-corrected partitioned analysis.**
Figure 3.7. Improvement in coupled model predictions achieved through bias-corrected partitioned analysis.

5. Meso- and Macro-scale Coupling of VPSC and ABAQUS FE Codes

5.1. Meso-scale VPSC Code

The VPSC code, developed by Lebensohn and Tomé (1993), predicts the texture evolution of highly anisotropic polycrystalline material. VPSC operates under the assumption that a polycrystalline material can be represented by a set of orientations of individual single-crystal grains, each of which can then be treated as an inhomogeneity embedded within a homogeneous effective medium. With this assumption, interaction equations are formulated to linearly relate the stress and strain rate of a single grain to the stress and strain rate of the surrounding effective medium. The VPSC formulation uses an integral approach to update the grain shape effect and evolution of the polycrystal orientations with deformation, enabling the prediction of texture evolution for the metallic materials. Applying viscoplastic deformation, the stress-strain response and
microstructure evolution are predicted at the single crystal using the following constitutive relationship (Tomé et al. 2001):

\[ \dot{\varepsilon}_{vp} = \dot{\gamma}_0 \sum s m^s_j \left( \frac{m^s : \sigma}{\tau^s} \right)^n \]  
(Eq. 7)

where \( s \) is the number of active slip and twinning systems, \( n \) is the inverse of the rate sensitivity, \( \tau^s \) is the threshold shear stress, \( m^s \) is the Schmid tensor, \( \sigma^t \) is the Cauchy stress deviator, and \( \dot{\varepsilon}_{vp} \) is the viscoplastic strain-rate. The threshold shear stress, \( \tau^s \) in Eq. 7 is affected by the deformation modes active during hardening. A reference hardening function is defined by:

\[ \tau^s = \tau^s_0 + (\tau^s_1 + \theta^s_1 \Gamma) \left( 1 - \exp \left( -\frac{\theta^s_0 \Gamma}{\tau^s_1} \right) \right) \]  
(Eq. 8)

where \( \tau^s_0, \theta^s_0, \theta^s_1 \) and \( \tau^s_1 + \tau^s_1 \) are the initial critical resolved shear stress (CRSS), initial hardening rate, asymptotic hardening rate, and back-extrapolated critical resolved shear stress, respectively. Each of these parameters takes a different value for each active deformation system. Anisotropic zirconium at room temperature has three active slip and twinning modes (prismatic, pyramidal, and tensile twinning) each with a hardening function of its own containing the four hardening parameters. These hardening parameters are poorly known and thus must be calibrated against physical experiments.

5.2. Macro-scale ABAQUS Code

At the macro-scale, ABAQUS calculates the total strain increment, \( \Delta \varepsilon \), which can be partitioned into elastic, \( \Delta \varepsilon_{el} \), and viscoplastic, \( \Delta \varepsilon_{vp} \) components:

\[ \Delta \varepsilon = \Delta \varepsilon_{el} + \Delta \varepsilon_{vp} = C^{-1} : \Delta \sigma + \Delta \varepsilon_{vp}(\sigma) \]  
(Eq. 9)

For each iteration at a given strain increment, \( \Delta \varepsilon \), the stress increment, \( \Delta \sigma \) is determined:
\[ \Delta \sigma = \sigma^{t+\Delta t} - \sigma^{t} \]  

(Eq. 10)

5.3. Coupling Between VPSC and ABAQUS

Using a Newton-Raphson iterative scheme, the VPSC and ABAQUS codes are coupled with the following convergence criteria \( X(\Delta \sigma) = 10^{-6} \) (i.e. \( \Delta \varepsilon \approx \Delta \varepsilon^{FE} \)):

\[ X(\Delta \sigma) = \Delta \varepsilon - \Delta \varepsilon^{FE} = C^{-1} : \Delta \sigma + \Delta t \dot{\varepsilon}_{vp}^{(px)} (\alpha^t + \Delta \sigma) - \Delta \varepsilon^{FE} \]  

(Eq. 11)

After convergence in stress equilibrium is reached at each time step, viscoplastic strain-rate \( \dot{\varepsilon}_{vp} \), hardening variables and crystal orientations \( q \), and tangent stiffness matrix \( C \), are accepted for every integration point, allowing ABAQUS to repeat the iteration process at the next time step, \( t+\Delta t \), with an increased displacement, \( u+\Delta u \) as illustrated in Figure 3.8.

Coupling between the two scales occurs as the FE model provides VPSC with updated stress \( \sigma \), and VPSC provides the FE model with updated viscoplastic strain-rate, \( \dot{\varepsilon}_{vp} \), hardening variables and crystal orientations \( q \), and tangent stiffness matrix \( C \), as shown in Figure 3.8. Specifically, the VPSC model supplies a texture-sensitive constitutive relationship between stress and viscoplastic strain-rate (see Eq. 7). This constitutive relationship takes both slip and twinning between crystals into account, yielding an accurate representation of the time-dependent, irreversible deformations of the poly-crystalline material (Tomé et al. 2001). Figure 3.9 illustrates the domain of each of the models and their corresponding separate- and integral-effect experiments.
6. Experimental and Numerical Campaign

Separate-effect experimental data for calibration of the VPSC meso-scale constituent model are collected in a series of uniaxial tension-compression tests and integral-effect experimental data for validation of the coupled model are gathered from the four-point bending test of a zirconium beam. Cylinders used in the uniaxial test, as
well as the beam used in the four-point bending test, are cut from a plate of zirconium processed by clock rolling and vacuum annealing processes to produce highly textured properties (Kaschner et al. 2001).

6.1. Uniaxial Tension and Compression Tests of a Zirconium Cylinder: Separate-effect Experiments and VPSC model

Uniaxial tension/compression tests are completed on cylindrical zirconium specimens to collect stress and plastic strain data for in-plane compression (IPC) and in-plane tension (IPT). Tensile specimens are cut to a nominal gauge length of 17.7 mm and a diameter of 2.25 mm; compression samples are cut to a length of 5 mm and a diameter of 5 mm. Tests are conducted at a temperature of 293 K with a strain rate of 0.001 s⁻¹. Zirconium samples are deformed up to a plastic strain of 25% along the testing direction (Tomé et al. 2001). Loading curves for in-plane compression and in-plane tension collected from the experimental tests are shown in Figure 3.10.

![Figure 3.10. Uniaxial tension and compression tests data.](image)
6.2. Four Point Bending of a Zirconium Beam: Integral-effect Experiments and Multi-scale FE-VPSC Model

A zirconium plate is cut into beams with dimensions of 6.35x6.35x50.8 mm and then vacuum encapsulated and heat treated, producing an equiaxed grain structure containing grains with a mean size of approximately 25 µm. Roller bearings and hardened steel dowel pins are placed at four locations within the frame to minimize the friction that may be produced due to large strains and high forces. Load is applied by upper pins located 6.35 mm to the left and right of the center, which are displaced 6 mm while the lower pins, located 12.7 mm from the center on both sides, remain stationary. Experiments are performed such that the nominal strain rate at the outer fibers of the beam is $10^{-3}$ s$^{-1}$ (Kaschner et al. 2001).

Tests are conducted with the beam being bent parallel to the crystal axis. Prior to bending the beam is marked with a 161 point grid, composed of 7 columns with 23 indentions each. Columns are spaced 1.016 mm apart and each point in the column spaced 0.254 mm apart. After bending, the displacement of these points is measured to calculate the experimental strain. Plastic strain is measured at the centerline of the beam after the maximum displacement is reached (Figure 3.11). The initial and final positions of the dot grid, measured using dot-matrix deposition and mapping, are used to calculate strain at each marked point of the beam face. Figure 3.12 highlights the dot matrix used for strain measurements on the test specimen.
Figure 3.11. Four point bending test experimental plastic strain data.

Figure 3.12. Zr beam after four-point bending experiment.

The ABAQUS FE model simulating macro-scale behavior is composed of a mesh of 32×4×4 C3D20R element with 20 nodes (Figure 3.13). The VPSC polycrystal model is integrated in the FE model using a user-defined material subroutine (UMAT) at every Gauss integration point (Knezevic et al. 2012) as previously explained in Section 5.3.

Figure 3.13. Macro-scale FE model.
7. Bias-Corrected Partitioned Analysis of Multi-scale Plasticity Model

7.1. Calibration of the VPSC Model

For our application in modeling the time-dependent irreversible deformation of a zirconium beam, the stand-alone VPSC model is calibrated using separate-effect experiments, i.e. uniaxial tension and compression tests of a zirconium cylinder described earlier in Section 6.1. As illustrated in Figure 3.14, the control parameter is stress, $\sigma$ at varying levels of which, the strain-rate measurements are available.

$$\Omega_V(\sigma, \theta)$$

Figure 3.14. Separate-effect calibration with input of polycrystal material properties, $\theta$, into the VPSC solver and comparison of stress-plastic strain output to experimental data.

Potential parameters for calibration are the twelve hardening parameters as well as the parameter $n$, representing the inverse of rate sensitivity parameter, seen in Eq. 7. Among these candidate parameters, appropriately selecting the parameters for calibration is critical. Here, we evaluate the sensitivity and uncertainty of parameters in a manner reminiscent to the Parameter Identification and Ranking Table (Boyack 1998, Atamturktur et al. 2012, Hegenderfer and Atamturktur 2013). A parameter that exercises little influence on the available experiments will not be properly calibrated and possibly cause ill-conditioning - on the other hand, a parameter whose value is known with little uncertainty should not be calibrated. Hence, the most logical approach is calibrating only
those parameters that are sensitive to available experiments and uncertainty to the analyst. The inverse of rate sensitivity parameter, $n$, in Eq. 7 is not only poorly known but also has been shown to be significantly influential on the VPSC model predictions of stress and texture in previous studies (Atamturktur et al. 2013, Atamturktur 2015a, 2015b). Hardening parameters for the threshold shear stress (Eq. 8) are also uncertain. The sensitivity of these parameters is determined through a main-effect analysis of variance test of the twelve hardening parameters. Results of the sensitivity analysis indicate $\tau_0$, $\tau_1$, and $\theta_1$ in the prismatic slip system to be the main contributors to the variance in model outputs, as shown in Table 1, effectively reducing the problem to the calibration of four parameters ($n$ and prismatic $\tau_0$, $\tau_1$, and $\theta_1$).

### Table 3.1. Sensitivity analysis of VPSC model hardening parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$R^2$ Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prismatic slip</td>
<td></td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>41.5 %</td>
</tr>
<tr>
<td>$\tau_1$</td>
<td>30.50 %</td>
</tr>
<tr>
<td>$\theta_0$</td>
<td>0.60 %</td>
</tr>
<tr>
<td>$\theta_1$</td>
<td>26.90 %</td>
</tr>
<tr>
<td>Tensile twinning</td>
<td></td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>0.69 %</td>
</tr>
<tr>
<td>$\tau_1$</td>
<td>0.32 %</td>
</tr>
<tr>
<td>$\theta_0$</td>
<td>0.08 %</td>
</tr>
<tr>
<td>$\theta_1$</td>
<td>0.01 %</td>
</tr>
<tr>
<td>Pyramidal slip</td>
<td></td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>0.03 %</td>
</tr>
<tr>
<td>$\tau_1$</td>
<td>0.01 %</td>
</tr>
<tr>
<td>$\theta_0$</td>
<td>0.00 %</td>
</tr>
<tr>
<td>$\theta_1$</td>
<td>0.01 %</td>
</tr>
</tbody>
</table>

Herein, MCMC sampling is used to explore the parameter domain, drawing 10,000 samples. To reduce the computational demand of MCMC, a fast-running GPM as explained in Section 4.1 is used as an emulator in place of the VPSC model. The GPM is
trained with 100 VPSC runs (50 in the tension range and 50 in the compression range) obtained using Latin Hypercube sampling to ensure the parameter domain is adequately explored. Prior distributions of hyperparameters for the model GPM (Eq. 5) and discrepancy GPM (Eq. 3) proposed in Gattiker (2008) are used. Uniform prior distributions are assigned for the four calibration parameters, with upper and lower bounds as listed in Table 2. Posterior distributions of the four calibration parameters are shown in Figure 3.15 and the main statistical properties of these posterior distributions are listed in Table 2. Figure 3.16 illustrates the improvement obtained in the stand-alone VPSC model predictions after calibration.

Figure 3.15. Posterior distributions of calibration parameters.
Table 3.2. Prior and posterior mean for calibration parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Prior</th>
<th>Posterior</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Lower Bound</td>
<td>Upper Bound</td>
</tr>
<tr>
<td>n</td>
<td>0</td>
<td>20</td>
</tr>
<tr>
<td>Prismatic τ₀</td>
<td>0</td>
<td>28</td>
</tr>
<tr>
<td>Prismatic τ₁</td>
<td>0</td>
<td>24</td>
</tr>
<tr>
<td>Prismatic θ₁</td>
<td>0</td>
<td>80</td>
</tr>
</tbody>
</table>

Figure 3.16. Stand-alone VPSC model predictions (left) prior to calibration and (right) after calibration with separate-effect uniaxial experiments.

7.2. Implementation of Bias-corrected Partitioned Analysis

Mean values of the posterior distributions for uncertain parameters of the meso-scale model (Table 2) are entered as the input for the coupled multi-scale VPSC-ABAQUS model, effectively improving the agreement between coupled model predictions and integral-effect experiments as shown in Figure 3.18. While calibration improves the agreement to experiments, the model continues to underestimate the plastic strain particularly at the extremes of the distribution, as detailed in Table 3. However, note that thus far, bias in constituent models’ predictions is not accounted for. A portion
of this underestimation can be explained by the discrepancy remaining between VSPC simulations and separate-effect experiments even after calibration.

It should be noted that the separate-effect experiments available are only for the in-plane crystal orientation, which relates to a single direction of the stress and strain tensors of the numerical model. Therefore, bias correction in this study is only applied in this direction. The discrepancy model to represent this bias is inferred with stress as the control variable and plastic strain as the response feature. This inference is completed at the same time as the uncertain input parameters are calibrated through the procedure explained previously in Section 4. Discrepancy is accounted for through bias correction of the meso-scale constituent model at every iteration, such that for every calculated stress point, the corresponding plastic strain is corrected (Figure 3.17). The discrepancy function trained for VPSC model is used to correct plastic strain according to the stress supplied by the macro-scale ABAQUS model. In this case, a constant correction factor is applied for the tensile and compression regions, where plastic strain is increased by 40% in tension and decreased by 10% in compression. The calibrated and bias-corrected VPSC-ABAQUS model predictions are shown in Figure 3.18. Also shown in Figure 3.18 is the prediction uncertainty determined by considering the uncertainty remaining in calibrated parameters (by one standard deviation). Most notably, the bias-corrected model with mean calibration parameter values from Table 2 is shown to improve predictions at the maximum tensile and compressive plastic strains, which are the locations of highest concern for analyzing the failure of this system (Table 3).
Figure 3.17. VPSC-ABAQUS coupling interactions with discrepancy accounted for in the meso-scale.
Figure 3.18. Results of coupled VPSC-ABAQUS model predictions (a) after VPSC model calibration but prior to bias correction and (b) after VPSC model calibration and bias correction.
Table 3.3. Predictions of maximum tensile and compressive plastic strains compared with experimental measurements.

<table>
<thead>
<tr>
<th></th>
<th>Maximum Plastic Strain</th>
<th>Percent Difference from Experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Top of Beam (Compression)</td>
<td>Bottom of Beam (Tension)</td>
</tr>
<tr>
<td>Experiment</td>
<td>-0.148</td>
<td>0.194</td>
</tr>
<tr>
<td>Uncalibrated Model</td>
<td>-0.062</td>
<td>0.066</td>
</tr>
<tr>
<td>Calibrated Model</td>
<td>-0.078</td>
<td>0.082</td>
</tr>
<tr>
<td>Calibrated Model with Bias correction</td>
<td>-0.086</td>
<td>0.125</td>
</tr>
</tbody>
</table>

In this particular application, a significant limitation is the presence of multiple dependent parameters between VPSC to ABAQUS constituent models, namely viscoplastic strain-rate, $\dot{\varepsilon}_{vp}$, crystal and texture properties, $q$, and tangent stiffness matrix, $C$, (recall Figure 3.8) and the absence of separate-effect experimental data available for each of these dependent parameters. Therefore, the other directions of the viscoplastic strain-rate tensor, as well as the crystal orientations and tangent stiffness matrix, are left uncorrected, thus limiting the extent to which the bias in constituent predictions can be remedied. Despite this limitation, the effect of partially correcting for discrepancy at the meso-scale propagates to produce improvements in the predictions of the coupled model. It is expected that if experiments were to be available for all components of the coupling, predictions would further improve and reach better agreement with experiments.

To demonstrate this aspect, consider a pair of numerical equations containing multiple dependent parameters being coupled as to represent a scenario similar to that of
the VPSC-ABAQUS coupled model. As shown in Figure 3.19, parameters $B$ and $C$ are each dependent upon parameter $A$, which is likewise dependent upon parameters $B$ and $C$. Synthetic experiments are created by using “true” values for $A$, $B$, and $C$, while biased simulations are created by altering the physics behind $B$ and $C$. Hence, the meso-scale constituent model is taken to be biased.

Let us consider two scenarios. In the first scenario, only experiments for output $B$ are available and in the second scenario, experiments are available for both $B$ and $C$, allowing for full correction of the model. Figure 3.20 shows the results for the first scenario. When only $B$ is corrected, the coupled simulation is not able to achieve agreement with the experiments, as the average error in the coupled model predictions is only reduced, though not entirely corrected. After correcting both dependent outputs $B$ and $C$, however, the simulation and experiments show improved agreement (assuming the quality and quantity of separate-effect experiments is sufficient for accurately training discrepancy).

![Diagram](image)

*Figure 3.19. Example with multiple components of constituent model coupled.*
8. Conclusion

With coupled modeling coming to the forefront of engineering practices as systems become more and more complex, a systematic framework for calibration and bias correction of partitioned models stands to make a significant impact in many engineering fields. Each constituent of a coupled model has its own unknown parameters and missing physics and engineering phenomena, resulting in bias and uncertainty that may impede the predictive capability of the coupled model, if left unaccounted for. Additionally, neglecting to account for bias during calibration may result in parameters being calibrated to incorrect values to compensate for bias.

This paper demonstrates that calibration and bias correction of the constituent level model through the use of separate-effect experiments mitigates the accumulation of error and improves the predictive capabilities of not only the constituents, but also the
coupled model. The application presented herein illustrates a real-life scenario where bias-corrected partitioned analysis utilizing separate-effect experiments improves the predictive capability of a multi-scale plasticity model. Implementation of the bias-corrected partitioned analysis paradigm allowed a 38.5% improvement in the fidelity of predictions for a highly anisotropic zirconium beam exposed to extreme loading. The improvement obtained in this application demonstrates the capability of the bias-corrected partitioned analysis framework to advance the predictive maturity of complex multi-scale models, therefore instilling confidence in these models as the basis for high-consequence decision making.

In complex systems, it is possible for constituent models to have multiple dependent parameters. Within the bias-corrected partitioned analysis framework, more than one dependent parameter involved in the coupling scheme requires not only sufficient quantity and quality of experiments for the constituent, but more specifically experiments related to each dependent parameter that is being transferred. When experiments are unavailable for some of the coupled parameters, only a partial bias correction may be completed. Often times partial bias correction is better than no correction at all. This procedure, however, should be done with much caution, taking into consideration the possible consequences of neglecting to correct the other parameters.

Aside from the biases and uncertainties in the constituents themselves, the coupling process may also introduce its own spectrum of biases and uncertainties due to an inability to perfectly model the physics of coupling operations. Implications of biases
and uncertainties introduced by the coupling interface have been neglected in this study, but should be investigated in future work.

References


CHAPTER FOUR

STATISTICAL INFERENCE OF EMPIRICAL CONSTITUENTS IN PARTITIONED ANALYSIS FROM INTEGRAL-EFFECT EXPERIMENTS: AN APPLICATION IN THERMO-MECHANICAL COUPLING

1. Introduction

Rapid advancements in parallel computing over the last two decades have enabled simulations of complex, coupled systems through partitioning. In partitioned analysis, independently developed constituent models communicate, representing dependencies between multiple physical phenomena that occur in the full system. Figure 4.1 schematically demonstrates a coupled system with two constituent models, each resolving different physical behavior. In this figure, the constituent model, denoted as the “consumer,” relies upon some input parameter that is being provided by the constituent model acting as a “feeder”. The role of the feeder model is to map operating conditions (i.e. those that are stimulating the process) to consumer inputs, thus providing functional inputs to the consumer model. Problems arise if the feeder model cannot be built—a challenge that is prevalent for highly complex systems in extreme operational conditions that push the limits of our understanding of underlying physical behavior. Often, these are also the situations where separate-effect experiments isolating the physical phenomena are not available; meaning that experimentally determining the unknown

7 The feeder/consumer constituent relationship shown here represents a weakly coupled system. The case of strongly coupled models, where feedback between constituents creates a loop that must be solved iteratively, is beyond the scope of this paper.
constituent behavior is not possible (Bauer and Holland, 1995), and that integral-effect experiments that reflect the behavior of the complete system tend to be the only available observations. In this paper, the authors advocate for the usefulness of integral-effect experiments in furthering model developer’s knowledge of the physics principles governing the system behavior of interest.

**Figure 4.1. Empirical representation of constituent model to simulate a coupled system through partitioned analysis.**

Thermo-mechanical coupling where the thermal model (feeder) influences the behavior of the mechanical model (consumer) is one such multi-physics application that plays a role in a wide range of engineering applications including shape memory alloys (Dunić et al., 2012), rock fracture behavior where temperature changes in a rock mass influence the elastic properties (Auricchio et al., 2007; Shen et al., 2014), and nuclear reactors where the high temperature loads experienced during irradiation change the material density, gas production, and thus mechanical behavior of fuel materials (Williamson et al., 2012; Galloway et al., 2015). Modeling of such coupled systems, where material properties are dependent upon temperature, often results in the scenario shown previously in Figure 4.1, as the precise effects of temperature on material properties in highly complex systems may be unknown and not possible to observe experimentally in an isolated manner. For example, changes in thermal conductivity of metallic fuels due to irradiation in a nuclear reactor is a physical process which is neither
theoretically well understood nor possible to isolate in experimental measurements, yet it is known to be influential in the reactor behavior (Bauer and Holland, 1995). In the absence of a thermal constituent model, the model representing the mechanical behavior would be bound to an incomplete (and thus, inaccurate) representation of reality, as the temperature dependency of its parameters are not accounted for. As a result, the mechanical constituent model, if calibrated with one dataset at a given temperature, would be unable to produce validated predictions of another dataset collected at a different temperature (as in the case documented in (Jackson et al., 2014)).

This paper presents a statistical inference method in which integral-effect experiments as well as the available mechanical model are used to empirically infer a mathematical representation for the thermal constituent model that is otherwise unattainable (i.e. empirical constituent model in Figure 4.1). This paper is organized as follows. The inverse analysis methodology is presented in Section 2 followed by a conceptual demonstration in Section 3. Section 4 focuses on a thermo-mechanical application where different temperatures experienced during system operations change a metallic material’s crystal properties, and therefore its mechanical behavior. The proposed methodology is applied in a case study of 5182 aluminum, which has an experimentally demonstrated dependence of the material behavior on both temperature and strain rate, for which constituent models are currently unavailable. Section 5 concludes the findings and presents a path forward for future work.
2. Methodology for Inferring Coupling Relationships through Inverse Analysis

2.1. Integral-Effect Experiment-Based Inference

The proposed approach seeks to learn the relationship of physics-based consumer constituent inputs to operational states. Such relationships would be represented as predictions of the feeder constituent model if it were to be available but instead become uncertain input parameters of the consumer model when the feeder model cannot be obtained (recall Figure 4.1). Of course, the consumer model could also have parameters that are not dependent upon the feeder model. Thus, two sets of uncertain input parameters must be considered for the consumer constituent: *constant parameters, $\theta_c$* that are not reliant upon other operational conditions and *functional parameters, $\theta_f$* that are reliant upon operational conditions (Figure 4.2). Similarly, the physics-based consumer model may also have two different types of operational parameters: parameters that the coupling depends upon (i.e. temperature in the thermo-mechanical example) that are denoted as *dependent operational parameters, $x_f$* and the parameters that the coupling does not depend that are be denoted as *independent operational parameters, $x_c$* (Figure 4.2).

![Figure 4.2. Variables of interest for the feeder and consumer models.](image)

Ultimately, the goal is to represent predictions of the missing feeder constituent model as functional parameter of the consumer constituent, such that $\theta_f \equiv \theta_f(x_f)$ (Brown
This is accomplished through inverse analysis using integral-effect experimental observations, \( y \), as our knowledge of the desired full-system behavior with uncertainty in the form of experimental error, \( e \) (Eq. 1). As shown in Eq. 1, where \( n \) is the discrete number of settings for experimental data points, the consumer constituent model, \( \eta \), effectively becomes a semi-empirical partitioned representation of the coupled system once \( \theta_f(x_f) \) is identified and included as an empirically derived feeder constituent.

\[
y(x_f^i) = \eta(x_f^i, \theta_f(x_f^i)) + e(x_f^i) \quad \text{where} \quad i = 1, 2, \ldots, n
\]

(Eq. 1)

In addition, the physics-based consumer constituent model may have its own parametric uncertainty as well as other operational states on which the feeder constituent does not depend. These uncertain physical parameters, \( \theta_c \) and the feeder constituent model, \( \theta_f(x_f) \) can be inferred simultaneously as shown in Eq. 2, where \( m \) indicates the discrete points at which experimental data is available in the control dimension of \( x_c \).

Consideration of the consumer model uncertainties concurrently with the empirical model inference will reduce the risk of unwarranted compensations that may otherwise degrade the realism of the empirical model. Inclusion of experiments across various control dimensions may also provide additional data points to inform the functional parameter inference.

\[
y(x_f^i, x_c^j) = \eta(x_f^i, x_c^j, \theta_f(x_f^i), \theta_c) \quad \text{where} \quad i = 1, 2, \ldots, n \quad \text{and} \quad j = 1, 2, \ldots, m
\]

(Eq. 2)

2.2. Gaussian Process Representation of Functional Parameters

Any available prior knowledge concerning the functional form of the empirical constituent \( \theta_f(x_f) \), perhaps in the form of expert opinion or predictions from legacy codes, can be incorporated during inference. For example, (Atamturktur et al., 2015) determined
a functional input parameter by calibrating coefficients of a functional form selected by expert opinion. If prior knowledge regarding the functional form of $\theta_f(x_f)$ is not available, however, a Gaussian process (GP) can be used without imposing restrictions on the functional form of $\theta_f(x_f)$ (MacKay, 1998; Neal, 1998; Kennedy and O’Hagan, 2001; Bastos and O’Hagan, 2009). In the case that a model has more than one missing constituent function, a separate GP and its associated hyperparameters would need to be inferred for each.

A GP is a stochastic process relating discrete points along some control dimension, $x$, where the nature of the relationship is specified by a mean and covariance function (Eq. 3). The GP applied herein adopts a squared exponential correlation function to relate points along the functional parameter, $\theta_f$, with respect to the dependent operational parameter, $x_f$. All input parameter values of the model are scaled to a unit hypercube for the inverse analysis, justifying the selection of a mean of 0.5 for the GP. The squared exponential correlation function (Eq. 4) is one of the most commonly implemented, as it provides a smooth, infinitely differentiable function capable of representing a wide range of continuous functions (Rasmussen and Williams, 2006; Swiler, 2006), with the dimensionality of the functional control parameter represented by $d$.

$$\theta_f \sim GP \left( 0.5, \lambda_{\theta_f}^{-1} R(x_f, x_f') \right)$$  \hspace{1cm} (Eq. 3)

$$R(x_f, x_f') = \exp \left\{ \sum_{k=1}^{d} -4\gamma_{\theta_f k} \left( x_{f_k} - x_{f_k}' \right)^2 \right\} \text{ where } k=1,2,\ldots,d$$  \hspace{1cm} (Eq. 4)
For simplicity, the remainder of this discussion assumes that $k$ is equal to one. The GP given in Eq. 4 has two hyperparameters, $\lambda_{\theta_f}$, the precision parameter which controls the magnitude of variations in $\theta_f$ and $\gamma_{\theta_f}$, the smoothness parameter which defines the length scale of $x_f$ across which $\theta_f$ is expected to vary, meaning that a larger value of $\gamma_{\theta_f}$ results in smaller correlations across $x_f$ (Williams and Rasmussen, 1996). These hyperparameters control the functional form of the GP for $\theta_f(x_f)$ and thus must be learned from the data. To do so, prior distributions are implemented for to the two GP hyperparameters, $\lambda_{\theta_f}$ and $\rho_{\theta_f} = e^{-\gamma_{\theta_f}}$. Herein, a beta hyperprior (Eq. 5) is applied to $\rho_{\theta_f}$, where the shape parameter $b_{\theta_f}$ can be used to enforce smoothness by shifting the distribution near one, and a gamma hyperprior (Eq. 6) to $\lambda_{\theta_f}$.

\[ \rho_{\theta_f} \sim \text{Beta}(1, b_{\theta_f}) \]  
\[ \lambda_{\theta_f} \sim \text{Ga}(a_{\theta_f}, b_{\theta_f}) \]  

(Eq. 5)  
(Eq. 6)

If the sampled $x_f$ values are identical (or near-identical), the correlation functions in the GP might have problems with matrix inversion due to singularity (or near-singularity), which is commonly avoided by the addition of some nugget parameter to the correlation function (Sacks et al., 1989; Neal, 1998; Santner et al., 2003). Herein, a nugget term in the form of a small white noise is added to the diagonal of the correlation matrix. The nugget term is scaled based on the smallest eigenvalue of the covariance with an exponential bound of $e^{20}$, following the form proposed in Ranjan et al. (2011).
2.3. Bayesian Inference for Inverse Analysis

The Bayesian solution to the inverse analysis in Eq. 2 can be inferred the posterior distributions of parameters conditioned upon prior knowledge and the experimental measurements (Eq. 7). The experimental data, \( y(x_f, x_c) \) are standardized to have a mean of zero and a standard deviation of one.

\[
P(\theta_c, \theta_f, \lambda_\theta, \rho_\theta | y(x_f, x_c)) \propto L(y(x_f, x_c) | \theta_c, \theta_f, \lambda_\theta, \rho_\theta) \times P(\theta_f) \times P(\theta_c) \times P(\lambda_\theta) \times P(\rho_\theta) \quad \text{(Eq. 7)}
\]

Posterior distributions given in Equation 7 can be obtained through Markov Chain Monte Carlo sampling of the parameter space requiring hundreds to thousands of runs depending on the dimensionality of the problem (Gilks et al., 1995; Higdon et al., 2004). In this study, Gibbs sampling, a specific case of the Metropolis-Hastings algorithm (Metropolis et al., 1953; Hastings, 1970; Geman and Geman, 1984), is used to sample the parameter space, where each step of the sampling is taken from a full conditional distribution of one parameter. Gibbs sampling cycles through each parameter individually to explore the domain (Gelfand and Smith, 1990). In the Gibbs sequence, each time hyperparameters of the GP for \( \theta_f \) are updated, the correlation matrix needs to be inverted, taking time proportional to \( n^3 \), where \( n \) is the size of the correlation function (i.e. number of data points in \( x_f \)), while full Gibbs scan for model parameters \( \theta_f \) take time proportional to \( n^2 \).

Noticing that additional Gibbs samples taken between hyperparameter updates adds only marginally to the computational cost, (Neal, 1998) suggested conducting subiterations (i.e. additional Metropolis steps) for vector-valued variables within the Gibbs sampler to potentially increase the rate of convergence. The effects of such additional Gibbs samples are discussed in Section 3.2.
3. Proof-of-Concept Demonstration

This section presents an academic proof-of-concept example with synthetically generated integral-effect experiments. Synthetically generating experiments allows the capability to control and know the true value of the empirical constituent to be inferred, thus providing a means for evaluation of the capability of the proposed inference methodology.

3.1. Model Definition and Integral-effect Experiments

Consider a consumer model, $\eta(\theta, x)$, that relates operational parameters to a system response, that has been captured by integral-effect experiments conducted at a finite number of select operational parameter settings (shown in Figure 4.3). The integral effect experiments demonstrate a dependence upon the control parameter, $x$, but this dependence is not represented in the available consumer constituent model. Predictions of this consumer constituent model where the functional relationship is currently unaccounted for and its prediction errors are shown in Figure 4.3.

![Figure 4.3. Integral-effect experimental data capturing coupled relationship.](image-url)
Figure 4.4. (Left) Physics-based model predictions where relationship to $x_f$ is unmodeled and (right) error resulting in the physics-based predictions due to these modeling assumptions.

The inverse analysis method discussed in Section 2 is implemented to construct the relationship between $\theta_f$ and $x_f$ from integral-effect experiments, shown in Figure 4.3, developing an empirical model to represent $\theta_f = f(x_f)$. Table 4.1 provides details of the parameter ranges for the inverse analysis, as well as the true functional form of a deterministic feeder model, which is currently missing and will be inferred empirically.

Table 4.1. Physics-based Model Parameter Values and Ranges

<table>
<thead>
<tr>
<th>State Variables (x)</th>
<th>Minimum</th>
<th>Maximum</th>
<th>True Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Independent Control ($x_c$)</td>
<td>0</td>
<td>4</td>
<td>-</td>
</tr>
<tr>
<td>Dependent Control ($x_f$)</td>
<td>0</td>
<td>4</td>
<td>-</td>
</tr>
<tr>
<td>Uncertain Model Parameters ($\theta$)</td>
<td>Function</td>
<td>1</td>
<td>5</td>
</tr>
</tbody>
</table>


3.2. **Inverse Analysis: Results and Discussion**

Twenty points are sampled along both $x_c$ and $x_f$, with the middle 20% of the data in both operational parameter space held out as a validation set (Figure 4.3). As discussed in Section 2, a GP and its associated hyperparameters are inferred to define the empirical constituent $\theta_f(x_f)$ rather than imposing a user-defined functional form. Prior distributions on the GP hyperparameters defined an *a priori* mean of 1 and standard deviation of approximately 0.45 for $\lambda_\theta$. During this inference, the functional parameter, $\theta_f$ is not confined by the prior bounds, as the sampling is allowed to explore beyond the initially defined minimum and maximum values. However, should the analyst prefer to place stricter boundaries on the functional parameter such restrictions may be implemented (Brown and Atamturktur, 2016).

Burn-in runs are completed for 2000 iterations followed by the drawing of 2000 samples, each of which utilizes ten subiterations during the $\theta_f$ sampling. Three Markov Chain Monte Carlo chains are carried out, each starting with different initial parameter values to ensure a converged solution and adequate mixing of the chains. Within each of these chains, every other sample is retained resulting in a collection of 3000 samples. The resulting posterior distribution of the empirical constituent model form generated from these samples is shown in Figure 4.5.
This empirically inferred feeder model, $\theta_f(x_f)$ can now be coupled to the consumer model. Mean predictions made with this new *experimentally augmented partitioned model* are shown in Figure 4.6, as well as the error remaining in these predictions. Compared to the simulations with the stand-alone consumer model operating without the functional parameter representation (recall Figure 4.4), the predictive capability of the model has greatly improved, with the average percent error reducing from 33.42% in stand-alone to 18.05% with the coupled empirical constituent and physics-based constituent system model, a 46% overall reduction in the prediction error. Not only was the predictive capability improved, but knowledge of the underlying coupling physics was also gained through the functional form of the previously unknown dependence.
3.3. Effect of Repeated Sampling of Functional Calibration Parameter

Recall from Section 2.3 that the functional parameter is sampled repeatedly with subiterations in accordance with the recommendations of (Neal, 1998) to improve the mixing of the Markov chain. Neal (1998) originally proposed subiterations to reduce computational costs in problems with high-dimensional parameter spaces with the assumption of a fast computation of the likelihood. In applying this method to engineering problems there are two scenarios that may be encountered; high-dimensional parameter space and computationally demanding model evaluations.

3.3.1. High-dimensional Correlations

First, as Neal (1998) presumed, the high-dimensional sampling of the dependent control parameter, or several dependent control parameters for a single functional
parameter, will result in a large covariance matrix requiring inversions for every sample of the GP hyperparameters. Often times an emulator may be employed for representing models of such high dimensions. Accordingly, a fast-running model (less than 0.001 second to evaluate) is assumed and an analysis of the effect of subiterations in large dimensional parameter spaces is completed. The nominal model presented in Section 3.1 is used as a baseline for comparison. Dimensionality of the problem is increased by sampling the dependent control parameter, $x_f$, on a finer grid to increase the size of the covariance. In every case shown, 20% of the data remains as a holdout set and the number of total samples of the functional parameter each (meaning the number of subiterations multiplied by the number of Gibbs iterations) is kept constant at 1000 for three chains with different starting values, producing a full distribution of 3000 samples. Figure 4.7 shows the degree to which the overall error of the empirical function is decreased with subiterations as well as the decrease in computational time required to complete the inference as the number of subiterations is increased, with the number of samples in the $x_f$ dimension (and therefore the size of the covariance matrix) is denoted by $N_x$. Table 4.2 further emphasizes this point, showing a continued decrease in computational time with increasing number of subiterations. Also shown in Table is that the error of the empirical model stabilizes at around four subiterations. In all of the different dimensionality cases tested, accuracy and computational efficiency are found to improve together as the number of subiterations increases. The first row of Table 4.2 shows the initial computational error and computational time resulting with one
subiteration and 1000 Gibbs iterations. Figure 6 and Table 2 illustrate the accuracy of the functional parameter by root mean squared error:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{N_x} (\theta_f^{\text{true}}(x_f^i) - \theta_f^{\text{inferred}}(x_f^i))^2}{N_x}}$$

(Eq. 8)

Figure 4.7. Convergence of parameter value error, standard deviation, and total computational time as number of subiterations of the $\theta_f$ parameter is increased.

Table 4.2. Accuracy and computational gains with increased parameter dimensionality.

<table>
<thead>
<tr>
<th>Number of Samples</th>
<th>20 samples</th>
<th>200 samples</th>
<th>2000 samples</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>% Decrease in Error</td>
<td>% Decrease in Comp. Time</td>
<td>% Decrease in Error</td>
</tr>
<tr>
<td>1</td>
<td>0.475</td>
<td>7.5 s</td>
<td>0.455</td>
</tr>
<tr>
<td>2</td>
<td>18.3%</td>
<td>33.8%</td>
<td>66.8%</td>
</tr>
<tr>
<td>3</td>
<td>69.2%</td>
<td>44.5%</td>
<td>81.6%</td>
</tr>
<tr>
<td>4</td>
<td>68.7%</td>
<td>49.9%</td>
<td>84.7%</td>
</tr>
<tr>
<td>5</td>
<td>66.9%</td>
<td>53.1%</td>
<td>85.8%</td>
</tr>
<tr>
<td>6</td>
<td>76.9%</td>
<td>55.1%</td>
<td>86.1%</td>
</tr>
<tr>
<td>7</td>
<td>76.9%</td>
<td>56.8%</td>
<td>86.7%</td>
</tr>
<tr>
<td>8</td>
<td>76.1%</td>
<td>57.9%</td>
<td>85.7%</td>
</tr>
<tr>
<td>9</td>
<td>76.5%</td>
<td>58.6%</td>
<td>86.4%</td>
</tr>
<tr>
<td>10</td>
<td>80.3%</td>
<td>59.6%</td>
<td>87.0%</td>
</tr>
</tbody>
</table>
3.3.2. Computationally Demanding Model

The second case worth investigating is when the computational cost of the physics-based model is on the order of a few seconds (such as that of the VPSC model presented in Section 4), and the analyst chooses to evaluate the model itself rather than bypassing it with an emulator during computation of the likelihood. The desire to maintain the physics through model evaluations rather than low-fidelity surrogates is evident in the push for high-fidelity model implementation as well as growing research in multi-fidelity models when possible (Ng and Willcox, 2014). Such is the situation to be investigated here.

Suppose a set number of Gibbs samples for every parameter and hyperparameter has been selected and set to 1000. However, the chain mixing may be found insufficient as convergence is not achieved with this setting. In this case, though the problem may be low dimensional, the analyst may choose to begin conducting subiterations of the functional parameter to improve the convergence, requiring an increased number of evaluations of the physics-based model within each Gibbs step. The results of such a decision are shown here for the nominal model presented in Section 3.1 with \( x_f \) sampled at 20 locations, 16 of which are used for the inference and 4 of which are kept as a holdout set, resulting in a low dimensional 16x16 covariance matrix.

Figure 4.8 illustrates the change in the resulting empirical constituent for a varying number of subiterations of the vector-valued parameter, \( \theta_f \). In this figure, every case utilizes three chains with different starting values and total 1000 samples of the functional parameter each (meaning the number of subiterations multiplied by the
number of Gibbs iterations always equals 1000) with 1000 total runs being used in the burn-in step followed by 1000 total runs in the sampling step. Although each of the figures are generated with 3000 total samples once the three chains are combined, the GPs trained with up to two Gibbs subiterations of $\theta_f$ or less exhibit unsatisfactory convergence, as shown by the fact that all 1000 samples for each chain overlay each other making the appearance of only 3 samples drawn rather than 3000. These findings indicate that the proposal distributions being generated with 1 or 2 subsamples are consistently rejected, causing the adaptive step-size to reduce towards zero and the proposals values to become constant. This problem is relived as the number of subiterations is increased.
Figure 4.8. Improved convergence of posterior distributions with increased subiterations of the $\theta_i$.

The small difference in samples from three subiterations to four, and likewise as subiterations continue to increase, is noticeable. Results demonstrate that once chains have sufficiently mixed and converged, little gains in prediction accuracy and precision may be gained from increased subsampling. Though the accuracy does not continue to improve with subiterations, the computational time does continue to decrease, demonstrating the capability of increased subiterations to support the use of more
computationally demanding models. Figure 4.9 illustrates this trend, where the computational time continues to decrease without gaining or sacrificing significant neither accuracy nor precision, where computational time is the total time required to sample the three distinct chains run in serial.

Table 4.3 further emphasizes this point, where computational time is the total time required to sample the three distinct chains. In addition to the accuracy of the functional parameter estimation, uncertainty remaining in the estimation is represented in Figure 8 by standard deviation, which is averaged over all $x_f$ points.

![Figure 4.9](image)

Figure 4.9. Convergence of parameter value error, standard deviation, and total computational time as number of subiterations of the $\theta_f$ parameter is increased.
Table 4.3. Change in inference results as number of iterations is increased.

<table>
<thead>
<tr>
<th>Number of Samples</th>
<th>RMS error</th>
<th>Percent Decrease in Error from 1 sample</th>
<th>Computational Time (seconds)</th>
<th>Percent Decrease in Computation Time from 1 sample</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.322</td>
<td>--</td>
<td>14.9</td>
<td>--</td>
</tr>
<tr>
<td>2</td>
<td>0.200</td>
<td>37.9%</td>
<td>9.18</td>
<td>38.4%</td>
</tr>
<tr>
<td>3</td>
<td>0.136</td>
<td>57.8%</td>
<td>7.25</td>
<td>51.3%</td>
</tr>
<tr>
<td>4</td>
<td>0.140</td>
<td>56.5%</td>
<td>6.36</td>
<td>57.3%</td>
</tr>
<tr>
<td>5</td>
<td>0.102</td>
<td>68.3%</td>
<td>5.95</td>
<td>60.1%</td>
</tr>
<tr>
<td>6</td>
<td>0.114</td>
<td>64.6%</td>
<td>5.63</td>
<td>62.2%</td>
</tr>
<tr>
<td>7</td>
<td>0.100</td>
<td>68.9%</td>
<td>5.43</td>
<td>63.6%</td>
</tr>
<tr>
<td>8</td>
<td>0.107</td>
<td>66.8%</td>
<td>5.10</td>
<td>65.8%</td>
</tr>
<tr>
<td>9</td>
<td>0.118</td>
<td>63.4%</td>
<td>5.03</td>
<td>66.2%</td>
</tr>
<tr>
<td>10</td>
<td>0.101</td>
<td>68.6%</td>
<td>5.06</td>
<td>66.0%</td>
</tr>
</tbody>
</table>

Figure 4.8 and Table 4.3 are computed with the nominal computer model, which operates at approximately $7 \times 10^{-4}$ seconds per model evaluation. This computational time is on the order of a surrogate model. However, the computation becomes more demanding as the physics-based model becomes increasingly demanding, such as the plasticity model to be discussed in Section 4. As such, the computational time of the physics-based model is increased and the analysis of the gains in accuracy and total computation time is assessed, results of which are shown in Table 4.4, where the initial computational time with one subiteration and 1000 Gibbs iterations is shown in the row where number of samples is equal to one. This table serves to demonstrate the consistent trend in the percent decrease in computational time across the varied model run times, although this trend is difficult to see in Figure 4.9 due to the drastically different initial total computational times for each of the models. Another notable observation from Table 4.4 is that the rate at which computational demands decrease becomes less as the time required for a single model evaluation increases, though the trend of continued gains in total computational time is still observed. These findings indicate that subiterations may alleviate the computational demands associated with the implementation of physics-based
models and reduce the need to use surrogate models in the functional parameter sampling.

### Table 4.4. Reduction in computational demands with the addition of subiterations.

<table>
<thead>
<tr>
<th>Number of Samples</th>
<th>0.01 s per evaluation</th>
<th>0.05 s per evaluation</th>
<th>0.10 s per evaluation</th>
<th>0.50 s per evaluation</th>
<th>1.00 s per evaluation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>443 s</td>
<td>2,132 s</td>
<td>4,217 s</td>
<td>21,040 s</td>
<td>42,050 s</td>
</tr>
<tr>
<td>2</td>
<td>15.1%</td>
<td>14.4%</td>
<td>14.3%</td>
<td>14.3%</td>
<td>14.3%</td>
</tr>
<tr>
<td>3</td>
<td>19.9%</td>
<td>19.0%</td>
<td>18.9%</td>
<td>18.9%</td>
<td>18.9%</td>
</tr>
<tr>
<td>4</td>
<td>22.5%</td>
<td>21.6%</td>
<td>21.5%</td>
<td>21.5%</td>
<td>21.4%</td>
</tr>
<tr>
<td>5</td>
<td>24.0%</td>
<td>23.1%</td>
<td>22.9%</td>
<td>22.9%</td>
<td>22.9%</td>
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<tr>
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<td>24.1%</td>
<td>23.7%</td>
<td>23.7%</td>
<td>23.7%</td>
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<tr>
<td>7</td>
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<td>25.0%</td>
<td>24.3%</td>
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<td>25.8%</td>
<td>24.9%</td>
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<td>25.0%</td>
</tr>
<tr>
<td>9</td>
<td>25.8%</td>
<td>25.6%</td>
<td>24.7%</td>
<td>24.8%</td>
<td>24.8%</td>
</tr>
<tr>
<td>10</td>
<td>26.9%</td>
<td>26.5%</td>
<td>25.7%</td>
<td>25.7%</td>
<td>25.7%</td>
</tr>
</tbody>
</table>

### 4. 5182 Aluminum Alloy with Temperature and Strain Rate Dependencies

#### 4.1. Viscoplastic Self-Consistent Model and Experiments

The viscoplastic self-consistent (VPSC) model predicts texture evolution of highly anisotropic polycrystalline materials. One such material is the 5182 aluminum alloy, which in addition to exhibiting viscoplastic behavior also displays temperature and strain rate dependencies, captured by experiments conducted by (Chen et al., 1998) (Figure 4.10). In an effort to identify the cause of the dependence, (Stout et al., 1998) collected texture measurements in combination with the mechanical measurements. Texture measurements revealed that 5182 aluminum favors the classic (101) deformation texture at temperatures below 300°C but transitions to a combination of the classic (101) and static recrystallization (001) textures at temperatures above 400°C (Figure 4.10). Available experimental stress-strain curves reveal this temperature dependence at two separate strain rates (0.001 and 1 s⁻¹), as shown in Figure 4.10. Stress values are collected.
at 30 points along each of the four curves, with strains ranging from 0 to 0.58 and samples spaced 0.02 apart. Despite this known temperature dependence, there is currently no constituent model for the thermal analysis available to couple with VPSC and represent the effects of temperature on material behavior (the current model configuration is shown in Figure 4.11).

![Graph](image)

(a) Strain Rate = 1s⁻¹  
(b) Strain Rate = 0.001s⁻¹

Figure 4.10. Uniaxial compression experimental tests of 5182 Al and different strain rates and temperatures.

The VPSC model predicts the behavior of polycrystals with viscoplastic deformations using the governing equation shown in Eq. 9:

\[
\dot{\varepsilon} = \dot{\gamma}_o \sum_{s=1}^{2} m^s \left( \frac{m^s \sigma}{\tau_0^s} \right)^n_{\sigma} \text{sgn}(m^s; \sigma)
\]  

(Eq. 9)

where \( \sigma \) is the stress applied to the crystal, \( \dot{\varepsilon} \) is the strain rate, \( s \) is the number of slip and twinning systems active in the material (which is two in the case of the glide-only 5182 aluminum model), \( m^s \) is the Schmid tensor associated with glide, \( \tau_0^s \) is the critical resolved shear stress, the exponent, \( n_\sigma \), represents the inverse of rate-sensitivity for glide activity, and \( \dot{\gamma}_o \) denotes a normalization factor. The strain rate equation is summed over all active slip systems, \( N_s \). Within this equation two parameters associated
with the glide behavior $n_g$ and resolved shear stress for the first deformation system, $\tau_o^1$ are uncertain. While the glide parameter remains constant throughout the domain (Atamturktur et al., 2015), the critical resolved shear stress represents a hardening function and therefore is the parameter related to the changing texture evolution with respect to temperature and strain rate. This thermo-mechanical coupling between hardening parameters, temperature and strain rate on texture development can be accounted for through an empirical constituent model making $\tau_o^s$ a function of $T$, thus resulting an experimentally augmented partitioned model.

![Physics-based VPSC model](image)

**Figure 4.11. Current physics-based VPSC model without thermal constituent to represent thermo-mechanical coupling.**

### 4.2. Inference of VPSC Weakly Coupled Physics: State-Aware Problem Formulation

Incorporating the empirical model with the physics-based plasticity model, the experimentally augmented coupled model may be written as:

$$\sigma = \eta (\varepsilon, \dot{\varepsilon}, n_g, \tau_0(T))$$  \hspace{1cm} (Eq. 10)

where stress is the prediction to be compared with experiments (recall Figure 4.10). The roles of the input parameters in the inverse procedure and their respective ranges for the analysis are detailed in Table 4.5. Uniform prior distributions are assumed for both parameters with upper and lower bounds as indicated in Table 4.5. No constraints are placed on the form of the empirical feeder model inferred to represent the
thermal constituent. These large ranges and minimal constraints leave much flexibility to
the inverse analysis, making it possible to learn as much as possible from the
experimental data.

Table 4.5. VPSC model parameter values.

<table>
<thead>
<tr>
<th>State Variables (x)</th>
<th>Parameter</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Independent Control (x_i)</td>
<td>Strain (ε)</td>
<td>0</td>
<td>0.58</td>
</tr>
<tr>
<td>Dependent Control (x_j)</td>
<td>Temperature (T) [°C]</td>
<td>180</td>
<td>570</td>
</tr>
<tr>
<td>Uncertain Model Parameters (θ)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Constant Parameter (θ_c)</td>
<td>n_g</td>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>Functional Parameter (θ_f)</td>
<td>τ_0 [MPa]</td>
<td>2</td>
<td>1500</td>
</tr>
</tbody>
</table>

Prior distributions on the GP hyperparameters for the functional parameter, τ_0, defined an *a priori* mean of 1 and standard deviation of approximately 0.45 for λ_θ. Burn-in runs are completed for 800 iterations followed by the drawing of 1000 samples, each of which utilized ten subiterations of the θ_f sampling. Three MCMC chains are carried out, each starting with different initial values of all the parameter values to ensure that a converged solution is reached, ultimately leading to a collection of 3000 samples. To confirm the accuracy of the inverse procedure 20% of the experimental data (ranging from a strain of 0.24 to 0.34) is held out during the inverse analysis for all temperature settings.

4.3. Results of Inverse Analysis

The posterior distribution of the τ_0 function is shown in Figure 4.12, where grey lines illustrate 3000 realizations and the solid black and dashed black lines denote the mean and one standard deviation of the posterior, respectively. Posterior distributions of the GP hyperparameters are shown in Figure 4.13. Statistics of the posterior for the
empirical thermo-mechanical model at the available temperature settings are provided in Table 4.6.

**Figure 4.12.** Posterior distribution of the functional parameter $\tau_0$ at a strain rate of 1 s$^{-1}$.

**Figure 4.13.** Posterior distributions of the empirical GP model hyperparameters.

Recall that the parameter $n_g$ in the physics-based VPSC model is also uncertain though it has no dependence on the operational settings. The posterior distribution obtained for $n_g$, shown in Figure 4.14, is relatively non-informative when the inverse
analysis is completed at a strain rate of 1 s\(^{-1}\). Inability to calibrate \(n_g\) implies that the model’s stress predictions are insensitive at this strain rate value, which is confirmed by an analysis of variance conducted at the both strain rate settings. The sensitivity of model output to \(n_g\) indeed varies greatly as a function of strain rate: \(\tau_0\) contributes to 100% of the variability in model predictions at a strain rate of 1 s\(^{-1}\) while the R\(^2\) values in the main effect screening at a strain rate of 0.001 s\(^{-1}\) are 42% and 58% for \(\tau_0\) and \(n_g\), respectively. Posterior distributions of the constant and functional parameters with respect to experiments at a strain rate of 0.001 s\(^{-1}\) are shown in Figure 4.15. Comparison of the calibrated parameter values and remaining uncertainty at both strain rate settings is shown in Table 4.6, where the mean and standard deviation of posteriors for the functional parameter are shown at available temperature settings, as the posterior varies throughout the operational domain. The difference in the \(\tau_0\) functions for the two strain rates is to be expected given the known dependence on strain rate (Atamturktur et al., 2015; Chen et al., 1998; Lebensohn et al., 2010; Stout et al., 1998).

![Figure 4.14. Posterior distribution of constant VPSC physics-based model parameter when operating at a strain rate of 1s\(^{-1}\).](image-url)
In Table 4.6, the difference in standard deviations of inferred parameter values, indicating uncertainty remaining in the predictions, are worth noting for the two different strain rate settings. When the inverse analysis is completed with respect to experiments conducted at a strain rate of 1 s\(^{-1}\) (where the model is highly sensitive to \(\tau_0\) and not at all sensitive to \(n_g\)) the standard deviation of \(\tau_0\) is on average 18.3\% of the mean value while the standard deviation of \(n_g\) is 24.9\% of the mean value. The uncertainty in these parameters swaps when the model is calibrated with respect to experiments conducted at a strain rate of 0.001 s\(^{-1}\) (where the model also becomes sensitive to \(n_g\)) with the standard deviation of \(\tau_0\) being on average 40.4\% of the mean value while the standard deviation of \(n_g\) is reduced to 10.7\% of the mean value. Results of this analysis suggest that the model calibration would improve if both strain rate settings could be considered simultaneously. Provided the opportunity for more data at other strain rate settings, training a function for \(\tau_0\) dependent upon both temperature and strain rate would be the best path forward.

![Figure 4.15. Posterior distributions of the (left) constant VPSC model parameter, \(n_g\) and (right) functional parameter \(\tau_0\) inferred for operations at a strain rate of 0.001 s\(^{-1}\).](image)

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Table 4.6. Comparison of the empirical thermo-mechanical constituent model and uncertain VPSC model parameter for inverse analysis with different strain rates.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Temperature Setting (°C)</th>
<th>Strain Rate = 1 s⁻¹</th>
<th>Strain Rate = 0.001 s⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>Standard Deviation</td>
<td>Mean</td>
</tr>
<tr>
<td>Constant Parameter (θₙ)</td>
<td>--</td>
<td>3.57</td>
<td>0.89</td>
</tr>
<tr>
<td>Functional Parameter (θₕ)</td>
<td>200</td>
<td>102.2</td>
<td>11.23</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>75.70</td>
<td>8.29</td>
</tr>
<tr>
<td></td>
<td>400</td>
<td>49.44</td>
<td>7.68</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>28.28</td>
<td>10.05</td>
</tr>
</tbody>
</table>

With the model parameters and corresponding GP hyperparameters determined through the inverse analysis, the resulting GP model for τ₀(T) is implemented as an empirical thermal constituent model and coupled with the existing physics-based VPSC plasticity model. The newly available experimentally augmented partitioned model simulating the thermo-mechanical coupling is shown in Figure 4.16. Figure 4.17 illustrates ultimate stress predictions of the coupled model compared with the available experimental data. Ultimate stress is the stress value obtained at the last strain value, which is typically the prediction of highest interest to decision makers as it relates to the point at which failure is most likely to occur. Table 4.7 provides statistics of the predictions of the newly available experimentally augmented model with the GP thermal constituent coupled to the VPSC mechanical constituent. This table captures an averaged picture of results of the empirically augmented model across all strain settings as opposed to only the final strain shown in Figure 4.17.
Figure 4.16. Coupled thermo-mechanical model, composed of an empirical thermal constituent and physics-based plasticity constituent, for predicting mechanical behavior of 5182 aluminum alloy at varying temperature settings.

![Diagram](image)

Figure 4.17. Ultimate stress predictions taken at the maximum strain value with remaining uncertainty.

Table 4.7. Statistics of the experimentally augmented GP-VPSC thermo-mechanical model.

<table>
<thead>
<tr>
<th>Temperature Setting (°C)</th>
<th>Predictions of Coupled Thermo-mechanical Model [(\sigma(T, \varepsilon))]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RMS Error (MPa)</td>
</tr>
<tr>
<td>200</td>
<td>34.9</td>
</tr>
<tr>
<td>300</td>
<td>14.9</td>
</tr>
<tr>
<td>400</td>
<td>3.50</td>
</tr>
<tr>
<td>500</td>
<td>2.29</td>
</tr>
</tbody>
</table>
5. Conclusions

Model developers are recognizing more than ever the need to account for interrelated physics and scales through coupled modeling. Partitioned analysis presents an attractive solution for these complex problems. However, the physics of one or more constituent in these relationships is sometimes unknown and therefore cannot be modeled directly. The omission of a constituent model degrades the predictive capability of the full system; a problem that becomes more pronounced as the complexity of the system increases and knowledge regarding the underlying physics becomes increasingly incomplete. For instance, the physics-based model may be a legacy code that cannot be easily changed. Missing coupling relationships can occur in legacy codes when, for example, new materials or systems are being implemented in the code where an operational state, which was not influential previously, becomes influential, or when new experiments become available showing dependence that was previously unknown. Furthermore, the empirical model will be intrinsically application-dependent based on the integral-effect experiments used in the inverse analysis. Therefore, different empirical models may be inferred for a variety of applications and partitioned analysis makes swapping empirical models for different applications a simple process.

The notion of treating the empirically derived function as an independent constituent model is attractive as it isolates the empirical components (conditioned upon experiments) from the physics-based components (based on first principle understanding). This transparency, which would be lost if the empirical relationship was directly integrated into the physics-based model with a monolithic approach, allows for easy
updating of the empirical model as new data becomes available and also provides clear indication to future code developers and designers of which components of the coupled model is conditioned upon experiments.

The inverse analysis proposed herein infers, from readily available integral-effect experimental measurements, the functional relationships neglected in physics-based models, providing the model developer with an empirical constituent model that can be coupled to the existing physics-based model to account for important dependencies. In addition to yielding a more accurate computer model, inferring this unknown relationship from observations provides insight into a more complete mathematical representation of the nature of missing physical relationships, furthering the scientific understanding of these processes. Furthermore, the GP approach developed herein is capable of providing not only GP hyperparameter values, but also recommendations of parametric model forms for future use as the empirical constituent is coupled to the existing physics-based model. The advantage of beginning the functional exploration with a GP is the few number of hyperparameters required, allowing the MCMC to deal with smaller dimensional parameter spaces thus maintaining feasible computational times.

The proposed methodology has demonstrated the capability to infer a physical dependence of 5182 aluminum material properties on the temperature at which the material is being loaded, producing an empirical model to be coupled with the existing VPSC physics-based model. These results show the promise of Gaussian process inverse analysis to demystify influential thermo-mechanical relationships underlying complex materials implemented in engineering and science today. The case study presented with
5182 aluminum also illustrates a path forward for continued development of the method to provide empirical constituent models dependent upon more than one operational state. Furthermore, the possibility of missing physics of the computer model as a consequence of missing model parameters resulting in a level of discrepancy bias remaining is recognized. Hence, discrepancy should also be included in this calibration framework.

References


CHAPTER FIVE

STATISTICAL INFERENCE OF EMPIRICAL CONSTITUENTS IN
PARTITIONED ANALYSIS: STRONGLY COUPLED MODELS

1. Introduction

In many engineering applications, multiple physical constituents collectively form a more complex, strongly coupled system by interacting with each other. In this context, a constituent may mean physical phenomena (i.e. thermal and mechanical behavior), fields (i.e. fluid and structure), scales (i.e. micro and macro scales) or simply different functional components (i.e. aircraft wings and body) that govern the behavior. The nature of these strongly coupled systems makes their numerical representations amenable for decomposition into independent, isolated computational constituents, which are first solved in an independent manner and then made to communicate with each other. Such communication typically takes place through the exchange of model inputs and outputs with iterative coupling operations. The computational process of solving the response of a complex system by means of iterative evaluations of simpler constituents is known as partitioned analysis (Felippa et al., 2001). Partitioned analysis comes with many benefits such as the ability to use existing legacy codes developed and validated independently by subject matter experts for each computational constituent as well as the flexibility to choose the most suitable solvers, spatial meshes, time discretizations and/or boundary conditions in each constituent.

8 Conversely, monolithic analysis involves the development of a single code that requires all constituents to advance in time in a synchronous manner.
Partitioned approach has been gaining popularity (Farhat and Lesoinne, 2000; Matthies and Steindorf, 2002; Joosten et al., 2009) and has been shown to yield realistic representation of reality for many engineering applications (for example, see studies completed by Döscher et al. (2002); Bunya et al. (2010); Andrade et al. (2011); Knezevic et al. (2012)). Partitioning relies on the basic premise that at the very least either expert knowledge or mature models are available for all constituents of interest. This premise has largely been unquestioned in the partitioned analysis literature, due perhaps to being an integral requirement of any mechanistic modeling effort. However, there are many engineering problems that lend themselves to partitioning, but lack the mechanistic knowledge necessary to develop computational models for all constituents, therefore yielding an incomplete partitioned representation of the coupled system. Often times, these situations are compounded with additional difficulties when experimentally observing the response of the constituents is not possible, rather integral-effect experiments entailing the whole system behavior, inherently including the coupling of all constituents, are the only possible form of observation.

The goal of this paper is to generate partitioned models of strongly coupled systems through inference from integral-effect experiments. Herein, we propose an approach that can alleviate the dilemma posed by the unavailability of a constituent model in a partitioned system, where experimental observations of the coupled system can be used to infer an empirical approximation of its response. This empirical approximation is functional in nature, reflecting how the input of a constituent model should change throughout the domain of applicability due to interactions occurring
among the physical constituents. The proposed approach is essentially a functional inverse analysis of the output response of the missing constituent with respect to its inputs, which also explicitly recognize the uncertainties prevalent throughout the process and incorporates them in the analysis.

The remainder of this paper discusses the details of the proposed a functional inverse analysis of a constituent model and demonstrates its applicability on both academic and practical applications. Section 3 extends the Bayesian inverse analysis presented in Chapter 4 to function for applications with strong, two-way coupling. Section 4 details a case study of an elasto-plastic analysis in which the elastic behavior is captured by a finite element macroscale constituent model, but the plasticity constituent model is unavailable and needs to be determined. The inverse analysis and resulting constituent plasticity model are discussed in Section 5. Section 6 concludes the findings and presents a path forward for future work.

2. Perspectives on Coupled Model Calibration

2.1. Shared Parameters in Partitioned Analysis

In this study, input parameters within strongly coupled systems will be thought of in three categories. Uncertain parameters, \( \theta \), are the input parameters of the constituent models for which the precise value is unknown and requires calibration. Uncertain parameters, often related to physical properties of a system, such as definition of materials and boundary conditions, are those that will be mitigated through calibration against experiments. Control parameters, \( x \), are those that control the operational conditions, such as temperature or loading applied to the system in hand. Finally,
remaining parameters of the system that are needed to execute the model but neither uncertain nor control parameters are referred to as general input parameters and denoted as $z$.

The main objective of coupling iterations is to determine the correct values for the inputs and outputs that are exchanged among constituents, which are henceforth referred to as dependent parameters. Likewise, parameters that do not depend on other constituents are referred to as independent parameters. Dependent parameters can take any of the two categories of inputs: control parameters, $x$, and remaining parameters, $z$. Iterative coupling occurs when parameters from any of these three groups are passed back and forth between constituent models until a convergence criterion is met.

Now, consider a strongly coupled system where two constituent models, $\Omega_A$ and $\Omega_B$, exchange parameters. Figure 5.1 illustrates nine ways in which these parameters can be shared between the two constituents, where the subscript letter denotes the model that is acting as the feeder of this parameter and the other is the consumer. At least one parameter must be shared in each direction for the system to be strongly coupled, however, the coupling can include the exchange of more than one parameter. Also, dependent parameters can be scalar or vector valued. For example, $X_A$, could be a single temperature prediction or a full temperature field that is predicted by $\Omega_A$ to control the predictions of $\Omega_B$. This iterative process introduces uncertainties to the system model. Herein, we will specifically focus on uncertainties resulting from poorly known parameters.
Starting with the most simple of the nine scenarios, Scenario 1 involves both models exchanging only general input parameters, $z$. This scenario means that although the models are informing one another, one is not stimulating the other. Scenario 2 is the exact opposite, where both models are exchanging control parameters (i.e., stimulating each other). An example of such a system would be a coupled dynamical system where $\Omega_A$ predicts a force to be applied to $\Omega_B$ and then $\Omega_B$ in turn predicts a displacement that is applied to $\Omega_A$. Scenarios 3 and 4 are essentially the same, where one constituent controls the next but the feedback received is a general model input, not a control parameter. Scenarios 5-8 illustrate the different ways in which these two parameters types can be paired. Finally, Scenario 9 presents the most comprehensive of the group with both models sharing general and control parameters.

Figure 5.1. Scenarios for coupling two constituent models.
Take note that in our formulation, there are no $\theta$ parameters shared in any of these scenarios, meaning that dependent output of a constitutive model to be entered as an input to another constituent is not treated as uncertain input parameter. This is because any uncertainty in a dependent parameter will be mitigated by learning the parameter values through the feeder model predictions.

However, if a constituent model, say $\Omega_B$ in Scenario 3, were to be unavailable, the parameter, $Z_B$ that would be a prediction of $\Omega_B$ would instead become an uncertain parameter of $\Omega_A$ (Figure 5.2). This missing physical relationship, $Z_B(X_A)$ is indeed relevant to the true physical process and necessary to obtain simulations representative of experimental measurements of the system the model is intended to represent.

![Figure 5.2. Introduction of uncertain inputs to the coupling interface due to a missing constituent model.](image_url)

### 2.2. Transparency of Experiments in Relation to Coupling Parameters

Intuitively, separate-effect experiments can be used to improve constituent models and integral-effect experiments can be used to improve the coupled model (Farajpour and Atamturktur, 2013; Hegenderfer and Atamturktur, 2013, others?). Confining model development to this straight-forward mindset, however, significantly limits benefits that partitioning stands to offer. Bias-corrected partitioned analysis, introduced in Stevens et
al. (2016) provided an interesting insight, establishing a link between separate-effect experiments and coupled predictions.

Building upon this work, the previous chapter illustrated a new link between integral-effect experiments constituent models by proposing that integral-effect experiments do not have to be confined to improving existing coupled models but can actually be used to infer constituent models. Herein, the final portion of this research study pushes the barrier even further, exploring the limitations on how much information regarding constituent models can be gained from integral-effect experiments. The focus of the proposed methodology is on systems where the input to any constituent model that will be empirically inferred is a control input. Figure 5.3 shows the inference options for each of the possible coupling scenarios available with the framework proposed herein.

Figure 5.3. Constituent model inference opportunities using the proposed methodology.
3. Methodology for Inferring Constituent Models in Strongly Coupled Systems

3.1. Conceptual framework

Let the dependent predictions of the constituent models be denoted as $\alpha$ for the available physics-based constituent and $\beta$ for the unavailable constituent. The coupling relationship between these models is illustrated in Figure 5.4 where the prediction of the physics-based model, $\alpha$, is dependent on a prediction of the missing constituent, $\beta$, which in turn would be dependent upon $\alpha$. Herein lies the main difference of inverse constituent model analysis for strongly coupled models from that of weakly coupled model\(^9\). With a strongly coupled system, the inference is seeking to identify a relationship in which the available physics-based model is reliant upon its own predictions as the functional control parameter. However, in weakly coupled systems the inference is a simpler and more straight-forward, as the functional control parameter will simply be an operational state driving predictions of the physics-based constituent.

The goal is to empirically derive the previously unknown representation of $\beta$, as a function of the available physics-based outputs, $\alpha$. Figure 5.4 (left) illustrates the given information for the inverse analysis, where only the physics-based constituent and integral-effect data are available. The currently unknown coupling relationship shown by the grey box will be replaced by an empirically derived constituent model, as shown in Figure 5.4 (right), meaning that $\alpha$ becomes the dependent control parameter in the framework described in Stevens et al. (2016b). This empirical constituent model will then

\(^9\) The reader is referred to Stevens et al. (2016) for a detailed methodology on the empirical constituent model inference for a weakly coupled system.
be represented as a functional calibration parameter, resulting in a new experimentally-augmented physics-based model $\Omega_\Lambda$ with the coupling relationships incorporated.

Figure 5.4. Formulation of empirical constituent model for the development of a partitioned representation of a strongly coupled system.

The inference problem is posed such that the currently available physics-based constituent is compared against available integral-effect experiments. An assumption in this process is that the available integral-effect data measures a system response of the physics or scale that can be predicted by the existing physics-based model. Therefore, the newly developed coupled model may be expressed as a relationship of the model predictions, $\eta$, to experimental measurements, $y$, at $N$ discrete points in the independent control domain.

$$y_{\text{int}}(x^i) = \eta( x^i, \theta_c, \theta_f(\alpha(x_c))) + \epsilon \quad \text{for } i = 1, 2, \ldots, N$$  \hspace{1cm} (Eq. 1)

where For applications presented herein, we will assume all observation errors are independent and Gaussian distributed. Take note that this formulation also accounts for uncertainty in the physics-based model independent of the coupling, $\theta_c$, as well as uncertainty in the form of experimental error, $\epsilon$, so that all of these sources of uncertainty are accounted for in conjunction with the empirical model inference.
3.2. Bayesian Modeling

A Bayesian approach is taken to learning the form of the functional parameter as well as the value for the constant parameter so that both sources of uncertainties, as well as model and experimental uncertainties, may be considered simultaneously (Brown and Atamturktur, 2016; Stevens et al., 2016b). Bayesian inference also allows for any prior knowledge and constraints to be incorporated to inform the sampling. For example, if a functional form of the constituent model is known, a parametric structure can be imposed (such as that demonstrated in Atamturktur et al. (2015)). If the form of the function is unknown, one may prefer to use nonparametric models where the functional form may be learned from the data. Gaussian Process (GP) models are one form of emulator that has been recommended by Kennedy and O’Hagan (2001) for being a well-suited, flexible model form when the true form is not known. Similar to the way a Gaussian distribution is defined with a mean and standard deviation, a GP is defined with a mean and a covariance function. Any prior knowledge regarding the expected general tendencies of the functional form to be inferred (such as the degree of smoothness of the function) can be incorporated through the selection of the form of the GP covariance. The exponential covariance structure is often preferred in applications that have smooth, continuous functional forms for its infinitely differentiability. Other covariance structures may be implemented as suitable for the application at hand. Once a covariance structure is selected, any prior knowledge regarding the precision and smoothness of the empirical function can be implemented through prior distributions on the hyperparameters. In addition, constraints can be place such as upper and lower boundaries on the functional
parameter value at any given $x_f$ (see Brown and Atamturktur (2016) for demonstration). If general knowledge of the shape of the function is available, such as the function should be increasing or decreasing in a given region of the domain, then derivatives may be included in the covariance structure to better inform the proposal draws (Golchi et al., 2015), or sampling can be completed using a truncated normal distribution so that only physically meaningful functions are evaluated.

Herein, a GP with a squared exponential covariance structure is used to determine the functional form of the missing constituent model (Eq. 2).

$$\theta_f \sim \text{GP} \left( \mu, \lambda_{\theta_f}^{-1} R(x_f, x_f') \right)$$  \hspace{1cm} (Eq. 2)

The mean function, $\mu$, can be initially defined to meet any known constraints on the functional form through a prior distribution and refined throughout the inference. The squared exponential covariance has two hyperparameters, $\lambda_{\theta_f}$ and $\gamma_{\theta_f}$, which influence the model precision and smoothness, respectively. A different set of hyperparameters may be used in the case of a different covariance form, but the following methodology remains applicable. Using this GP in combination with constant uncertain parameter, $\theta_c$, and given control input settings, a distribution of predictions of the physics-based model, $\Omega$, may be represented as:

$$\left( \Omega(x_f, x_c) | \theta_f, \theta_c, \lambda_y \right) \sim \mathcal{N} \left( \eta(\theta_f(x_f), \theta_c, x_c), \lambda_y^{-1} I \right)$$  \hspace{1cm} (Eq. 3)

where $\lambda_y$ is the precision of the physics-based model predictions. Algorithm 1 presents the process for Bayesian inference of the uncertain model parameters and GP
hyperparameters for a generic case. Constraints from prior information may be integrated into this general algorithm as best fit for a given application.

**Algorithm 1. Constituent Model Inference**

**Inputs:** Initial values: \(a, b, \lambda, \rho, \theta_f(x_f), \theta_c\)

Prior distributions: \(\lambda, \rho \sim \text{Beta}(1, 1), \theta_c \sim U(0, 1), \theta_f \sim \text{GP}(\mu, \lambda^{-1}_f \mathbf{R})\)

Simulator precision distribution parameters: \(a, b\)

**Step 1.** Determine physics-based model precision parameter

\[
a^*_\eta = a + \frac{N}{2}
\]

\[
b^*_\eta = b + \frac{1}{2}(y_{\text{int}} - \eta(\theta_f, \theta_c))^T(y_{\text{int}} - \eta(\theta_f, \theta_c))
\]

\[
\lambda_y = \text{Ga}(a^*_\eta + b^*_\eta^{-1})
\]

**Step 2.** Compute covariance

\[
\mathbf{R}(x_{f_i}, x_{f_j}) = \exp\left\{\sum_{k=1}^{d} -4y_{f_{ik}}(x_{f_{ik}} - x_{f_{jk}})^2\right\}
\]

where \(d\) is the dimensionality of \(x_f\)

**Step 3.** Subiterations to sample \(\theta_f\)

For \(i = 1, \ldots, I\) where \(I\) is the predefined number of subiterations

**Step 3.1. Propose** \(\theta_f^* \sim \mathcal{N}(\theta_f, \lambda^{-1}_f \mathbf{R})\)

Draw \(\theta_f^*\) by spectral decomposition

\[
\frac{1}{2} \mathbf{R}^{-1} = \mathbf{U} \Lambda \mathbf{U}^T
\]

\[
\theta_f^* = \mathbf{c}_f \mathbf{U}^{1/2} \mathbf{z} + \theta_f\ \text{where} \ \mathbf{z} \sim \mathcal{N}(0, 1)
\]

**Step 3.2. Calculate log-likelihood**

\[
\log\left(\pi(\theta_f^* | \lambda, \rho, \theta_f)\right) = -\frac{\lambda_y}{2}(y_{\text{int}} - \eta(\theta_f^*, \theta_c))^T(y_{\text{int}} - \eta(\theta_f^*, \theta_c))
\]

\[
-\frac{\lambda_y}{2}(\theta_f^* - 0.5)^T \mathbf{R}^{-1}_s(\theta_f^* - 0.5)
\]

where \(\mathbf{R}_s\) is the covariance with a nugget term added to avoid singularity

**Step 3.3. Determine acceptance**

Calculate the density ratio

\[
\frac{\pi(\theta_f^* | \lambda, \rho, \theta_f)}{\pi(\theta_f^* | \lambda, \rho, \theta_f)} = \exp\left(\log\left(\pi(\theta_f | \lambda, \rho, \theta_f)\right) - \log\left(\pi(\theta_f | \lambda, \rho, \theta_f)\right)\right)
\]

If: density ratio \(\geq 1\), Set: \(\theta_f = \theta_f^*\)

Else: Draw \(U \sim \text{Unif}(0, 1)\)

If density ratio \(\geq U\), Set: \(\theta_f = \theta_f^*\)

Else: Keep \(\theta_f = \theta_f\)

End loop over \(i\)
Step 4. Propose new $\theta_c$ from conditional distribution with updated $\theta_f$

Draw on complementary log-log scale

$t_c = \log(-\log(\theta_c))$

$t_c^* = c_\theta z + t_c$  where $z \sim \mathcal{N}(0,1)$

$\theta_c^* = \exp(-\exp(t_c^*))$

Step 4.2. Calculate log-likelihood

$$
\log \left( \pi(t_c^*|\theta_f, \theta_c) \right) = -\frac{\lambda_f}{2} \left( y_{int} - \eta(\theta_f, \theta_c^*) \right)^T \left( y_{int} - \eta(\theta_f, \theta_c^*) \right) + t_c^* - \exp(t_c^*)
$$

Step 4.3. Determine acceptance

Calculate the density ratio

$$
\frac{\pi(t_c^*|\theta_f, \theta_c)}{\pi(t_c|\theta_f)} = \exp \left( \log \left( \pi(t_c^*|\theta_f, \theta_c) \right) - \log \left( \pi(t_c|\theta_f) \right) \right)
$$

If: density ratio $\geq 1$,  Set: $\theta_c = \theta_c^*$

Else: Draw $U \sim \text{Unif}(0,1)$

If density ratio $\geq 1$, Set: $\theta_c = \theta_c^*$

Else: Keep $\theta_c = \theta_c$

Step 5. Propose new GP hyperparams from conditional distribution with updated $\theta_f$ and $\theta_c$

Step 5.1. Update $\lambda_{\theta_f}^* \sim \Gamma(a_{\lambda}^*, b_{\lambda}^*)$ where

$a_{\lambda}^* = a_{\lambda} + \frac{N}{2}$  where $N =$ number of samples along $x_f$

$b_{\lambda}^* = b_{\lambda} + \frac{1}{2} \left( \theta_f - 0.5 \right)^T R^{-1} \left( \theta_f - 0.5 \right)$

Step 5.2. Propose $\rho_{\theta_f}$: $p_{\theta_f}^* \sim \mathcal{N}(p_{\theta_f}, c_p^2)$  where $\rho_{\theta_f} = e^{-\lambda_{\theta_f}}$

Draw on complementary log-log scale

$p_{\theta_f} = \log \left( -\log(p_{\theta_f}) \right)$

$p_{\theta_f}^* = c_p z + p_{\theta_f}$  where $z \sim \mathcal{N}(0,1)$

$\rho_{\theta_f}^* = \exp \left( -\exp(p_{\theta_f}^*) \right)$

Step 5.3. Compute proposed covariance

$\gamma_{\theta_f}^* = -\log(p_{\theta_f}^*)$

$R^*(x_f, x_f') = \exp \left\{ \sum_{k=1}^d p_{\theta_f}^* \left( x_{f_k} - x_{f_k}' \right)^2 \right\}$

Step 5.4. Calculate log-likelihood

$$
\log \left( \pi(p_{\theta_f}^*|\theta_f, p_{\theta_f}) \right) = \frac{1}{2} |R^*| - \frac{\lambda_{\theta_f}}{2} (\theta_f - 0.5)^T R^{-1} (\theta_f - 0.5)
$$

$$
+ (b_{\rho} - 1) \log \left( 1 - \rho_{\theta_f}^* \right) + p_{\theta_f}^* - \exp(p_{\theta_f}^*)
$$
3.3. Proof-of-concept demonstration

Consider a physical system in which two phenomena are interacting and their response is captured through integral-effect experiments (Figure 5.5). Suppose a numerical model for one of the constituents is available, however a model for the second constituent that is necessary to develop a partitioned model is unavailable, as represented in Figure 5.4(left). We infer the relationship of this missing constituent to map the iterative behavior of outputs of constituent \( \Omega_A \) to affect its own input parameters in a feedback loop.
Figure 5.5. Integral-effect experimental data to be used for mapping $\Omega_\Lambda$ dependent output, $\alpha$, to its own input parameters, $\theta_f(\alpha(x))$.

Figure 5.6. True form of the functional input which we intend to infer through an empirical GP model.

In this controlled problem, the true form of the functional input parameter, $\theta_f = f(\alpha(x_\Lambda))$ is known and shown in Figure 5.6. The available physics-based model, in addition to the uncertainty resulting from the missing constituent’s predictions as a functional
input parameter, also has uncertainty in its existing parameters. Therefore, the inference problem for the available model may be described as:

$$\Omega_A = 1.3\beta[\alpha(x_A)]x_A^3 + 1.5\sin(\theta_c x_A) + 3$$  \hspace{1cm} (Eq. 4)

where $\theta_f(x) = \beta(\alpha(x_A))$ and $\theta_c$ are the unknown parameters to be inferred. A GP with a prior constant mean of 0.5 and squared exponential covariance matrix dependent upon a precision hyperparameter $\lambda_{\theta_f}$, and length parameter, $\rho_{\theta_f}$ is used to represent the functional form of $\beta(\alpha(x_A))$. Bayesian inference is implemented to form posterior distributions of the GP hyperparameters, $\beta$ and $\theta_c$ simultaneously (refer to Stevens et al. (2016b) for full details on the Bayesian formulation of this inverse problem). Details on the boundaries and prior distributions for these parameters used in the Bayesian Inference are provided in Table 5.1.

| Table 5.1. Model Parameter Boundaries and Prior Distributions for Bayesian Inference |
|------------------------------------------|---------|---------|---------------------------------|
| **State Variables (x)**                  | Minimum | Maximum | Prior Distribution |
| Independent Control ($x_c$)              | 0       | 1       | -                 |
| Dependent Constituent Prediction ($\alpha$) | 3       | 14      | -               |
| **Uncertain Model Parameters ($\theta$)** | Minimum | Maximum | Prior Distribution |
| Functional Parameter ($\theta_f$)        | 5       | 20      | Uniform(5,20)    |
| Functional Parameter ($\theta_c$)        | 1       | 5       | $\theta_f \sim GP \left(\mu, \lambda_{\theta_f}^{-1}R\right)$ |
| **GP Empirical Constituent Hyperparameters** |         |         |                   |
| Precision ($\lambda_{\theta_f}$)        | -       | -       | Gamma(5,5)       |
| Smoothness ($\rho_{\theta_f}$)          | -       | -       | Beta(1,0.1)      |

Posterior densities of the GP hyperparameters are shown in Figure 5.7. Posterior distributions derived for $\theta_f$ and $\theta_c$ are shown in Figure 5.8. Figure 5.9 compares the statistics of these inferred parameter values to the true parameter values. Take note that
Figure 5.7 illustrates the posteriors with respect to the prior bounds while Figure 5.8 shows the distributions for comparison to the true values. Once the GP representing the empirical constituent model for $\beta(a(x_A))$ is determined it is incorporated to $\Omega_A$ model to produce coupled predictions, which are shown in comparison to integral-effect experiments in Figure 5.10.

![Figure 5.7. GP hyperparameter posterior densities.](image)
Figure 5.8. GP predictions of the functional form $\beta(\alpha(x_A))$ and posterior density of the constant parameter $\theta_c$.

Figure 5.9. Inferred $\beta(\alpha(x_A))$ with one standard deviation uncertainty bounds compared with the true function and constant parameter compared to true parameter value.
4. Multi-scale Plasticity of Anisotropic Elasto-plastic Material

The importance of representing complex material behavior beyond the elastic range has long been recognized and has become a prominent field of study in material science and modeling (Dawson, 2000; McDowell, 2010; Roters et al., 2010; Panchal et al., 2013). These models are necessary for understanding complex material behavior under extreme loadings (Asayama and Hasebe, 2000). Partitioned models are particularly useful when a material has a clear separation of scales contributing to the elastic and plastic components (Wang et al., 2010).

Two hurdles, however, may face the development of such multi-scale partitioned models in practice due to the high complexity and immense computational resources required for implementing these models; (i) knowledge of first principle physics may not be available for each constituent domain to develop the constituent models and (ii) separate-effect experiments isolating behavior of the constituents are not possible to
conduct. Development of smaller-scale (be that meso-, micro-, or nano-) material models requires expert knowledge of the specific material behavior at hand as well as significant resources for the development of the meso-scale constituent model. Some model developers (see Krätzig and Pölling (2004) for example) choose to bypass this challenge by determining dependent parameters based on small scale separate-effect experiments to characterize the advanced material properties. However, these separate-effect experiments are not always feasible (or even possible) to conduct (Bauer and Holland, 1995). Given these challenges, a means to account for the coupling between the meso- and macro-scale without requiring the development and implementation of a physics-based meso-scale model would prove highly valuable for practical applications.

4.1. Integral-effect Experimental Data

The experimental setup (shown in Figure 5.11) is modeled after the four point bending test conducted on a zirconium beam in (Kaschner et al., 2001). Herein, inference is to be made about the behavior of the plasticity constituent throughout the loading process, therefore time dependent strain measurements are synthetically generated with a coupled FE-plasticity model. The experimental sample is a zirconium beam that is 50.8 mm long with a 6.35 mm x 6.35 mm square cross section. A four-point bending test is conducted in which supports under the beam are place 12.7 mm from the centerline and load is applied at two points 6.35 mm from the centerline (Figure 5.11). The test is displacement controlled, meaning that the load is applied until the loading points have been displaced 3 mm. Integral-effect experiments generated from this simulation are shown in Figure 5.12.
Figure 5.11. Experimental setup for collection of integral-effect data.

Figure 5.12. Integral-effect data capturing the midsection strain throughout loading.
4.2. Multi-scale Elasto-plastic Coupling

In this multi-scale elasto-plastic problem, a macro-scale finite element model is the only currently available constituent to compare with the above experimental data. On its own, the macro-scale model is only capable of elasticity calculations. A meso-scale model, if available, would contribute plasticity calculations through the form of plastic strain predictions. In the problem presented herein, a meso-scale plasticity model is the missing constituent to be inferred as an empirical model represented through a functional parameter value. Figure 5.13 illustrates the nature of the coupling between the two scales. The coupling, if a constituent model were to be available, would take place as the macro-scale finite element model predicts stress, $\sigma$, which then acts as a dependent control parameter for a plasticity model that in turn predicts plastic strain, $\varepsilon_{\text{pl}}$. The plastic strain would then be added to the elastic strain determined by the finite element model to compute a total strain, $\varepsilon$, for each loading step and the simulation would progress to the next time step (Stevens et al., 2016a). However, given the absence of a plasticity model or expert knowledge to develop such a model, the plastic strain dependent input to the macro-scale model can be inferred empirically.

The macro-scale elasticity model developed herein is an ABAQUS model composed of 32x4x4 C3D20R solid elements with 20 nodes. The macro-scale calculations are to take place at every integration point within the model, such that the functional parameter will be applied relating to the stress at that point to predict the relative plastic strain. The simulation is controlled by displacement applied to the upper nodes at the two loading points, thus making displacement the independent control
parameter, $x_c$, known in both the simulations and experiments. This parameter will be used to relate the centerline strain distribution of the numerical model to the strain distribution of the experiments at known loading steps.

![Diagram](image)

**Figure 5.13. Representation of multi-scale coupling through empirically derived plasticity constituent model.**

### 4.3. Fast-running Metamodel for Finite Element Constituent Model

If the computer model, $\eta(\cdot, \cdot)$ is fast-running, it is unnecessary to emulate the model since simulations can be quickly performed to determine the actual model prediction. However, in applications such as this one, where evaluation of a finite element model with over 10,000 integration points would be required, the computational demands associated with the model evaluations become prohibitive. To work around this limitation, a fast-running metamodel can be trained using computer runs available at a limited number of input settings, and then used to estimate what the computer model output would be at input settings where actual output from the finite element model is not available (Kennedy and O’Hagan, 2001; Bayarri et al., 2007). For this purpose, we use
another GP in lieu of the physics-based finite element model and take the mean predictions of this GP to be used in place of $\eta(\cdot,\cdot)$.

While a plethora of literature exists for generating efficient parameter design spaces for training metamodels where parameters represent only constant, averaged values (Sacks et al., 1989), there is very limited, if any, previous work on design of computer experiments to explore parameter spaces for training runs of functional parameters. The issue that arises in deciding on a parameter space for the training runs is that the metamodel must accept a vector of parameter values relating the functional form and predict a model output that is representative of the true model. Consider, for instance the case where $\theta_f(x_f)$ is a function sampled across 50 $x_f$ settings. In this case, the metamodel would be required to accept a vector of 50 values to make up the full $\theta_f$ function and the model predictions would be dependent upon all of the values in the functional order that they occur.

Keeping in mind that the samples for $\theta_f(x_f)$ will be drawn from a GP with a covariance prescribed from $\lambda_{\theta_f}$ and $\rho_{\theta_f}$ parameters sampled with a scale factor of $c_{\theta}$ (recall Step 3.1 of Algorithm 1), a justifiable means for generating the training data is creating functions by sampling a parameter space of the GP hyperparameters and step size. Generating a set of training runs with $\theta_f(x_f)$ sampled in this manner will ensure that the training functions are representative of those that are intended to be sampled. In addition to these three parameters, generation of functional draws from the GP depends on an initial mean function and as such the training runs also required a variety of initial functions to be used. A Latin Hypercube design is used to develop a parameter space of 80 runs using the
parameter ranges provided in Table 5.2. These 80 runs are then applied to six different initial functions to generate a design space of 480 total training runs. The parameter functions $\theta_f(x_j)$ for each of these runs are generated with draws following the form shown in Eq. 5, where the covariance matrix is a square exponential form parameterized with the smoothness parameter, $\rho_{\theta_f}$, is of the form shown in Eq. 6. The resulting training runs are seen in Figure 5.15.

$$\theta_f \sim \mathcal{N}(\mu_{\text{initial}}, \mathbf{C}_{\theta_f} \rho_{\theta_f}^{-1} \mathbf{R})$$  \hspace{2cm} (Eq. 5)

$$\mathbf{R}(x_{f_i}, x_{f_j}) = \rho_{\theta_f}^4 (x_{f_{i_k}} - x_{f_{j_k}})^2$$  \hspace{2cm} (Eq. 6)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_\theta$</td>
<td>0.05</td>
<td>1.5</td>
</tr>
<tr>
<td>$\lambda_{\theta_f}$</td>
<td>0.05</td>
<td>3.0</td>
</tr>
<tr>
<td>$\rho_{\theta_f}$</td>
<td>0.80</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table 5.2. Parameter Ranges for Generating Metamodel Design of Experiments

Figure 5.14. GP generated (left) training and testing (right) parameter functions for developing a GP metamodel of ABAQUS stand-alone model simulations taking functional input data.
The GP metamodel that is trained for representation of the stand-alone finite element model is a zero mean Gaussian process with a squared exponential covariance structure. To validate the goodness of the metamodel training for accurately representing predictions of the finite element model with a variety of functional inputs half of the design of experiments were used for training the metamodel (Figure 5.14 left) and the other half were held out for cross-validation (Figure 5.14 right). Cross-validation is completed at all 20 of the displacement settings of the simulation so that the goodness of the model as a function of stress can be assessed. Figure 5.15 shows this cross-validation, where predictions of the stand-alone finite element model with a given functional input are represented on the x-axis and predictions of the metamodel with the corresponding functional input are provided on the y-axis. The 45-degree line shown in black represents the ideal match between metamodel and model predictions. As seen in the figure, the metamodel and model continuously fall along this line, providing confidence in the capability of the trained metamodel to accurately represent the numerical model with functional inputs.
Figure 5.15. Cross-validation of GP metamodel for ABAQUS stand-alone model at increasing displacements.
4.4. Bayesian Inference of Empirical Gaussian Process Plasticity Model

Following the framework presented in Algorithm 1, the functional form of the plasticity model is inferred, with the metamodel trained in Section 4.3 being called for every representation of $\eta$. Recall from Section 3.2 that a GP is desirable in Bayesian inference because it allows the flexibility of not imposing a functional form as well as the control to impose constraints for all information that is available. Table 5.3 provides the details of all necessary parameter ranges and prior distributions input to the constituent model inference algorithm.

Table 5.3. Parameter Information and Prior Distributions for Plasticity Model Inference

<table>
<thead>
<tr>
<th>Macro-scale Elastic Model Parameters</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Prior Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Independent Control ($x_c$)</td>
<td>Displacement (u) [mm]</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>Dependent Control ($x_f$)</td>
<td>Stress ($\sigma$) [MPa]</td>
<td>0</td>
<td>270</td>
</tr>
<tr>
<td>Functional Parameter ($\theta_f$)</td>
<td>Plastic Strain ($\varepsilon_{pl}$)</td>
<td>0</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>$\theta_f \sim GP (\mu, \lambda_{\theta_f}^{-1}R)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>GP Empirical Constituent Hyperparameters</th>
<th>$\lambda_{\theta_f}$</th>
<th>$\rho_{\theta_f}$</th>
<th>Prior Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-</td>
<td>-</td>
<td>Gamma(5,5)</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td>-</td>
<td>Beta(1,0.1)</td>
</tr>
</tbody>
</table>

In the case of the plasticity model to be inferred for the present application, the following additional information is known and should therefore be imposed on the GP inference:

(i) Plastic strain is zero when the stress is zero; therefore the function should be bounded to be negligible at the lower end.

(ii) Plastic strain should not exceed 0.5; therefore the function should be bounded to a maximum of 0.5 across the entire domain.
(iii) Plastic strain is irrecoverable by nature; therefore the function should be 
monotonically increasing.

The first two constraints are implemented simply by bounding the sample so that no 
values outside these ranges at the appropriate areas of the domain can be drawn. The third 
constraint, monotonicity is implemented by encouraging monotonic GP sampling through 
a process developed by Golchi et al. (2015). The process utilizes an expanded covariance 
matrix to learn about the derivatives of the GP. The new form of the covariance matrix is 
shown in Eq. 7, where $\mathbf{R}$ is the normal covariance presented in Algorithm 1. Using this 
modified covariance, draws are taken from a normal distribution with covariance 
including derivatives and a mean vector that includes the derivatives $\theta'_f$ at selected 
sampling locations, $x'_f$, which do not have to be the same as $x_f$ Eq. 8)

$$
\Sigma = \begin{bmatrix}
R(x_i, x_j) & \frac{\partial R}{\partial x_j}(x_i, x'_j) \\
\frac{\partial R}{\partial x_i}(x'_i, x_j) & \frac{\partial^2 R}{\partial x_i \partial x_j}(x'_i, x'_j)
\end{bmatrix} 
$$

(Eq. 7)

$$
\begin{bmatrix}
\theta_f^* \\
\theta'_f^*
\end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix}
\theta_f \\
\theta'_f
\end{bmatrix}, \lambda_{\theta_f}^{-1}\Sigma\right)
$$

(Eq. 8)

The result of these draws is a new sample of the functional parameter, $\theta^*_f$ as well 
as the corresponding derivatives of this function, $\theta'_f^*$. A monotonicity indicator $m(x'_f)$ is 
developed which equals one when a derivative at a point $x'_f$ is positive and zero if it is 
negative. Monotonicity is then encouraged by applying $m$ as a penalty term to the 
likelihood if the function is decreasing rather than increasing (Eq. 9). For example, when 
$\theta'_f^*$ is negative at a given point, $m$ will be equal to 0, making log($m$) negative infinity, 
therefore causing the log-likelihood to be largely negative. However, when $\theta'_f^*$ is positive
at a given point, \( m \) will be equal to 1, making \( \log(m) \) equal to zero, thus having no effect on the log-likelihood. Furthermore, Algorithm 1 is updated such that \( \Sigma \) is used in the place of \( R \) throughout the entire formulation and \( \begin{bmatrix} \theta_f \\ \theta'_f \end{bmatrix} \) is used in place of \( \theta_f \) except in the model evaluations \( \eta(\theta^*_f) \).

\[
\log \left( \pi \left( \theta_f^* | \lambda_{\theta_f}, \rho_{\theta_f}, \theta_f \right) \right) = -\frac{\lambda_y}{2} (y_{\text{int}} - \eta(\theta^*_f, \theta_c))^T (y_{\text{int}} - \eta(\theta^*_f, \theta_c))
\]

\[
-\frac{\lambda_{\theta_f}}{2} \left( \begin{bmatrix} \theta_f^* - 0.5 \\ \theta'_f^* \end{bmatrix} \right)^T \Sigma^{-1} \left( \begin{bmatrix} \theta_f^* - 0.5 \\ \theta'_f^* \end{bmatrix} \right) + \log(m) \quad \text{(Eq. 9)}
\]

5. Results and Conclusions

The constituent model inference is completed with 1000 burn-in runs and 1000 sampling runs, each with 5 subiterations of \( \theta_f(x_f) \) (Neal, 1998; Stevens et al., 2016b), and prior distributions presented in Table 5.3. Figure 5.15 shows the posterior distribution of the functional parameter value as well as the mean and standard deviation of this distribution at control locations, \( x_f \) compared to the true function, which was the plasticity model implemented to generate the integral-effect experimental data. The posterior distribution in these figures are shown within the plastic strain range of 0 to 0.5 to illustrate the reduction in uncertainty from the initial prior with a uniform distribution from 0 to 0.5. Additionally, posterior densities of the GP hyperparameters are shown in Figure 5.17.

The posterior distribution observed is populated primarily by linear functions, which goes along with the posterior density of \( \rho_{\theta_f} \) strongly 1 as well as the imposed monotonicity constraint. While a density of \( \rho_{\theta_f} \) of 1 is typically desired to impose
smoothness in the function, the combination a prior distribution heavily weighted to 1 and a monotonicity constraint also causing a trend in the functions to maintain positive derivatives, there is a chance that the two constraints are confounding one another causing the restriction to linear functions. Considering the confinement of posterior samples to linear functions, the general trend of the plastic strain development is being captured, as shown in Figure 5.16 (right). The mean $\theta_f(x_j)$ function of the posterior distribution follows a linear trend through the center of the true function. Furthermore, the true function is enveloped within one standard deviation.

![Graph showing posterior draws and statistics of the empirical plasticity constituent model compared to the true functional form.](image)

**Figure 5.16.** Posterior draws (left) and statistics (right) of the empirical plasticity constituent model compared to the true functional form.
Predictions of the finite element model augmented with the mean function of the inferred emulator are shown in comparison to integral-effect experiments in Figure 5.18, where points falling along the 45-degree demonstrate a perfect match of predictions to experiments. Predictions are shown at four different heights of the beam midsection where integral-effect data was collected. Overall, the coupled predictions tend to match experiments reasonably well, despite the fact that the mean function used to generate these coupled predictions is a linear function while the true plasticity function is non-linear. This observation raises some concern about nonidentifiability in the model given different plasticity functions.
6. Conclusions

Partitioned analysis is providing model developers with the opportunity to represent the strongly coupled physical relationships observed in our complex engineering and science systems better than ever before. The ability to take advantage of existing mature models of constituents within a system so that the focus of new model development efforts may be on the coupling among constituents rather than redeveloping already validated models with a monolithic approach. However, the flexibility of partitioned analysis falls apart when a constituent model is not available and conducting separate-effect experiments for generation of data to empirically derive a constituent is not feasible.

This paper presents a novel statistical analysis method to infer the important coupling relationships between an existing physics-based model and its missing constituent through Bayesian inference leveraging integral-effect experimental data. The capability to infer the physics of a constituent model in the form of a functional input parameter dependent upon the physics-based model’s own predictions is unlike any other technology existing today. The potential of the proposed methodology has been
demonstrated for the development of a meso-scale plasticity model for representation of a multi-scale elasto-plastic system.

While the results demonstrate the promise of this new method, there is clearly still work to be done. As such, the discussion in this paper also serves to identify many paths for future research as this notion of functional parameter inference continues to be developed. First, the physics-based constituents likely to be implemented in this inference process will typically be too computationally demanding to operate thousands of times during the sampling steps raising a need for metamodels. Methods for generating sufficient design of experiments in functional parameter spaces, however, are not currently well established. Producing a training data set from a set of GP models with hyperparameters guiding the design selection has been demonstrated, but other more refined approaches are needed. Second, training of the constituent model form through GP model hyperparameters provides a combination of flexibility and control as the functional form is not restricted, but any known constraints can be implanted. The interaction of the prior information on the GP hyperparameters, such as encouraging monotonicity in the likelihood along with smoothness through the priors, is not yet well understood and should be further studied as methods continue to mature.

References


CHAPTER SIX

CONCLUSION

1. Summary of Research

Coupled modeling has come to be a fundamental piece of engineering design and analysis as systems are becoming increasingly complex and interrelated. However, partitioned methods for operating these models depend on the availability of well-defined constituent models with minimal uncertainty or bias. Each constituent of a coupled model has its own unknown parameters and missing physics resulting in uncertainty and bias that, if not accounted for, may impede the predictive capability of the full system. Furthermore, development of a coupled model may be prohibited when one or more of the necessary constituents is unavailable. In such cases, the coupling relationships are often neglected in favor of uncertain model parameters calibrated to constant values and resulting in model bias.

This dissertation discusses the causes of uncertainty and bias in coupled models and presents two methodologies for enabling accurate predictions from coupled models in the face of uncertainty. First, bias-corrected partitioned analysis is a novel method leveraging the transparency of partitioned analysis by taking advantage of separate-effect experiments to reduce parametric uncertainty and quantify systematic bias at the constituent level followed by an integration bias-correction to the coupling framework. Next, a statistical inference methodology for inferring neglected coupling relationships is presented. The capability to infer relationships breaks the mold of traditional inverse analysis methods and opens a door to interpreting the unknown causes of bias in our
existing physics-based models. Beyond the scope of model development and calibration, this inverse inference stands to contribute the existing scientific knowledge base by identifying and explaining fundamental dependencies of which we currently lack knowledge. In particular, the arguments made focusing on constituent models within partitioned systems are significant. A breadth of literature has focused on methods to bring constituent models together, only beginning to realize the complications this brings to analyzing uncertainties. This is the first work of its kind to take a step back from merging models to analyze what information can still be gained from the individual components as they exist in the full system.

Methods proposed herein are applied to advanced plasticity models, one representing anisotropic elasto-plastic behavior of zirconium and another representing temperature dependent mechanical properties of 5182 aluminum alloy. These simulations are used to represent the material behaviors under extreme loadings, such as those encountered in failure scenarios. Predictions under these conditions often inform decision-making in high consequence scenarios and therefore require evaluation of the accuracy of model predictions compared to available experimental data as well as uncertainty in the model predictions.


The research campaign resulting from this dissertation has produced the following contributions:
Findings from the review of literature on verification and validation practices for partitioned models (Chapter 2):

- Careful selection of the iterative coupling scheme to be implemented in a partitioned model is important, as schemes exhibit not only distinct convergence behaviors, but also differences in the propagation of uncertainty and error between constituent models, possibly leading to convergence to different incorrect solutions.

- Partitioned analysis presents a new challenge to solution verification when domain-specific spatial and temporal discretizations are used, leading to mismatched or embedded meshes and unaligned or staggered time steps, respectively.

- Refinement of models requires simultaneous consideration of plans for further code development to reduce model bias as well as actions to calibrate and validate the models with new experimental data. Furthermore, partitioned analysis requires that each of these aspects take into consideration selection of the constituent models to that are most efficient to improve with respect to the possible gains in predictive capability.

- The large body of knowledge on methods for partitioned analysis has escalated the development and implementation of coupled models, in turn raising awareness of problems that result from uncertainties and errors within partitioned models.

- Existing methods to address these uncertainties and errors are premature, thus development systematic frameworks leveraging both separate-effect and integral
effect experiments, combined with efficient allocation of resources for further experimentation and code development specifically catered towards partitioned models is identified as an area of interest for future research.

Findings from the development of a methodology for bias-correcting constituent models within iterations of partitioned analysis (Chapter 3):

- Uncertainties and biases from constituent models can accumulate or compensate with one another during iterative coupling procedures, causing complications in identifying the root cause of errors in model predictions.

- The proposed framework takes advantage of the unique transparency of partitioned analysis to exploit separate-effect experiments for calibration and bias-correction of constituent models in addition to integral-effect experiments for validation of coupled predictions.

- This transparency allows for the root cause of uncertainties and bias to be identified within the constituent models so that uncertainty may be reduced prior to coupling and bias can be corrected for at every exchange between constituents.

- The proposed bias-corrected partitioned analysis is demonstrated with a multi-scale plasticity model in which a visco-plastic self-consistent (VPSC) material model is embedded in every integration point of a finite element model. Separate-effect experiments of uniaxial tension and compression tests of zirconium coupons were used to calibrate and reduce uncertainty of the VPSC model and infer the model bias as a function of the stress parameter being input from
ABAQUS, enabling correction for this bias to avoid propagation through the analysis.

- Implementation of the proposed method improved the fidelity of coupled predictions to integral-effect experiments of a highly anisotropic zirconium beam exposed to creep loading, representative of the behavior of fuel cladding exposed to high loads in nuclear reactors.

*Findings from the development of an inverse methodology for inference of empirical constituents to establish coupled models (Chapters 4 and 5):*

- When unavailable due to lack of theoretical knowledge or ability to conduct separate-effect experiments, empirical constituent models can be inferred through inverse analysis of available physics-based constituent models and integral-effect experiments.

- Carrying out the inverse analysis for constituent model inference in a Bayesian context provides a means of quantifying uncertainty in the empirical model.

- The proposed inverse analysis methodology is first applied to develop a coupled model for thermo-mechanical analysis of 5182 aluminum alloy at high temperatures. Mechanical properties of this material are used in a physics-based VPSC model to predict stresses, but the constituent model representing the relationship of material properties to operational temperature was unavailable.

- Temperature-dependent predictions with quantified uncertainty are made possible by coupling the newly developed empirical thermal constituent to the mechanical
VPSC constituent, demonstrating the applicability of the proposed method to thermo-mechanical modeling.

- Constituent models can also be inferred for strongly coupled, iterative relationships. Empirical representation of a constituent in an iteratively coupled model stands to produce representations of previously unknown constituent interactions, providing a means for the development of partitioned models of strongly coupled systems coupling that are currently infeasible.

- Bayesian inference of a plasticity constituent model is demonstrated for an application to an elasto-plastic beam by extracting information from integral-effect experiments of strain measurements during creep loading.

- Design of experiments for a functional parameter space is demonstrated through sampling of hyperparameters of a Gaussian Process and implemented for the development of a fast-running metamodel of a stand-alone finite element code with a functional plasticity input parameter.

3. Limitations and Recommendations for Future Work

3.1. Limitations and Assumptions

The methodologies developed herein are designed to be generally applicable for any partitioned model; however, there are remaining limitations and assumptions that must be recognized. First and foremost, model verification should always take place prior to implementation of these methods or any type of calibration and validation study. Though beyond the scope of this dissertation, the VPSC and finite element models used in the case studies presented underwent verification by model developers in earlier
studies. Once a model is properly prepared for calibration, the capability of the methods proposed herein to improve the predictive capability assumes that sufficient quality and quantity of experimental data is available. A final assumption that should be mentioned is that uncertainties and biases of the coupling interface have been considered negligible in all the applications presented.

Limitations remaining in the proposed methods are also recognized. In the majority of applications presented, constituent models shared only three or less parameters in the coupling process. As systems become more complex, such as expansion from two constituent models up to a full-system hierarchical model with countless interdependencies, the number of parameters involved in coupling is expected to increase. This increase in complexity of the coupling and additional uncertainties could lead to higher risk of compensations between parameters in the bias-corrected methodology as well as in the inference of empirical constituent models. Further on this point, the inverse analysis of constituent models proposed is currently limited to inference of constituent models dependent upon only one parameter. Finally, discrepancy has not yet been incorporated into the methodology for inferring constituent models. A model in which one or more of these assumptions was not upheld would require modifications to the implementation of the methodologies, though the rationale behind the methods should be upheld.

The degree to which the proposed methods could be explored and the models could be improved was somewhat limited by the availability of experimental data. Specifically, separate-effect experiments of the zirconium material were only available
for one direction, limiting the application to partial-bias correction rather than correcting all directors of the tensor. In inferring the thermal constituent model for the aluminum alloy, data was only available at two strain-rates, making inference of a functional form of the threshold hardening stress on strain-rate unreasonable. Should more data have been available for these case studies the methods proposed could have been explored in more detail.

3.2. Suggestions for Future Work

This dissertation provides novel insights into the behavior of uncertainties and errors in coupled models. Future studies can build on the work presented in these discussions and continue to develop the methods into mature frameworks.

The major suggestions for future work focus on the inverse analysis of constituent relationships, as this is a topic that is entirely new and in the initial stages of development and is sure to be a promising area of research for years to come. First, we recognize that no model is perfect and as such some level of discrepancy should be accounted for during the inverse analysis. The Bayesian methodology applied herein lends itself to incorporation of a discrepancy term and this is a natural next step in the algorithm development. Next, expansion of the methodology to higher complexity problems is recommended. Increased complexity may come in two forms: (i) higher dimensionality in the dependence where parameters may vary as function of more than one control parameter and (ii) more involved relationships between model settings and outputs where correlations existing in the system should be accounted for. As the problems taken on with this methodology continue to increase in complexity the use of fast-running
emulators in place of the complex physics-based models will become increasingly critical. With this in mind, sophistication of methods for designing computer experiments for the exploration of functional parameter spaces is a new field opening up for further research.

In closing, the methods and associated algorithms presented herein provide a step forward for our capabilities to simulate the behavior of complex systems with confidence. Model validation and uncertainty quantification of coupled systems is an active research topic just starting to grow. Partitioned analysis has become standard practice in nearly every engineering field, but the methods addressing the additional challenges and exploiting the new opportunities associated with this analysis are lagging behind the modeling capabilities. As such, the model validation and uncertainty quantification community stands to benefit from discussions on development and uncertainty in partitioned models presented in this dissertation. The assumptions, limitations, and paths forward for future work discussed here are intended to promote continued endeavors in this new and exciting field.