Project No. 11-3056

Multiscale Modeling and Uncertainty Quantification for Nuclear Fuel Performance

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

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Final Report NEUP Project 11-3056
Principal Investigator: Don Estep

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Project Objective:	In this project, we will address the challenges associated with constructing high fidelity multiscale models of nuclear fuel performance. We (*) propose a novel approach for coupling mesoscale and macroscale models, (*) devise efficient numerical methods for simulating the coupled system, and (*) devise and analyze effective numerical approaches for error and uncertainty quantification for the coupled multiscale system. As an integral part of the project, we will carry out analysis of the effects of upscaling and downscaling, investigate efficient methods for stochastic sensitivity analysis of the individual macroscale and mesoscale models, and carry out a posteriori error analysis for computed results. We will pursue development and implementation of solutions in software used at Idaho National Laboratories on models of interest to the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program.

1. Project Summary, Personnel, and Tasks

1.1 Summary Developing sustainable nuclear fuel cycles is a principal priority of the Office of Nuclear Energy in the Department of Energy. The use of model simulations of fuel behavior can be a cost-effective means to accelerate development by reducing the need for prototypes and large-scale experiments. But, model simulations must undergo a rigorous process of validation and uncertainty quantification in order to assess their predictive capability. This is a difficult undertaking. As energy is converted into heat in the fission process, there are significant microstructure and composition changes in the fuel that affect the chemical, thermal and mechanical properties of fuels. Predictive simulation of nuclear fuel forms must account for these changes.

Existing fuel performance models are mostly semi-empirical and are calibrated by materials data collected under a wide range of conditions. This leads to significant limitations in terms of predicting behavior in the dynamic environment in nuclear reactors. This has motivated new efforts to develop high-fidelity models of nuclear fuels that are multiscale in nature, and integrate the fundamental radiation damage and defect behavior at the crystal lattice level into the continuum (engineering) scale via sophisticated mesoscale models of microstructure evolution in irradiated fuel.

Multiscale models raise a number of significant challenges. Both developing high fidelity models for each scale and formulating coupling methods between models at different scales that yield high fidelity behavior are difficult problems. Multiscale models are complex nonlinear systems with complicated dynamical behavior and computing accurate numerical solutions is another difficult challenge. Another significant complication for modeling fuel performance is that any model is inherently stochastic because of experimental error, modeling error, and the statistical nature of some components. The consequence is that multiscale modeling of nuclear fuel performance is computationally intensive undertaking.

In this project, we will address the challenges associated with constructing high fidelity multiscale models of nuclear fuel performance. We propose a novel approach for coupling mesoscale and macroscale models, devise efficient numerical methods for simulating the coupled system, and devise and analyze effective numerical approaches for error and uncertainty quantification for the coupled multiscale system. As an integral part of the project, we will carry out analysis of the effects of upscaling and downscaling, investigate efficient methods for stochastic sensitivity analysis of the individual macroscale and mesoscale models, and carry out a posteriori error analysis for computed results. While we pursue development of the methodology in the context of a particular multiscale model of interest to the Idaho National Laboratory and, more broadly, to the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, our techniques will apply to a wide class of multiscale models for nuclear fuel performance.

1.2 Project Personnel

The project team underwent several major transitions. First, the original Co-Principle Investigator at Idaho National Laboratory, Michael Pernice, retired and John Peterson took over that role. Second, Dr. El-Azab and Dr. Xiu both changed universities.

Principle Investigator:	Donald Estep, Colorado State University
Co-Principle Investigators:	Anter El-Azab, Florida State University, Purdue University
	Michael Pernice, Idaho National Laboratory
	John Peterson, Idaho National Laboratory
	Peter Polyakov, University of Wyoming
	Simon Tavener, Colorado State University

Dongbin Xiu, Purdue University, University of Utah
Postdocs: Will Newton, Colorado State University
Troy Butler, Colorado State University
Yeonjong Shin, University of Utah
PhD Students: Kevin Lenth, University of Wyoming
Charles Vollmer, Colorado State University

1.2 Project Tasks Listed in Proposal and Related Milestones

During the course of this project, the project reporting system was changed three times. During the last change, we have to remap the original Task List described in the proposal to a set of Milestones. The work was organized around the original Task List but broken up to address each Milestone. Below I present the original list of Tasks and then list the associated Milestones. I left off the Milestones associated with reporting.

NEUP Task 1 Develop and implement algorithms for coupling mesoscale and macroscale models and derive and implement a posteriori estimates for solution
Milestones: M3NU-11-CO-CSU_-0402-026, M2NU-11-CO-CSU_-0402-0219

NEUP Task 2 Development and implementation of methods for stochastic analysis of macroscale and mesoscale models and derive a posteriori estimates for stochastic results
Milestones: M3NU-11-CO-CSU_-0402-029, M3NU-11-CO-CSU_-0402-025, M3NU-11-CO-CSU_-0402-024, M3NU-11-CO-CSU_-0402-0210

NEUP Task 3 Derive and implement algorithms for iterative solution of coupled stochastic macroscale and mesoscale models
Milestones: M2NU-11-CO-CSU_-0402-0211

NEUP Task 4 Study coupling aspects including formulation of consistent upscaling and downscaling transformations, choice of representative volume element for mesocale model, choice of boundary conditions for representative volume element, choice of discretization resolutions
Milestones: M2NU-11-CO-CSU_-0402-0219, M2NU-11-CO-CSU_-0402-0218, M3NU-11-CO-CSU_-0402-027, M2NU-11-CO-CSU_-0402-0216

NEUP Task 5 Implementation of algorithms in MOOSE/BISON/MARMOT codes and testing on realistic problems
Milestones: M3NU-11-CO-CSU_-0402-028, M2NU-11-CO-CSU_-0402-0214, M2NU-11-CO-CSU_-0402-0217, M3NU-11-CO-CSU_-0402-025

NEUP Task 6 Organizing project and products: including obtaining INL accounts for team members, creating Wiki, project web page, code archive and QA, collaborations and schedule of meetings

2. Activity and Progress

Task 1

In the first year of the project, we proposed an algorithm for coupling of **existing** macroscale and mesoscale stochastic models, and implemented the algorithm in a C++ code. However, early investigations revealed several issues that had to be resolved for this task, including:

- Formulation of mesocale models. It turns out that there a number of models being considered in the research community at large, making it difficult to focus on one as a target for a posteriori error analysis, and also to settle on a specific approach to coupling. Note the choice of model affects the kinds of information passed between the scales. This work was presented in several interim reports.
- Efficient solution of Cahn-Hilliard-type mesoscale models: The current numerical solution of the Cahn-Hilliard equation in MOOSE/BISON is too slow to allow for realistic computations, which means we do not have a good choice of discretization for a posteriori error analysis. We addressed this partially by implementing various numerical improvements in MOOSE/BISON (Task 5).
- But the most significant issue revealed by our early investigations was the need to develop mathematically justified approaches for incorporating molecular scale radiation damage into models of void damage and migration occurring at the engineering scale.

Our investigations led to the conclusion was that existing micro-mesoscale models have serious modeling and mathematical difficulties, and we refocused our efforts on developing alterative models that have a strong mathematical and physical foundation. This has evolved into two different but related projects:

- A. El-Azab described a consistent modeling framework for the stochastic source terms representing molecular scale radiation effects in the Cahn-Hilliard mesoscale model. El-Azab has continued working with CSU graduate student Charlie Vollmer on constructing a source term reflecting damage events that drives the Cahn-Hilliard model. Charlie has constructed a stochastic process/time series model that feeds damage information to the mesoscale model based on well-validated simulation software for single microscale damage events. Over the past year, Charlie obtained a copy of the FORTAN Cahn-Hilliard code and implemented his time series model as the driving term in the Cahn-Hilliard model and carried out both validation studies and initial numerical investigations. Charlie has carried out simulations using both the old paradigm for coupling (putting a damage simulation at each node of a discretization of a PDE) to the new paradigm of coupling through statistical quantities computed from a point process model of damage formed on an independent scale. He has made great progress on writing a manuscript describing the point process model and the coupling along with the numerical results [9]. This forms the first part of Charlie's PhD thesis [8].

- Charlie Vollmer has independently developed a mesoscale stochastic process model for the void formation and migration that uses microscale damage events. The model is simple and employs only a few parameters, but allows for a very rich library of behaviors. The goal is twofold. First, we are considering the coupling of the mesoscale Cahn-Hilliard model to time series data created from the mesoscale stochastic process model, rather than coupling directly to the microscale damage event process. We can think of the stochastic mesoscale model as a consistent stochastic upscaling procedure. Second, we are considering the stochastic mesoscale models as an independent macroscale model of void migration. This could be useful for validation studies for the Cahn-Hilliard equation. Charlie has focused his attention on analyzing properties of the stochastic process model – focusing on medium and long time stability properties that are essential to coupling to a PDE. These subjects form the second part of Charlie's PhD thesis [8]. We anticipate producing two manuscripts, one addressing theoretical properties of the model and one applying the model to void damage and migration.

Task 2

Task 2 involved activity in stochastic analysis and uncertainty quantification on a broad range of fronts. Papers [1,3,6,7,11,13] and PhD thesis [2] extended stochastic analysis and efficient computation of stochastic problems in a number of directions. [1] describes a new approach to the formulation and solution of stochastic inverse problems for parameters in a model. The thesis [2] developed a perturbation method for describing the effects of uncertainty in a model parameter. [3] presents a rigorous framework to estimate the upper and lower bounds for system responses subject to epistemic uncertainty. [6] develops bounds on the variance in a stochastic parameter in a model required for the computation to convergence. [7] focuses on efficient computation of the forward propagation problem for a model. [11] presents theory for a new efficient computational method for the propagation of uncertainty through a model based on a posteriori error analysis and generalized adaptive error control. [13] presents an a posteriori error analysis for an approximate p quantile computed from a model with stochastic parameters along with an adaptive error control algorithm.

Two of the projects described as milestones that we proposed to pursue did not pan out. Milestone M3NU-11-CO-CSU_-0402-029 was concerned with the use of PC/KL expansions for treatment of stochastic evolution problems by decomposition. We produced a manuscript but the numerical method was simply too slow to be competitive, so we did not pursue it. Milestone M2NU-11-CO-CSU_-0402-0218 was concerned with the development and analysis of a smooth stochastic spline mesoscale representation of unresolved microscale behaviors. This is an issue that is central to the stochastic modeling of material properties and we submitted a number of interim reports describing our preliminary work. However, as noted, we focused our efforts on a modeling problem that was much more important to this project.

Task 3

In Monte Carlo simulations of nonlinear models, it is generally assumed that the model solutions are computed exactly. In previous work, Estep and collaborators have analyzed the effect of numerical solution of the nonlinear models, assuming the discrete nonlinear models are solved exactly. The effect of using finite iteration in the solution of coupled macro/mesoscale models falls under a more general problem: given a nonlinear model that is solved iteratively using a fixed point iteration, what the effect of using a finite number of iterations in the solve on a Monte Carlo analysis? This is a complicated issue because the operator defined by a finite number of fixed point iterations defines a different sigma algebra than the full nonlinear operator, and hence defines different probability spaces. There are events that are measurable with respect to one of the two operators and not the other. In addition, there are at least two approaches to solving coupled stochastic models: a "sample" based approach where each sample is computed using the iteration and a "distribution" based approach that attempts to iterate probability distributions in an associated system.

We have developed a systematic mathematical formulation of the various iterative approaches and have analyzed the convergence and the effect of finite iteration on accuracy. We have a draft manuscript that only needs polishing [15].

Task 4

Though we worked on a number of examples (described in a number of manuscripts submitted with project reports), we did not discover a way to quantify the modeling properties of a stochastic upscaled microscale model in terms of its statistical properties. However, we realized that there is related problem that is very important. Namely, when using a representation of microscale behavior in a mesoscale model, practical choices of the representation and upscaling procedure details has to be made. We constructed an inverse problem to choose those representation parameters along with parameter values in [10]. We also investigated error estimation for numerical methods employing multidiscretization methods for coupled systems of reaction-diffusion equations, such as those used to model void migration [12] and the use of adjoint problems solved on discretizations with significantly different time scales for use in a posteriori error estimation [14].

Task 5

This task was completed [4,5]. We implemented some of the algorithms we have developed as part of the project for representing solutions of stochastic Allen-Cahn equations in MOOSE/BISON. The former student Kevin Lenth (U. Wyoming) was hired as a research scientist at University of Wyoming to work with INLpersonnel on implementation. He traveled to INL for about a month in June, and collaborated closely with John Peterson (INL). We also implemented substantial improvements to the time integration schemes in MOOSE/BISON.

Task 6

The project team maintained an active and fulfilling collaboration with Idaho National Laboratory personnel and between the different university partners. During the project, there was a steady stream of visits between institutions. The investigators, postdocs, and students were very active in attending professional meetings and giving talks about the project research. The project supported a number of young researchers and students.

- Will Newton completed a draft paper related to Task 3 and went to work at *Total Benchmark Solution*. He visited INL several times.
- Kevin Lenth finished his dissertation and worked at INL for a month to implement his results in MOOSE/BISON.
- Troy Butler took a tenure track position at University of Colorado Denver while continuing to work on the project.
- During his PhD studies, Charlie Vollmer worked at Los Alamos May-July 2015 and at Sandia National Laboratory from June-August, 2016. ***The work at Sandia has resulted in a research paper and a patent (so far)***. Charlie is interested in pursuing a career in a DOE laboratory. Charlie plans to finish his PhD thesis by August, 2018.

3. Products

1) *A numerical method for solving a stochastic inverse problem for parameters,* T. Butler and D. Estep, Annals of Nuclear Energy, 2012, 10.1016/j.anucene.2012.05.016
2) *Application of a perturbation method to nonlinear stochastic PDE*s, PhD Thesis, Keven Lenth, University of Wyoming.
3) *On upper and lower bounds for quantity of interest in problems subject to epistemic uncertainty*, J. Li, X. Qi, and D. Xiu, SIAM J. Sci. Computing, 2015, 10.1137/120892969
4) Error estimation and time step selection in MOOSE was improved significantly.
5) A simplified Allen-Cahn mesoscale model was implemented in MOOSE, and a stochastic analysis was conducted.
6) *On a Perturbation Method for Stochastic Parabolic PDE*, D. Estep and P. Polyakov, Communications in Mathematics and Statistics: 3 (2015), 215-226
7) *Non-Adaptive Quasi-Optimal Points Selection for Least Squares Linear Regression and Its Application to Stochastic Collocation*, Yeonjong Shin and Dongbin Xi. DOI:10.1137/15M1015868, 2016.
8) *Properties of Discrete Time and Discrete Space Contact Processes,* Charles Vollmer, PhD thesis (pending)
9) *Source Representation in Phase Field Models of Void Dynamics under Irradiation,* Anter El-Azab, Don Estep, Charlie Vollmer, in preparation
10) *Quantifying Upscaling Uncertainties of Random Data: A Cahn-Hilliard Case Study with Random Initial Conditions,* Troy Butler, Don Estep, Nishant Panda, draft
11) *Nonparametric density estimation for randomly perturbed elliptic problems III: Convergence, complexity, and generalizations,* D. Estep, M. Holst, A. Malqvist, Journal of Applied Mathematics and Computing 38 (2012), 367-387

12) *A posteriori analysis of an iterative multi-discretization method for reaction-diffusion systems*, D. Estep. V. Ginting, J. Hameed, and S. Tavener, Computer Methods in Applied Mechanics and Engineering, 267 (2013), 1-22
13) *Uncertainty quantification for approximate p-quantiles for physical models with stochastic inputs*, D. Elfverson, D. Estep, F. Hellman, A. Malqvist, SIAM ASA Journal on Uncertainty Quantification, 2 (2014), 826–850
14) *A posteriori error analysis of two stage computation methods with application to efficient resource allocation and the Parareal Algorithm*, J. H. Chaudhry, D. Estep, S. Tavener, V. Carey, and J . Sandelin, SIAM Journal on Numerical Analysis, 54 (2016), 2729-3122
15) *Approximation Properties of Distributions Arising From a Fixed Point Iteration*, D. Estep, J. Chaudhry, W. Newton, S. Tavener, in preparation.