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George Em Karniadakis
BROWN UNIVERSITY IN PROVIDENCE IN STATE OF RI AND PROVIDENCE PLANTATIONS

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Final Report

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14. ABSTRACT
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formulation; (2) Numerical solution of SPDEs; (3) Reduced-Order modeling; (4) Estimation/Inverse problems; and (5) Robust optimization and
control. This work sets the mathematical foundations of Uncertainty Quantification methods used by many diverse communities in computational
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MULTI-SCALE FUSION OF INFORMATION FOR UNCERTAINTY QUANTIFICATION AND MANAGEMENT IN LARGE-SCALE SIMULATIONS AFOSR GRANT NUMBER: FA9550-09-1-0613 (*FINAL REPORT)*

GE Karniadakis, JS Hesthaven & B Rozovsky, *Brown University*; AT Patera & K Willcox, *MIT*; N Zabaras, *Cornell University*; T Hou, *Caltech*

Abstract

We developed an integrated methodology for uncertainty quantification (UQ) that proceeds from initial problem definition to engineering applications. Towards this goal, we worked on five research areas: (1) Mathematical analysis of SPDEs and multiscale formulation; (2) Numerical solution of SPDEs; (3) Reduced-Order modeling; (4) Estimation/Inverse problems; and (5) Robust optimization and control. This work set the mathematical foundations of Uncertainty Qantification methods used by many diverse communities in computational mechanics, fluid dynamics, plasma dynamics, and materials science. We have pioneered methods for efficient high-dimensional representations of stochastic processes, established Wick-Malliavin approximation for nonlinear SPDEs, theoretical error estimates for multiscale parametric and stochastic PDEs, a new approach to design of experiment and UQ on parametric manifolds, multi-fidelity optimization-under-uncertainty, a data-driven Bayasian framework and probabilistic graphical models for UQ, and information-based coarse graining methods. We have also demonstrated an integration of our UQ methodology and all five areas for a benchmark problem. We have published more than **150 papers** in top mathematical journals, obtained one patent (MIT), and have established one software company (MIT).

Contents

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1 Status/Progress

In the following we provide some research highlights in each of the five research areas of the MURI.

1.1 Mathematical analysis of SPDEs and multiscale formulation

Wick Malliavin Approximations to nonlinear Stochastic PDEs (Brown leads) An important achievement is the development of completely new nonlinear Malliavin calculus. This type of calculus is important for the analysis and simulation of stationary and/or "causal" systems. It allows effective treatment of systems perturbed by nonlinear functions of colored Gaussian noise. We have also developed an effective methodology for homogenization of random elliptic PDEs with deterministic multi-scale structure of the coefficients.

Approximating nonlinearities in Stochastic Partial Differential Equations (SPDEs) via the Wick product has often been used in quantum field theory and stochastic analysis. The main benefit is simplification of the equations but at the expense of introducing modeling errors. We have shown that the Wick solutions have accuracy comparable to linear stochastic perturbation series solutions. However, number-theoretical renormalizations, e.g., based on Catalan numbers for the Wick-Navier-Stokes (WNS) equations, can improve the accuracy by orders of magnitude. The propagator of Wick approximations to nonlinear SPDEs has the same structure as the system of equations for the coefficients of formal power series solutions. Moreover, the structure of this propagator is seemingly universal, i.e., independent of the type of noise. We also introduced new high-order stochastic approximations via Wick-Malliavin series expansions for Gaussian and uniformly distributed noises, and demonstrate convergence as the number of expansion terms increases. Our results are for Burgers and Navier-Stokes (NS) equations but the same approach can be adopted for other nonlinear SPDEs with polynomial nonlinearities and more general noises.

Multiscale Data-Driven Methods (Caltech leads) We made significant progress in developing effective numerical methods for solving stochastic partial differential equations and multiscale problems. In particular, we have developed (i) a dynamically bi-orthogonal method for time-dependent SPDEs; (ii) a data-driven stochastic method for multi-query stochastic problems; (iii) a multiscale model reduction method for PDEs with nonseparable multiscale solutions. We have also made progress in deriving a multiscale closure for the 3D incompressible Navier-Stokes equations and in developing data-driven time-frequency analysis by exploiting the intrinsic sparse structure of multiscale data. Below we will give some details on project (i):

We proposed a dynamically bi-orthogonal method (BO) to study time dependent SPDEs. This was inspired by ongoing work in the MURI on dyamicallly orthogonal expansions (DO). The objective of both BO and DO methods is to exploit some intrinsic sparse structure in the stochastic solution by constructing the sparsest representa- tion of the stochastic solution via a bi-orthogonal basis. These methods essentially track the Karhunen-Loeve expansion dynamically without the need to form the covariance matrix or to compute its eigen-decomposition. In the first part of the work, we derived the dynamically bi-orthogonal formulation for SPDEs, discussed several theoretical issues, such as the dynamic bi-orthogonality preservation and the consistency between the BO formulation and the original SPDE.We also gave some numerical implementation details of the BO methods, including the representation of stochastic basis and techniques to deal with eigenvalue crossing. In the second part, we presented an adaptive strategy to dynamically remove or add modes, performed a detailed complexity analysis, proposed a parallel implementation of DyBO, and discussed various generalizations of this approach. We have applied the BO method to solve the 1D stochastic Burgers equation, 2D incompressible Navier-Stokes equations and the Boussinesq

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approximation with Brownian motion forcings. These numerical examples demonstrate that the BO method solves these nonlinear time-dependent SPDEs accurately and efficiently. In subsequent work, the group at Brown derived an exact equivalence between the BO and DO methods and developed a hybrid approach that combines the best computational features of both methods.

1.2 Numerical solution of SPDEs

We devloped methods to solve the Navier-Stokes and other nonlinear SPDEs in more than 100 dimensions! Several other dvelopments include advances in the generalized polynomial chaos and its variance as well as in Bayesian type methods. In the following, we provide a partial list and in the references we provide all methods we have devloped in this MURI.

The *Cornell* PIs focused on sparse Bayesian kernel techniques (relevance vector machines, RVM) for the solution of SPDEs. Each dimension of the multivariate response was modeled using local kernels centered on top of each data point. The missing scale parameters of the kernels were selected by maximizing the joint marginal likelihood of all dimensions of the response. To address issues with high dimensionality and non-informative variance, these algorithms were later extended to weighted mixture of Gaussian processes.

The *Brown group* focused on high-dimensional problems using adaptive ANOVA with applications to the performance analysis of the horn problem, fluid flows and electromagnetic scattering, and also in developing new polynomial chaos methods for white noise. In the context of the horn benchmark, ANOVA was combined with the reduced basis method to enable a similar parametric reduction of the high dimensional problem to allow the development of a certified reduced basis methods for the critical components of systems with many scattering bodies. This allowed for the development of reduced basis methods for problems with many parameters as has been demonstrated for the acoustic horn problem (see below). Another approach to tackling the curse-of-dimensionality is the formulation of PDF equations for colored noise (joint solution-excitation; fractionals PDEs) and solve them using ANOVA or Proper Generalized Decomposition.

The *Caltech group* worked on two methods: Data-Driven Stochastic Multiscale Method (DSM) and Multiscale Multi-Level Monte Carlo Method (MsMLMC), respectively. The second method can be incorporated into the first to boost its applicability and efficiency, especially for tough problems involving randomness and multiscales simultaneously. An important aspect of DSM is the re-usability of the constructed stochastic basis for different deterministic forcing functions. For computational efficiency, a low-rank approximation method is used (developed in compressed sensing) to exploit the low-rank structure of the covariance matrix. Both DSM and MsMLMC have been applied to the horn benchmark with the latter giving up to 100 times speed-up compared to standard MC.

Uncertainty Quantification for Multiscale PDEs using a Graph Theoretic Approach (Cornell leads) We developed a probabilistic graphical model based methodology to efficiently perform uncertainty quantification in the presence of both stochastic input and multiple scales. Both the stochastic input and model responses were treated as random variables in this framework. Their relationships were modeled by graphical models which give explicit factorization of a high-dimensional joint probability distribution. The hyperparameters in the probabilistic model were learned using sequential Monte Carlo (SMC) method locally in the graph. Coarse graining (stochastic homogenization) was addressed in a non parametric way using hidden variables in a way that naturally arises within the Bayesian graph theoretic framework. Finally, we made predictions from the probabilistic graphical model using the belief propagation algorithm rather than Monte Carlo integration. Belief propagation has the potential of almost linear scaling in certain applica-

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tions. Numerical examples were investigated to show the accuracy and efficiency of the predictive capability of the developed graphical model. Many interesting extensions of this framework were investigated that potentially could lead to a transformative way for UQ in multiscale/multiphysics PDE systems.

Information Theoretic Coarse Graining: Relative entropy (Cornell leads) Relative entropy has been shown to provide a principled framework for the selection of coarse-grained potentials. Despite the intellectual appeal of it, its application has been limited by the fact that it requires the solution of an optimization problem with noisy gradients. When using deterministic optimization schemes, one is forced to either decrease the noise by adequate sampling or to resolve to ad hoc modifications in order to avoid instabilities. The former increases the computational demand of the method while the latter is of questionable validity. In order to address these issues and make relative entropy widely applicable, we proposed alternative schemes for the solution of the optimization problem using stochastic algorithms. Cluster expansions are simplified, Ising-like models for binary alloys in which vibrational and electronic degrees of freedom are coarse grained. The usual practice is to learn the parameters of the cluster expansion by fitting the energy they predict to a finite set of ab initio calculations. In some cases, experiments suggest that such approaches may lead to overestimation of the phase transition temperature. We presented a novel approach to fitting the parameters based on the relative entropy framework which, instead of energies, attempts to fit the Boltzmann distribution of the configurational degrees of freedom. We showed how this leads to T-dependent parameters.

Numerical Methods for High-Dimensional PDF Equations (Brown leads) In this task we addressed the problem of computing the numerical solution to kinetic partial differential equations involving many phase variables. These types of equations arise naturally in many different areas of mathematical physics, e.g., in particle systems (Liouville and Boltzmann equations), stochastic dynamical systems (FokkerPlanck and DostupovPugachev equations), random wave theory (MalakhovSaichev equations) and coarse-grained stochastic systems (MoriZwanzig equations). We proposed three different classes of new algorithms addressing high-dimensionality: The first one is based on separated series expansions resulting in a sequence of low-dimensional problems that can be solved recursively and in parallel by using alternating direction methods. The second class of algorithms relies on truncation of interaction in low-orders that resembles the BogoliubovBorn-GreenKirkwoodYvon (BBGKY) framework of kinetic gas theory and it yields a hierarchy of coupled probability density function equations. The third class of algorithms is based on high-dimensional model representations, e.g., the ANOVA method and probabilistic collocation methods. A common feature of all these approaches is that they are reducible to the problem of computing the solution to high-dimensional equations via a sequence of low-dimensional problems. The effectiveness of the new algorithms was demonstrated in numerical examples involving nonlinear stochastic dynamical systems and partial differential equations, with up to 120 variables.

An adaptive hybrid bi-orthogonal/dynamically-orthogonal method for the stochastic Navier-Stokes equations (Brown leads) A new hybrid methodology for SPDEs was developed based on the dynamically orthogonal (DO) and bi-orthogonal (BO) methods; both approaches are an extension of the Karhunen-Lo‘eve (KL) expansion and hence they capture a low-dimensional structure of the solution by tracking the KL expansion of the solution at any given time on-the-fly. It has been shown that DO and BO are equivalent in the sense that one method is an exact reformulation of the other through a matrix differential equation. However, DO suffers numerically when there is a high condition number of the covariance matrix while BO suffers when there is an eigenvalue crossing. To this end, we proposed a unified hybrid framework of the two methods

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by utilizing an invertible and linear transformation between them. We also presented an adaptive algorithm to add or remove modes dynamically to better capture the transient behavior. Several numerical examples including the Navier-Stokes equations were presented to illustrate this new adaptive hybrid BO-DO method.

1.3 Reduced-Order modeling

Certified Basis (MIT leads)

Uncertainty Quantification (UQ) in almost all forms and approaches is perforce a many-query context. It thus follows that UQ is very well suited to the offline-online strategy afforded by model order reduction (MOR) techniques. In the past, application of MOR to UQ has been inhibited by fundamental restrictions in MOR methodology: MOR could treat only a rather limited class of partial differential equations (PDEs); MOR could treat problems characterized by only relatively few parameters. In our MURI effort we have substantially expanded the capabilities of MOR techniques and furthermore proposed new frameworks in which MOR can serve well the goals of UQ. We have also further improved our *a posteriori* error estimators so as to better assess and control the "self-uncertainty" introduced by model order truncation.

Our accomplishments in the area of expanded classes of problems focus on coupled and nonlinear problems, as well as implementations for supercomputers but also deployed platforms. Our accomplishments in the area of increased parameter dimensionality are twofold: related to parameter-domain decomposition, the development of an "*h*-*p*" reduced basis approximation; related to spatial-domain decomposition, the development of the port-reduced static-condensation reduced-basis element (PR-SCRBE) method for linear problems and also eigenproblems. Our accomplishments in the area of frameworks for uncertainty quantification focus on data assimilation for state estimation. Finally, our accomplishments in the area of *a posteriori* error estimation focus on exact bounds, and on space-time techniques for long-time evolution problems.

We consider these accomplishments in more detail below and more details can be found in the publications of Patera's group.

A1. Expanded problem classes. We have expanded the reduced basis method to consider long-time evolution of nonlinear problems (such as the incompressible Navier-Stokes equations), and also coupled problems (convection-conduction) related to heat exchanger design. We have also expanded the reach of our approach by considering optimized implementations of the reduced basis method on supercomputers and also deployed platforms (for real-time computation).

A2. Treatment of many parameters. Most of this effort falls within two methodological thrusts.

The "*h*-*p*" reduced basis method. This breaks the parameter domain into optimal parameter subdomains and then applies the reduced-basis method on each parameter subdomain. The method permits higher parameter dimensionality due to the smaller domain (hence less rich solution variation) associated with each approximation.

The Port-Reduced Static Condensation Reduced-Basis Element Method (PR-SCRBE). The PR-SCRBE approach is a component-based system synthesis approach which exploits model order reduction at two levels: at the level of ports (the interfaces at which components connect), informed by evanescence arguments; at the level of the component interiors, informed by low-dimensional parametric manifolds. The method can address many parameters, and indeed also topology variations, thanks to the component decomposition and associated divide-and-conquer strategy: we solve many problems with a few parameters rather than one problem with many parameters. The method is also equipped with error estimators both for the port and interior truncations.

A3. Data Assimilation. Most of this effort has been focused on the development of a new data assimilation approach, the Parametrized Background Data Weak method, and an associated

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rigorous theory of stability and approximation. The distinguishing feature of the method is the effective incorporation of low-dimensional parameter manifolds identified, and approximated, by methods developed within the context of reduced basis methods. The PBDW method is non-intrusive in the sense that the PDE appears only in the offline stage and furthermore provides real-time response in the online stage. The method has been applied within our group to physical systems, in particular to acoustics experiments, with considerable predictive success.

A4. Improved a posteriori error estimators. Most of this effort falls within two methodological thrusts.

The first thrust is the development of a formulation in which the reduced-basis error bound is measured with respect to the exact solution of the PDE. In earlier approaches, the reduced-basis error bound is measured relative to a highly refined "truth" finite element approximation. The new approach, proposed and developed by Dr Masa Yano, is preferred not only for the increased rigor, but also because the formulation naturally suggests a simultaneous finite-element reduced-basis adaptive refinement strategy.

The second thrust is the development of improved error estimates for weakly stable evolution problems. In the past, error bounds for weakly stable evolution problems exhibited exponential growth such that only short-time estimates were meaningful. In the new approach, we consider a space-time formulation informed by an optimal inf-sup parameter which considers worst-case growth not from timestep to timestep but rather over the entire time interval and consistent with the governing equation: long-time evolution may thus be pursued.

Stochastic/Multiscale UQ for Wave Dynamics (Brown leads) In this research task we focused on three separate but connected efforts. The continued development of certified reduced basis methods in general and with a particular focus on wave problems. We have demonstrated the effectiveness of such methods for a variety of problem types, including parameterized geometries and the use of such models for uncertainty quantification during scattering. A substantial effort has been in the development and application of certified reduced methods for integral equations, including the development of methods that allows the computation of scattering by a collection of scatterers. The challenges associated with the development of reduced models for parametrized models with a high-dimensional parameter space has also been considered. We have developed methods that dramatically accelerate the greedy approximation in the reduced basis development and demonstrated the ability to handle problems with many parameters. In a related work we have shown how to combine reduced models with ANOVA expansions to allow the effective estimation of parametric sensitivity, leading to parameter compression to allow the development of a reduced model for relevant parameters only. A major part of this effort has been devoted to the development and analysis of high-order accurate multi-scale finite element methods. The work is based on a new and more direct high-order multi-scale expression and the analysis confirms optimal behavior. We have considered both the classic Poisson problem as well as completed the first analysis of multi-scale finite element methods for the wave Helmholtz equation. We have also demonstrated how reduced basis methods can be used to reduce the computational overhead associated with heterogeneous multi-scale behavior.

1.4 Estimation/Inverse problems

Bayesian Techniques (Cornell leads)

Fully Bayesian Uncertainty Quantification Framework/Gaussian Processes with correlated outputs: Computer codes simulating physical systems usually have responses that consist of a set of distinct outputs (e.g., velocities and pressures) that evolve also in space and time and

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depend on many unknown input parameters (e.g., physical constants, initial/boundary conditions etc.). Furthermore, essential engineering procedures such as UQ, inverse problems or design are notoriously difficult to carry out mostly due to the limited simulations available. The aim of this work was to introduce a fully Bayesian approach for treating these problems which accounts for the uncertainty induced by the finite number of observations. Our model was built on a multi-dimensional Gaussian process that explicitly treats correlations between distinct output variables as well as space and/or time. The proper use of a separable covariance function enabled us to describe the huge covariance matrix as Kronecker product of smaller ones leading to efficient algorithms for carrying out inference and predictions. The novelty of this work is the recognition that the Gaussian process model actually defines a posterior probability measure on the function space of possible surrogates for the computer code and the derivation of an algorithmic procedure that allows us to sample it efficiently. We demonstrated how the scheme can be used in uncertainty quantification tasks in order to obtain error bars for the statistics of interest that account for the finite number of observations.

Sparse Bayesian Techniques. Multi-output sparse Bayesian techniques (extension of relevance vector machines) that are able to automatically identify the most relevant of a set of basis functions (using either localized kernel functions or an optimal orthogonal polynomial basis). When using an optimal orthogonal polynomials basis, our techniques may be thought as a Bayesian, tree-based extension of generalized Polynomial Chaos (gPC). This combines the optimal convergence of the gPC for smooth functions, with locality capturing discontinuities and the Bayesian framework allowing the quantificaiton of epistemic uncertainty. Our numerical experiments demonstrated that this is a powerfull combination. The sparsity of the resulting surrogate: 1) may be intuitively interpretable and 2) are super-fast to evaluate.

Treed Multi-output Gaussian Process: We developed an efficient, Bayesian Uncertainty Quantification framework using a novel treed Gaussian process model. The tree is adaptively constructed using information conveyed by the observed data about the length scales of the underlying process. On each leaf of the tree, we utilize Bayesian Experimental Design techniques in order to learn a multi-output Gaussian process. The constructed surrogate can provide analytical point estimates, as well as error bars, for the statistics of interest. We numerically demonstrated the effectiveness of the suggested framework in identifying discontinuities, local features and unimportant dimensions in the solution of SPDEs.

Solution of Inverse Problems with Limited Forward Solver Evaluations: A Bayesian Perspective. Solving inverse problems based on computationally demanding forward solvers is ubiquitously difficult since one is necessarily limited to just a few observations of the response surface. This limited information induces additional uncertainties on the posterior distributions. The main contribution of this work is the reformulation of the solution of the inverse problem when the expensive forward model is replaced by a set of simulations. The proposed solution is based on the idea of a Bayesian surrogate that replaces the code. We derived three approximations of the reformulated solution with increasing complexity and fidelity. We demonstrated numerically, that the proposed approximations indeed capture the epistemic uncertainty on the solution of inverse problem induced by the fact that the forward model is replaced by a set of simulations and that they converge to the true solution as the number of simulations is increased.

1.5 Robust optimization and control

Design under Uncertainty (MIT leads)

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Under this thrust we have pursued two main research topics: multifidelity methods to accelerate the cost of solving optimization under uncertainty problems, and a goal-oriented approach to inference of distributed parameters. Our multifidelity approaches build on the methods, tools and applications developed in the Model Reduction thrust of the MURI project.

In optimization under uncertainty problems, computing the mean, variance, or other statistics of the high-fidelity model output for every change in the design variables is computationally expensive due to the large number of model evaluations needed. In many practical situations, a low-fidelity model is available to provide useful information about the output of the high-fidelity model at a lower cost. Multifidelity Monte Carlo simulation is a modification of the control variate method that takes advantage of the correlation between the output of the low-fidelity model and the output of the high-fidelity model to reduce the computational cost of uncertainty propagation.

Engineered systems parametrized by distributed quantities represent a significant challenge for state-of-the-art computational methods and inverse problem formulations. An infinite-dimensional parameter is identified to predict output quantities of interest. Goal-oriented inference is the process by which these final outputs are exploited in the inference process. In the linear case, we have shown that the inference algorithm can be suitably modified to improve online efficiency without sacrificing accuracy in prediction of outputs. Our work focused on extending goal-oriented inference to the setting of nonlinear problems. Our work on the deterministic inverse problem formulation has focused on employing error estimation techniques popular in the mesh adaptation community to obtain a parameter estimate that has the correct prediction, but without converging the parameter. In the statistical setting, we extended recent work in Bayesian inference to identify a map from prior predictive to posterior predictive. One then would obtain samples of the posterior predictive directly from applications of the prediction model to prior samples and propagation through the identified map. The required map will generally have many fewer parameters than the analogous map from prior to posterior since it is applied in the prediction space.

1.6 Integrated UQ Methodology

In order to demonstrate advances on all five research areas we focused on the specific horn benchmark problem, hence addressing the design of wave-dominated problems under uncertainty. We tested new developments on nonlinear Malliavin calculus, combining reduced basis methods with ANOVA, model validation, on quantifying model uncertainty in inverse problems, on stochastic quantization for the Navier-Stokes equations, on learning techniques, and on stochastic multiscale modeling of materials.

We considered a frequency-domain acoustic planar horn problem first introduced and analyzed in (Udawalpola & Berggren, I. J. Num. Meth. Eng., 73:1571, 2008) in the deterministic framework. The horn consists of a straight waveguide followed by a flare section. The pressure field satisfies a Helmholtz equation with an incoming-wave condition at the waveguide inlet, zero-flow (Neumann) conditions on the horn walls, and a radiation condition for the farfield. We took for our input (stochastic) parameters the flare geometry, wavenumber k, and impedances $Z_{\mathrm{t}}, Z_{\mathrm{b}}$ of the top and bottom flare walls; we also must specify a parameter domain. We took for our output the effective reflection coefficient of the horn; the aim is to minimize reflection and hence maximize power transmission. First, we obtained a "truth" finite element (FE) approximation and subsequently we developed a reduced basis (RB) approximation to the FE approximation with corresponding rigorous *a posteriori* error bounds for the difference between the finite element and reduced basis output predictions. The results were reported in a previous progress report (2011).

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2 Personnel Supported During Duration of Grant

• Faculty: Karniadakis, Hesthaven, Rozovsky, Zabaras, Hou, Patera, Willcox.
• Postdocs (partial support): (Brown) D. Venturi, L. Grinberg, S. Zhang; B. Stamm, P. Gatto, S. Zhang,F. Zeng; (Caltech) Z. Zhang, F-N. Hwang, C. Liu, Z. Shi, Q. Li, G. Luo; (MIT) J. Eftang, D.B.P. Huynh, J.D. Penn, D.J. Knezevic, K. Smetana, T. Tonn, S. Vallaghe, M. Yano, T. Tom, M. Yano, Q. Liao .
• PhD Students (partial support): 14 at Brown; 6 at Cornell; 6 at Caltech; 3 at MIT.

3 Honors & Awards

• Hesthaven – SIAM Fellow (2014).
• Hou – AMS Fellow (2012); SIAM Fellow (2009); AAAS (2011).
• Karniadakis, SIAM Fellow (2010); USACM T.J. Oden Medal (2013); R. Kleinmann SIAM award (2015).
• Patera – USACM T.J.R. Hughes Medal (2013); Hans Kupczyk Guest Professorship Award 2010 from the University of Ulm (Germany); Honorary Member, Société de Mathématiques Appliquées et Industrielles (SMAI, France), 2012; Chaire d'Excellence (Senior Research Chair), Fondation Sciences Mathématiques de Paris, France, 2013–2015.
• Wllcox and Leo Ng (PhD student with Willcox) received second place in the AIAA Multidisciplinary Analysis and Optimization conference Student Paper competition, for his paper entitled "Multifidelity Uncertainty Propagation for Optimization Under Uncertainty." (September 2012).

4 AFRL Point of Contact

• Jordan, Jennifer L Dr CIV USAF AFMC AFRL/RWM , Energetic Materials Core Technical Competency Lead, Eglin Munitions Directorate visited Cornell and research collaborative plans are under way.
• Willcox discussed multifidelity methods with Ray Kolonay and Ed Alyanak from AFRL.
• Philip Beran, WPAFB, OH 45433, Phone 937-255-665. Visited and gave a talk at MIT in Fall 2010;
• Horie Yasuyuki, CIV USAF AFMC AFRL/RWMER (Yasuyuki.Horie@eglin.af.mil); Dutton, Rollie E Civ USAF AFMC AFRL/RXLMP (Rollie.Dutton@wpafb.af.mil); Cooper, William L Dr CIV USAF AFMC AFRL/RWMWH (william.cooper@eglin.af.mil). A short course on UQ was given by co-PI Zabaras at Eglin AFB and also at General Electric.

5 Transitions

• Karniadakis's group – http://sourceforge.net/projects/mepcmpackage/ The Multi-Element Probabilistic Collocation Method Package (MEPCMP) is a C++ package which can generate high dimensional, multi-element collocation points based on arbitrary probability density function for the application of Multi-Element Probabilistic Collocation Method (MEPCM).
• Patera's group – Several technology and software disclosures were made to the MIT Technology Licensing Office during the life of the grant. The MIT Office of Sponsored Research will file the official report on intellectual property. We note here a transition recipient.

Transition Organization: Akselos, Inc `http://www.akselos.com/company.html`

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MIT Case No. 15408 “SCRBE V1.1 Software”, by David John Knezevic.

• Hesthaven's group – Working closely with HyperComp, Inc to transition the use of reduced basis methods and related UQ technology into TEMPUS software. TEMPUS is used widely by AFRL. PhD student X. Zhu spent the summer at HyperComp as an intern working on transitioning reduced order modeling ideas and software into HyperComp Inc.

6 Acknowledgement/Disclaimer

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7 Publications

1. P. Chen, N. Zabaras and I. Bilionis, Uncertainty Propagation using Innie Mixture of Gaussian Processes and Variational Bayesian Inference”, Journal of Computational Physics, Vol. 284, 291-333, 2015.

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Program Manager

The AFOSR Program Manager currently assigned to the award

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Abstract

We developed an integrated methodology for uncertainty quantification (UQ) that proceeds from initial problem definition to engineering applications. Towards this goal, we worked on five research areas: (1) Mathematical analysis of Stochastic Partial Differential Equations (SPDEs) and multiscale formulation; (2) Numerical solution of SPDEs; (3) Reduced-Order modeling; (4) Estimation/Inverse problems; and (5) Robust optimization and control. This work sets the mathematical foundations of Uncertainty Quantification methods used by many diverse communities in computational mechanics, fluid dynamics, plasma dynamics, and materials science. We have pioneered methods for efficient high-dimensional representations of stochastic processes, established Wick-Malliavin approximation for nonlinear SPDEs, theoretical error estimates for multiscale parametric and stochastic PDEs, a new approach to design of experiment and UQ on parametric manifolds, multi-fidelity optimization-under-uncertainty, a data-driven Bayasian framework and probabilistic graphical models for UQ, and information-based coarse graining methods. We have also demonstrated an integration of our UQ methodology and all five areas for a benchmark problem. We have published more than 150 papers in top mathematical journals, obtained one patent (MIT), and have established one software company (MIT).

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Specific research highlights include:

Mathematical Theory: Quantization-renormalization of SPDEs; New evolution equations for joint-pdf of SPDEs; Nonlinear Malliavin calculus.

Reduced Basis Methods (RBM): Integral equations and multi-scattering problems; Robust design, parameter estimation, and model uncertainty.

Adaptive ANOVA: Convergence theory; Parameter compression and RBM; Fluid flows, porous media, multi-scattering.

Bayesian Framework: coarse-graining; Active learning + SPDEs; Adaptive SMC, dependent random variables, Model uncertainty in inverse problems.

Numerical SPDEs: Data-driven stochastic multiscale method, Multiscale multilevel MC, Probabilistic graphical models, Long-time integrators of SPDEs.

Software: MEPCM library (polynomial chaos + ANOVA); RBM libraries - RBOOMIT, RBAppMIT; Akselos, Inc; Random poly-crystals – RPCrystal; TEMPUS/Hypercomp.

In addition, we have extended the original proposal to introduce new concepts as follows:

Stochastic Delay ODEs & PDEs
Fractional PDEs – First Symposium on June 3-5, 2013 (Newport, RI)
Reduced Basis for design of experiments
Multiscale high-order FEM and Reduced Basis
A control-theoretic approach to "inference for prediction"
UQ for polycrystals using microstructure images and FFT
Probabilistic graphical models for UQ
Bayesian surrogates to compute epistemic uncertainty

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