FINAL REPORT FOR DOE AWARD NUMBER DE-SC0003452
ANALYSIS AND REDUCTION OF COMPLEX NETWORKS UNDER UNCERTAINTY

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1. Summary

This was a collaboration with Youssef Marzouk of MIT, Omar Knio of Duke University (at the time at Johns Hopkins University) and Habib Najm of Sandia National Laboratories. The objective of this effort was to develop the mathematical and algorithmic capacity to analyze complex networks under uncertainty. Of interest were chemical reaction networks and smart grid networks. The statements of work for USC focused on the development of stochastic reduced models for uncertain networks. The USC team was led by Professor Roger Ghanem and consisted of one graduate student and a postdoc. The contributions completed by the USC team consisted of **1)** methodology and algorithms to address the eigenvalue problem, a problem of significance in the stability of networks under stochastic perturbations, **2)** methodology and algorithms to characterize probability measures on graph structures with random flows. This is an important problem in characterizing random demand (encountered in smart grid) and random degradation (encountered in infrastructure systems), as well as modeling errors in Markov Chains (with ubiquitous relevance !). **3)** methodology and algorithms for treating inequalities in uncertain systems. This is an important problem in the context of models for material failure and network flows under uncertainty where conditions of failure or flow are described in the form of inequalities between the state variables.

2. Technical Contributions

2.1. **Random Eigenvalue Problem.** Two computationally efficient algorithms are developed for solving the stochastic eigenvalue problem. An algorithm based on the power iteration technique is proposed for the calculation of the dominant eigenpairs. This algorithm is then extended to find other subdominant random eigenpairs. The uncertainty in the operator is represented by a polynomial chaos expansion, and a similar representation is considered for the random eigenvalues and eigenvectors. The algorithms are distinguished due to their speed in converging to the true random eigenpairs and their ability to estimate a prescribed number of subdominant eigenpairs. The algorithms are demonstrated on two examples with close agreement observed with the exact solution and a solution synthesized through Monte Carlo sampling.

The robust predictive models for natural and engineered systems should incorporate the significant variabilities in the behavior of these systems induced because of the inherent variability of system components, inadequacy of the input-output models and inaccuracy of the numerical implementations (finite-dimensional approximation). Towards this end, efficient uncertainty quantification techniques have been developed that represent the uncertainty in the input, propagate it through the numerical models, and finally produce a probabilistic description for the system outputs and Quantities of Interest (QoI). In addition to the classical sampling techniques, such as Monte Carlo simulation and its improved derivatives, such as Markov chain Monte Carlo techniques, recently, there has been growing interest in the non-sampling spectral technique, named Polynomial Chaos Expansion. In this stochastic projection technique, the governing equation is projected onto truncated polynomial chaos coordinates, resulting in a finite-dimensional approximation of the sample space, which is amenable to numerical calculation .

Our objective in this work was to characterize the eigenspace of linear systems with parametric uncertainties. Such characterization can be used as the basis in various model reduction techniques, and thus significantly improve the computational cost of the analysis of large uncertain systems. Our particular interest was on random matrices that arise from finite-dimensional approximation (discretization) of continuous operator, such as partial differential operators, involving parametric uncertainty, as well as on those corresponding to a discrete random system, such as multi-degree of freedom oscillators. Generally, there is no closed-form expression for these random matrices.

Recently, Polynomial Chaos Expansion techniques have been applied to the solution of random eigenvalue problem where given a PC representation for the random matrix, the solution eigenvalue and eigenpairs are assumed to have similar spectral representation in the same vector space. The weak form of the eigenvalue problem is then obtained by Galerkin projection of the eigenvalue equation on the PC orthogonal basis, spanning the Hilbert space of input random variables, leading to a system of nonlinear algebraic equations. The PC coefficient of the solution eigenpairs are then obtained by the numerical solution of these systems. The resulting PC solution lends itself readily to accurate uncertainty representation of QoI and sensitivity indices, and is greatly advatangeous to other proposed methods.

In our approach, given a PC representation for the random matrix, instead of solving the system of algebraic equations for the PC coefficients, we utilize the idea of power iteration scheme in order to calculate the PC coefficients of dominant random eigenpair. Also, we propose an algorithm that calculates a prescribed number of dominant random eigenpairs, and thus arrive at an optimal approximation for a lower-dimensional subspace in which the random operator can be represented.

2.2. **Random Flows on Graphs.** Markov chains are ubiquitous in modeling phenomena that exhibit random fluctuations while evolving in time. Their value lies in their simplicity, both of interpretation and implementation. Indeed, the mere justification of finite memory with constant structure, allows the postulation of a Markovian model from which consistent sample paths for futures of the system can be realized. Decision processes associated with this behavior can also be readily formalized yielding elegant analytical insight. These Markovian models are typically parameterized by their initial state and the probabilities of transition between states. These so-called transition probabilities are usually estimated from the evolution of the Markov chain observed along a number of sample paths. Given the dichotomy between the simplicity of Markovian models, and the highly complex natural, man-made, and social phenomena to which they have been adapted, a framework for assessing the uncertainty in associated mode-based inferences is essential. One can contemplate two constructions of Markov chains that provide different perspectives on these uncertainties. The first construction maintains the belief that a Markov model is a suitable description of the underlying motives such as physical or social processes. In this case uncertainty is attributed to lack of knowledge (due perhaps to insufficient observations) of the true values of transition probabilities, which are themselves treated as random. An ensemble of Markov chains is thus obtained, that is in one-to-one correspondence with the ensemble of transition matrices. The second construction recognizes that a Markov model is merely a convenient representation of the processes of interest, and develops adaptation strategies as information is acquired. Accordingly, the transition matrix of the Markov chain is permitted to vary in time, effectively, refitting a new Markov chain. Clearly, in this construction, the amount of data available to re-fit a Markov chain is more limited than in the first construction, and uncertainty in the estimated transition probability can be significant. We referred to these two constructions as the time-invariant and to the time-variant models, respectively. We present a methodology for ascertaining the uncertainty in transition probabilities of Markov chains, and demonstrate its value in quantifying the uncertainty in the predicted steady-state dynamics and associated decisions.

Without loss of generality, we focus our attention on finite-state discrete-time Markov chains. The time evolution of the state probabilities from a time instance to the next is determined by the entries of the transition matrix which describe the transition rates between two states of the chain. These transition rates are usually estimated as deterministic model parameters using least squares, Maximum Likelihood, Most a-Posteriori, or Maximum Entropy (MaxEnt) arguments. Within the confines of probability theory our objective, then, is to characterize a probability measure for the transition matrix that is consistent, in some sense, with mathematical constraints and available evidence.

Our approach involves characterizing a probability measure over the set of all mathematically admissible transition matrices, constraining them to be valid stochastic matrices. We estimate this measure using the MaxEnt principle given the information on the mean values and possibly higher moments. We make use of no other assumptions in the estimation procedure. With a MaxEnt RTM available, a Markov chain can be constructed in two different ways, describing two distinct behaviors. In the first one, referred to as Markov chain with time-invariant RTM, a single sample of the random transition matrix is assumed to govern the

Markov chain's time evolution. In the second implementation, referred to as Markov chain with time-variant RTM, at each time step, a new independent sample is drawn from the RTM based on which the Markov chain makes a one-step transition. The second variation is also referred to as Markov chains in random environment.

We demonstrated the significance of this formalism on problems related to characterizing demand in a smart grid environment, the maintenance scheduling of civil infrastructure, the allocation of resources in a health care setting, energy management in the built environment, and random flows over a network. We also explored the value of probabilistic characterization to a multiscale perspective on data.

We also investigated a similar problem in the context of forest dynamics. In that context we adapted other methodologies based on upscaling of Markov processes developed in climate applications.

2.3. **Stochastic Inequalities.** Inequality constraints appear in many problems in science and engineering as manifestation of finite capacity, geometric confinement or the second law of thermodynamics. The theory of elasto-plasticity, for instance, uses inequalities to separate a regime of purely elastic material behavior, from post-yield inelastic behavior. In most problems of interest, on the other hand, uncertainties on model form, model parameters or data, are unavoidable and are a reflection of insufficient experimental information and physical resolution. While mathematical tools for the treatment of inequality constraints, and in particular Variational Inequalities (VIs), are well understood for the analysis of deterministic problems, there has been only little effort, to date, in extending them to the analysis of problems exhibiting uncertainty.

Stochastic projection methods have been found to be very effective for solving problems involving uncertainty. They typically involve formulating the governing equations as a variational equality in their stochastic dimension to construct new equations that govern the stochastic components of the problem. The projection of the variational equality thus obtained onto truncated Polynomial Chaos Expansions (PCEs) yields a finite-dimensional problem amenable to calculation. Stochastic projection approaches are sometimes more computationally efficient than sampling-based approaches, such as Monte Carlo simulation, and are particularly well-suited to analyze the sensitivity of the stochastic solution with respect to input stochastic properties, as required for resource allocation aimed at improving predictions.

Two main challenges are essential in problems with inequality constraints. First, the constraints are defined pointwise in the domain of the problem, which is not commensurate with the standard weak formulation of most boundary value problems. Second, inequality constraints destroy the linear structure of the underlying mathematical problems, and the solution is typically sought in a convex set, defined by the constraints, rather than in a linear space. Systems of partial differential equations with inequality constraints can thus not readily be formulated as a variational equality that can subsequently be discretized by projection.

Developments in deterministic VIs have, over the past few decades, overcome these difficulties and yielded a unified framework for the variational formulation of a wide class of problems from science and engineering whose mathematical formulation involves inequality constraints. The Signorini problem was the first problem involving a VI and pave the way for the subsequent development of the mathematical foundation of a theory of VIs, and associated numerical techniques. The VI theory has been extended and generalized in many directions, and has found applications in many branches of mechanics and physics, such as elasto-plastic material behavior, contact/impact problems, flow through porous media, and variational theories of crack initiation, as well as in network modeling, control, equilibrium modeling, finance, and game theory. The development of VIs has revealed fundamental properties of solutions to many of these problems, such as properties regarding their existence, uniqueness and regularity, and has also enabled the development of of highly efficient new methods for their numerical solution.

There has been only little effort, to date, in extending the theory of VIs to the analysis of problems exhibiting uncertainty The type of SVIs studied to date is quite different from those encountered in applications in mechanics and physics, or lacks effective solution strategies.

Our work on this topic is concerned with the systematic extension of the theory of VIs to the stochastic case. The main objective is to delineate a framework for the formulation of stochastic problems with inequality constraints as SVIs, and for their numerical solution via projection. While the framework that we developed is general, we demonstrated our approach on applications in elasto-plastic material behavior. An essential challenge, again, was to develop pointwise constraints on a solution defined only in the weak sense through projections.

The conclusion of our work no this topic is that (i) the statement of a stochastic problem with inequality constraints in the form of a SVI enables its discretization via projection onto PCEs, and (ii) the collocation of the inequality constraints enables their computationally efficient treatment in algorithms for the solution of SVIs.

3. Research Team

The USC team involved one dedicated student and a postdoc shared with another ASCR project. The student, Dr. Hadi Meidani, has recently accepted an offer to join the department of Civil and Environmental Engineering at the University of Illinois at Urbana-Champaign as assistant professor, while the postdoc, Dr. Maarten Arnst, is now Assistant Professor in Aerospace Engineering at the Université de Liège in Belgium. In addition, to these two individuals, Dr. Maud Comboul was partially supported on this effort, adapting multiscale Markov models to the problem of forest dynamics. She is currently a postdoc in the School of Earth Sciences at USC.

4. Scholarly Products

4.1. Journal Publications.

(1) Comboul, M. and Ghanem, R., "Multiscale Modeling for Stochastic Forest Dynamics,", *International Journal for Multiscale Computational Engineering,* Vol. 12, No. 4, pp. 319-329, 2014.
(2) Meidani, H. and Ghanem, R., "Random Markov decision processes for sustainable infrastructure systems," in press *Structure and Infrastructure Engineering*, DOI: 10.1080/15732479.2014.893445, 2014.
(3) Meidani, H. and Ghanem, R., "Spectral power iterations for the random eigenvalue problem," *AIAA Journal,* Vol. 52, No. 5, pp. 912-925, 2014.
(4) Meidani, H. and Ghanem, R., "Multiscale Markov models with random transitions for energy demand management," *Energy and Buildings,* Vol. 61, p. 267-274, 2013.
(5) Meidani, H. and Ghanem, R., "Uncertainty quantification for Markov chain models," *Chaos,* Vol. 22, No. 4, 2012.
(6) Ghosh, D., and Ghanem, R., "An invariant subspace-based approach to the random eigenvalue problem of systems with clustered spectrum," *International Journal for Numerical Methods in Engineering,* Vol. 91, No. 4, pp. 378-396, 2012.
(7) Arnst, M. and Ghanem, R., "A variational-inequality approach to stochastic boundary value problems with inequality constraints and its application to contact and elastoplasticity," *International Journal for Numerical Methods in Engineering,* Vol. 89, No. 13, pp. 1665-1690, 2012.

4.2. Papers in Conference Proceedings.

(1) Meidani, H. and Ghanem, R., "Uncertainty quantification of diffusion maps," *ICOSSAR'13: International Conference on Structural Safety and Reliability,* New York City, NY, June 16-20, 2013.
(2) Meidani, H. and Ghanem, R. "Modal Analysis of Structures under Uncertainties Using Spectral Stochastic Techniques" *14th AIAA Non-Deterministic Approaches Conference,* Honolulu, HI, April 23-26, 2012.
(3) Comboul, M. and Ghanem, R., "Multiscale modeling for stochastic forest dynamics," pp. 2627-2632 *in ICOSSAR'09: Safety Reliability and Risk of Structures, Infrastructures and Engineering Systems, Edited by Furuta, Frangopol and Shinozuka,* 2009.

4.3. Abstracts in Conference Proceedings.

(1) Ghanem, R. and Meidani, H., "Uncertainty Quantification and Decisions for Markovian Dynamics," *SIAM Conference on Applications of Dynamical Systems,* Snowbird, UT, March 21 2013.
(2) Meidani, H., and Ghanem, R., "Diffusion on Random Manifolds," *2012 SIAM International Conference on Data Mining,* Anaheim, CA, April 26-28.
(3) Meidani, H. and Ghanem, R., "Maximum entropy construction for data-driven analysis of diffusion on random manifolds," *SIAM First Conference on Uncertainty Quantification,* Raleigh, NC, April 2-5, 2012.
(4) Meidani, H. and Ghanem, R. "Markov Chains with random transition matrices - a maximum entropy formalism," *11th US National Congress on Computational Mechanics,* Minneapolis, MN, July 2011.

(5) Meidani, H. and Ghanem, R. "Algorithms for stochastic eigenvalue analysis with Polynomial Chaos," *Sixth M.I.T. Conference on Computational Fluid and Solid Mechanics, Cambridge, MA.* June 15-17, 2011.
(6) Comboul M. and Ghanem R., "Multiscale modeling for stochastic forest dynamics," *SIAM conference on Applications of Dynamical System,* Snowbird, UT, May 2011.
(7) Ghanem, R. and Meidani, H. "MaxEnt Formulation for Markov Chains in Random Environment," *SIAM Conference on Computational Science & Engineering,* Reno, NV, February 28-March 4, 2011.
(8) Ghanem, R. and Arnst, M., "An assessment of stochastic model reduction methods," *European Conference on Computational Mechanics,* Paris, France, May 16-21, 2010.
(9) Arnst, M. and Ghanem, R., "Formulation and solution of stochastic variational inequalities describing inelastic material behavior and contact/impact," *10th US National Congress on Computational Mechanics,* Columbus, OH, July 16-19, 2009.
(10) Meidani, H., Ghanem, R., and Arnst, M., "Computation of Network Equilibrium Using Variational Inequalities" *10th US National Congress on Computational Mechanics,* Columbus, OH, July 16-19, 2009.
(11) Comboul, M. and Ghanem, R., "Multiscale modeling for stochastic forest dynamics," *10th US National Congress on Computational Mechanics,* Columbus, OH, July 16-19, 2009.

4.4. **Technical Reports.**

(1) NRC Committee on Mathematical Foundations of Verification, Validation, and Uncertainty Quantification "Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification," *NRC Board on Mathematical Sciences and Their Applications Division on Engineering and Physical Sciences, 2012.*
(2) Ghanem, R. "A Report to NSF on Opportunities and Challenges in Uncertainty Quantification for Complex Interacting Systems," 2010.

4.5. **Keynote Lectures.**

(1) "UQ in Computational Science and Engineering," *Fourth International Conference on Scientific Computing and Partial Differential Equations (SCPDE11),* (plenary) Hong Kong, China, December 5-9, 2011.
(2) "V&V or a Psycho-Analysis of Predictions,", *European Conference on Computational Mechanics,* (semi-plenary) Paris, France, May 16-21, 2010.
(3) "Uncertainty Management in Predictive Simulations," (plenary) *Workshop on Quantification on CFD Uncertainties,* at the Vrije Universiteit Brussel, Belgium, October 29-30, 2009.

4.6. **Invited Talks.**

(1) "Stochastic representations of model-based predictions and associated data assimilation," *Institute for Computational Engineering and Science (ICES),* The University of Texas at Austin, September 13 2012.
(2) "Upscaling and Dimension Reduction for Stochastic Flows," *Department of Mechanical and Aerospace Engineering,* UCSD, October 29 2012.
(3) "A Perspective on Uncertainty Quantification and Model Validation," *Princeton University*, April 9 2012.
(4) "V&V or the Schizophrenia of Prediction Science: from Diagnosis to Therapy ," *MIT Distinguished Speaker Series in Computational Science and Engineering,* Cambridge, March 7 2012.
(5) "V&V in Predictive Models," *Department of Atmospheric, Oceanic and Space Sciences, University of Michigan*, Ann Arbor, April 7 2011.
(6) "A Computable Approach to Validation" *Frontiers in Computational & Information Sciences Seminar Series,* Pacific Northwest National Laboratory, Richland, WA, August 16 2010.
(7) "V&V or Investigation on the Multiple Personalities of Predictions," *ICeS: Institute for Computational Engineering and Science,* University of Texas, Austin, March 27-April 1, 2010.
(8) "V&V or a Psychology of Models," *Department of Mathematics, University of California, Berkeley, March 4, 2010.*
(9) "Back of the Envelope Calculations: When and How Big ?" Institute for Computational and Mathematical Engineering, Stanford University, November 16 2009.

(10) "Verification and Validation: A Paradigm for Trustworthy Predictions," *CAMS Colloquium,* USC, October 19, 2009.
(11) "An Approximation Theory for Model Validation," University of California Santa Barbara, CA, January 16 2009.

4.7. **Workshops.**

(1) "Reduced models for risk assessment of urban systems," *3^{rd} International Symposium on Advances in Urban Safety (SAUS2012),* Nanjing, China, November 24-26, 2012.
(2) "Random field representations and approximations for fixed point iterations," *Computational and Theoretical Challenges in Interdisciplinary Predictive Modeling Over Random Fields,* Texas Tech University, Lubbock, TX, October 26, 2012. r
(3) "Focus on objectives resolves the curse of dimensionality" *NASPDE12 (Numerical Solution of Stochastic PDEs)*, Warwick, UK, June 11-12, 2012.
(4) "Uncertainty in Reduced Order Models : A blessing or a curse ?" at *Workshop on Reduced Basis, POD and PGD Model Reduction Techniques: a Breakthrough in Computational Engineering ?* Cachan, France, November 16-17-18, 2011.
(5) "Uncertain Handshaking," *von Neumann Symposium on Multimodel and Multialgorithm Coupling for Multiscale Problems,* organized by the American Mathematical Society, Snowbird, Utah, July 4-7, 2011.
(6) "Uncertainty Quantification in Industrial Problems," *IMA Workshop on Quantification of Uncertainty in Indsutrial Problems and Energy Applications,* the Institute for Mathematics and Its Applications (IMA), University of Minnesota, June 2-4, 2011.
(7) "Uncertainty Quantification in Inverse Problems," *IMA Workshop on Large-scale Inverse Problems and Quantification of Uncertainty,* the Institute for Mathematics and Its Applications (IMA), University of Minnesota, June 6-10, 2011.
(8) "From deterministic to stochastic multi-scaling and uncertainty analysis," *NSF Workshop on Challenges in Computational Multiscale Materials Modeling (CCMMM)*, Arlington, VA, May 4 2011.
(9) "Dimension reduction and measure transformation in stochastic multiphysics modeling," BIRS Workshop on Stochastic Multiscale Methods, Banff, Canada, March 27-April 1 2011.
(10) "Data-Driven Stochastic Modeling and Simulation", I. Yadegaran and R. Ghanem, *Workshop on Uncertainty Quantification for Multiphysics and Multiscale Systems,* USC, Los Angeles, CA, March 8, 2011.
(11) "Comboul M. and Ghanem R., Stochastic models for natural and urban systems," *Workshop on Uncertainty Quantification for Multiphysics and Multiscale Systems,* USC, Los Angeles, CA, March 8, 2011.
(12) "Uncertainty Characterization for Markov Chain's Transition Probabilities," H. Meidani, R.G. Ghanem, *Workshop on Uncertainty Quantification for Multiphysics and Multiscale Systems,* USC, Los Angeles, CA, March 8, 2011.
(13) "Stochastic upscaling for waves in polycrystalline materials," *IPAM Workshop on Random Media: Homogenization and Beyond,* UCLA, Los Angeles, CA, January 24-29, 2011.
(14) The Los Alamos National Laboratory workshop on *Mapping Out Future Directions for Uncertainty Quantification in Scientific Inference*, Santa Fe, November 4 2010.
(15) "Uncertainty Challenges for SmartGrid," *Mathematics Challenges for SmartGrid,* Pacific Northwest National Laboratory, Richland, WA, August 17 2010.
(16) Plenary talk: "Construction and Identification of Stochastic Models," *SICON'09, University of Rome - La Sapienza,* September 23 2009.
(17) Comboul M., Ghanem R. and Becker T., "Crustal surface deformation time series analysis for transient detection," *SCEC annual meeting: transient detection exercise,* Palm Springs (California), September 2010.
(18) "Information-Driven Predictions for Urban Sustainability," *THU-USC Faculty Forum on Green and Smart for Sustainable Future,* Davidson Center, USC, April 3 2010.
(19) Invited participants at the AFOSR/AFRL "Multi-Scale Modeling Planning Workshop," Dayton, OH, December 9-10, 2009.

(20) "Ubiquitous Sustainable Cities," invited presentation to the *Second SmartGrid Symposium,* USC, October 6, 2009.

4.8. **Short Courses.**

(1) "Stochastic Representations," (3 hours) *UQ Summer School,* University of Southern California, Los Angeles, CA August 22-24, 2012.
(2) "Stochastic Computational Science," (6 hours) *SIAM Conference on Uncertainty Quantification,* Rayleigh, NC, April 1 2012.
(3) "Stochastic Representations of Model-Based Predictions and Associated Data Assimilation," (6 hours) *CIMPA UNESCO School in Applied Mathematics,* KAUST, Saudi Arabia, Spring 2012.
(4) "Uncertainty Quantification in Geosciences," (2 hours) *SIAM Conference on Geosciences,* Long Beach, California, March 21-24, 2011.
(5) "Uncertainty Quantification in Mechanics: Theoretical and Computational Aspects," (6 hours) *10^{th} US National Congress on Computational Mechanics* (with C. Soize), in Columbus, OH, July 15, 2009, and the *11^{th} USNCM* in Minneapolis, MN, July 24, 2011.