AFRL-AFOSR-VA-TR-2019-0110

Mathematical Methods for Predictive Simulation of Stochastic Turbulence Systems

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04/19/2019
Final Report

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Air Force Research Laboratory
AF Office Of Scientific Research (AFOSR)/ RTA2
Arlington, Virginia 22203
Air Force Materiel Command

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
30-05-2017

2. REPORT TYPE
Final report

3. DATES COVERED *(From - To)*
1 Sep 2016 through 28 Feb 2017

4. TITLE AND SUBTITLE
Mathematical Methods for Predictive Simulation of Stochastic Turbulence Systems

5a. CONTRACT NUMBER
FA9550-16-1-0355

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Catalin Trenchea

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
UNIVERSITY OF PITTSBURGH THE 3520 FIFTH AVE
PITTSBURGH PA 15213-3320

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
OFC OF NAVAL RSCH (ONRRO) CHICAGO
CHICAGO REGIONAL OFFICE
230 SOUTH DEARBORN, ROOM 380 CHICAGO IL 60605-1595

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT

We use a probability theory approach for uncertainty quantification (UQ) and focus on the broad research areas of algorithmic development and numerical analysis for the discretization of systems of linear or nonlinear SPDEs. We conduct comprehensive theoretical and computational comparison of the efficiency, accuracy, and range of applicability of non-intrusive methods (stochastic collocation methods) and intrusive techniques (stochastic Galerkin methods) for solving SPDEs and for UQ applications. The parameter identification problem provides a very useful mechanism for determining

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:

a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
					19b. TELEPHONE NUMBER *(Include area code)*

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MATHEMATICAL METHODS FOR PREDICTIVE SIMULATION OF STOCHASTIC TURBULENCE SYSTEMS

AFOSR GRANT FA 9550-16-1-0355

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Abstract

Mathematical modeling and computer simulations are nowadays widely used tools to predict the behavior of problems in engineering and in the natural and social sciences. All such predictions are obtained by formulating mathematical models and then using computational methods to solve the corresponding problems.

We use a probability theory approach for *uncertainty quantification* (UQ) since it is particularly well suited for SPDE models, and focus on the broad research areas of algorithmic development and numerical analysis for the discretization of systems of linear or nonlinear SPDEs, building upon and significantly extending our previous successful work.

We conduct comprehensive theoretical and computational comparison of the efficiency, accuracy, and range of applicability of *non-intrusive* methods, such as stochastic collocation methods, and *intrusive* techniques, such as stochastic Galerkin methods, for solving SPDEs and for UQ applications.

We extend the algorithmic and analysis advances wrought by these efforts to the even more challenging settings of optimal control and parameter identification problems for SPDEs. The parameter identification problem is especially important in the SPDE setting since it provides a very useful mechanism for determining statistical information about the input parameters from, e.g., measurements of output quantities. This effort builds on our previous work on adjoint and sensitivity-based methods for deterministic optimal control and parameter identification problems to develop similar methods for tracking statistical quantities of interest from the computational solutions of linear and nonlinear SPDEs driven by high-dimensional random inputs.

Status/Progress

We have developed approaches to modeling turbulence and predicting uncertainty in turbulence models. However, the current situation is that, even with the current best UQ algorithms, doing a full turbulent flow computation including generating the full PDF of both initial, parametric/model and forcing uncertainty for a full simulation of a complex flow (typical in engineering flows) over a long time interval is not possible within time and resource constraints.

Many applications central to predictive CFD today face the challenge of computing multiple realizations. These include modeling non-fully resolved processes with stochastic terms, Uncertainty Quantification, estimation of sensitivities, control, parameter identification, increasing skill of predictions and accounting for the effects of uncertain data and models. The fundamental and intractable issue is that each realization of a 3d, complex (often turbulent) flow can require large amount of computing time (even weeks) while performing enough realizations to generate a full PDF can require thousands of realizations. This is the fundamental and intractable competition between computing ensembles and the resolution required for a single accurate realization. The avoidance of addressing competition explains the very many papers on UQ in computational fluid dynamics that have tests limited to the 1d Burgers equation.

In the proposed research we continued the development of novel algorithms to address the choke point issues faced in modern computational fluid dynamics at the chaotic crossroads where theory and application meet. At this crossroads, data is uncertain and models must incorporate the effects of unresolved processes through various parameterization schemes. Both introduce uncertainty which must be quantified and impose a finite predictability horizon. Estimating uncertainty and extending predictability both require substantial ensemble calculations. Computing ensembles of flow data when each realization requires a fine mesh for accuracy introduces the conflict between high resolution single realizations and computing and ensemble of sufficient size for accurate statistics. One specific realization of this research is as follows. The main uncertainty in groundwater flow is the unknown and unknowable porous matrix.

The research performed by **Roxana Tanase** *in her Ph.D. thesis was to develop algorithms for estimating spatially varying permeability for elliptic and parabolic groundwater flow equations using Kalman filter Markov chain Monte Carlo and adjoint variable based algorithms. These algorithms [1, 2, 3, 4] were fully validated through analysis, error estimates and numerical simulations.*

The focus of her study was to analyze methods for the optimal control / parameter identification of systems governed by partial differential equations with random input data. She considered several identification objectives that either minimize the expectation of a tracking cost functional or minimize the difference of desired statistical quantities in the appropriate spatial-L^p *norm (including higher order moments, hence allowing to match any statistics, e.g., the variance, skewness, kurtosis, etc.). One specific problem of parameter identification of a linear elliptic PDE that describes flow of a fluid in a porous medium with uncertain permeability field was examined in full detail. The numerical results reveal [6] the consequences of the moment-tracking approximation and the significant increase in efficiency of the method. The stochastic parameter identification algorithm integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation mixed-FEM approach. She also derived rigorous error estimates for the fully discrete problems, using the Fink-Rheinboldt theory for the approximation of solutions of a class of nonlinear problems.*

The fundamental approach to turbulence modelling in various applications begins with an ensemble of solutions which is statistically averaged. Computing a full ensemble has, until our current work, not been realizable. Thus various ergodic hypotheses have been invoked and statistical averaging converted to time averaging. Following this, models, such as k-epsilon, are developed for time averages of flow quantities. The models have developed this way because there was no other path for progress. However, it has long been recognized that the assumption ergodicity is fundamentally false in the naïve form in which it has been applied. Further there are simple flows which are at statistical equilibrium that cannot ever be at steady state and thus equivalence of statistical and time averages once again fails. Clearly what is needed is a good theory that give a mathematically precise proof of ergodicity. Such a proof also gives very valuable information of how ergodicity fails and what extra terms must be incorporated into models when naïve ergodicity fails. There has been some recent progress in developing such a theory by Hairer and Mattingly. Again, the value of such a theory lies in its certainty and in its delineation of how models must be adapted to account for cases where ergodicity fails in its naïve setting.

Yong Li *developed ergodicity results [7] for the two-dimensional stochastic Boussinesq equation: formulated the problem in an appropriate functional setting and proved existence and uniqueness, via an approximating regularizing scheme. He also proved the existence of an invariant measure corresponding to the stochastic flow* $t \to (u(t), \theta(t))$ *an its uniqueness via coupling methods.*

Acknowledgement/Disclaimer

This work was sponsored (in part) by the Air Force Office of Scientific Research, USAF, under grant/contract number FA 9550-16-1-0355. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

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Yong Li	Graduate student, Univ. of Pittsburgh (currently Associate at Goldman Sachs)
Roxana Tanase	Graduate student, Univ. of Pittsburgh
Catalin Trenchea	Associate Professor, Univ. of Pittsburgh

Publications

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Honors & Awards Received

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