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# Computational Methods for Predictive Simulation of Stochastic Turbulence Systems

Catalin Trenchea
UNIVERSITY OF PITTSBURGH

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Final Report

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**14. 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.

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# GENERALIZED MATHEMATICAL AND COMPUTATIONAL METHODS FOR PREDICTIVE SIMULATION OF STOCHASTIC TURBULENCE SYSTEMS

## AFOSR GRANT FA 9550-12-1-0191

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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 fundamantal 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.

This competition thus introduces at least 3 problems where fundamental mathematical analysis is required for sufficient progress to have an impact on real applications: 1. Predictive algorithms are needed to reduce the cost of computing ensembles more than just incrementally. Analysis of the algorithms is critical because simple (evolutionary) approaches only trade lower cost per step for stability issues that create a need for many more time steps. Only careful analysis can delineate the precise balance between stability and complexity. 2. In cases where thousands of realizations are not possible within time and resource constraints, generation of a full PDF, while ideal, is impossible. Thus, the theoretical issue shifts to the question of what information can be reliably extracted from many fewer (hundreds or even tens) of realizations. We addressed analyzed ensemble algorithms for complex flows: improving models and algorithms for UQ for turbulence to expand their range of applicability. This hinges on further development of algorithms for breaking the competition of high resolution single realizations and computing ensembles. The first such algorithms known in the scientific literature were developed in the current AFOSR project.

Ensemble simulation algorithms reconnect numerics with the highly developed statistical theory of turbulence since it allows direct calculation of important quantities from the theory such as turbulent intensities, effective Lyapunov exponents (predictability), the self-organization hypothesis. The models and analysis developed in this project are the first for which a models solution has been proven rigorously to converge to statistical equilibrium and thus may have implications for the problem of spinup of atmosphere and ocean models.

Coupled flow problems arise in many setting of scientific, technological and engineering interest and uncertainty quantification for complex flows increases in importance and difficulty with problem complexity. The goal of this project is to develop practical methods for UQ of complex, even turbulent, flows. This means the fundamental problem of the cost of each realization must be addressed. This development has several sub-directions such as modeling of non-statistically steady turbulence and a new modular turbulence modeling approach. The methods developed included new approaches, distinct from the traditional monolithic solution methods and tailored for the real needs of applications. 1. Development of a theory of partitioned methods and new partitioned methods for the fluid flow problems. This theory differentiated between two separate approaches to partitioning based on so called IMEX methods and splitting methods. Analysis of stability and errors over long time intervals and for small parameters was performed. 2. The first rigorous energy analysis of time filters for evolution equations. This theory explains anomalies observed and reported in practical CFD computations. Interestingly, some anomalies previously thought to be due to nonlinear effects and nonlinear instabilities were shown to be linear phenomena. The extension of modular nonlinear filters modeling of turbulence to the near wall region in turbulent flows was accomplished.

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## Publications

REFERENCES

[1] Martina Bukač, W. Layton, C. Trenchea, **Marina Moraiti**, **Hoang Tran**, Analysis of partitioned methods for Biot system, *Numerical Methods for Partial Differential Equations* 31 (2015), no. 6, 1769-1813.

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[33] Max Gunzburger, Catalin Trenchea and Clayton G. Webster, Error estimates for a generalized stochastic collocation approach to identification and control problems for random elliptic PDEs, submitted (2015).

## Honors & Awards Received

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