



Goal-Oriented Probability Density Function Methods for Uncertainty Quantification

Daniele Venturi

BROWN UNIVERSITY IN PROVIDENCE IN STATE OF RI AND PROVIDENCE PLANTATIONS

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Final Report

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14. ABSTRACT During the performance period of the grant we developed the proposed goal-oriented probability density function method based on the Mori-Zwanzig formulation and applied it to stochastic partial differential equations (SPDEs) such as advection-reaction and Burgers equations. We also developed new algorithms to solve high-dimensional probability density function (PDF) equations and stochastic domain decomposition techniques to propagate uncertainty across heterogeneous domains. The main findings can be summarized as follows: The Mori-Zwanzig approach has the potential to overcome well-known limitations encountered in stochastic simulations of high-dimensional random systems, in particular the curse of dimensionality and the lack of regularity of the solution. This comes at the price of solving complex integro-differential PDEs whose computability relies on either analytical approximations or data-driven approaches. The new methods we developed for high-dimensional PDF equations can be used in many different disciplines, ranging from optimal control under uncertainty of nonlinear dynamical systems to plasma dynamics (numerical solution to the full Boltzmann equation).					
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Final Report

Goal-Oriented Probability Density Function Methods for Uncertainty Quantification

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1 Summary

During the performance period of the grant we developed the proposed goal-oriented probability density function method based on the Mori-Zwanzig formulation and applied it to stochastic PDEs such as advection-reaction and Burgers equations (see **section 1.2.1**). We also developed new algorithms to solve high-dimensional probability density function (PDF) equations (see **section 1.2.2**) and stochastic domain decomposition techniques to propagate uncertainty across heterogeneous domains. These research efforts resulted in two papers published in the Proceedings of the Royal Society of London A, two papers under review during performance period (one published now and one in press) and one book chapter (now in press). The main findings can be summarized as follows: The Mori-Zwanzig approach has the potential to overcome well-known limitations encountered in stochastic simulations of high-dimensional random systems, in particular the curse of dimensionality and the lack of regularity of the solution. This comes at the price of solving complex integro-differential PDEs - the Mori-Zwanzig equations - whose computability relies on either analytical approximations or data-driven approaches. We investigated the accuracy of analytical techniques based Kubo-Van Kampen operator cumulant expansions for Langevin equations driven by fractional Brownian motion and other noises, stochastic advection-reaction equations and stochastic Burgers equation. In the context of the Burgers equation, we studied numerically one- and two-point MZ-PDF equations and computed the statistical properties of random shock waves generated by high dimensional random initial conditions and random additive forcing terms. We also addressed the problem of computing the numerical solution to high-dimensional PDF equations. To this end, we developed three different classes of new algorithms: 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 (ADI) methods. The second class of algorithms relies on a truncation the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of coupled probability density function equations. The third class of algorithms is based on high-dimensional model representations, e.g., ANOVA and probabilistic collocation methods. A common feature of all these approaches is that allow us to compute the solution of high-dimensional PDF equations via a sequence of low-dimensional problems. This is a very important question which will find its way in many related works. For instance, we are currently using the alternating direction Galerkin method we developed for high-dimensional PDF equations in the context of stochastic optimal control. i.e., optimal control under uncertainty of nonlinear dynamical systems, and plasma dynamics (solution to the full Boltzmann equation).

1.1 Published Papers and Book Chapters

1. D. Venturi, H. Cho and G. E. Karniadakis, “Mori-Zwanzig approach to uncertainty quantification”, *Springer Handbook on Uncertainty Quantification*, 2016 In Press
2. H. Cho, X. Yang, D. Venturi and G. E. Karniadakis, “Numerical methods for propagating uncertainty across heterogeneous domains”, *SIAM J. Sci. Comput.*, 2015, In Press.
3. H. Cho, D. Venturi and G. E. Karniadakis, “Numerical methods for high-dimensional probability density function equations”, *J. Comput. Phys.*, 2016, **315**, pp. 817-837.
4. H. Cho, D. Venturi and G. E. Karniadakis, “Statistical analysis and simulation of random shocks in stochastic Burgers equation”, *Proc. R. Soc. A*, 2014, 470 (2171), pp. 1-21.
5. D. Venturi and G. E. Karniadakis, “Convolutionless Nakajima-Zwanzig equations for stochastic analysis in nonlinear dynamical systems”, *Proc. R. Soc. A*, 2014, **470** (2166), pp. 1-20.
6. D. Venturi and G. E. Karniadakis, “Convolutionless Nakajima-Zwanzig equations for stochastic analysis in nonlinear dynamical systems”, *Proc. R. Soc. A*, 2014, , 470 (2166) Supplement, pp. 1-13.

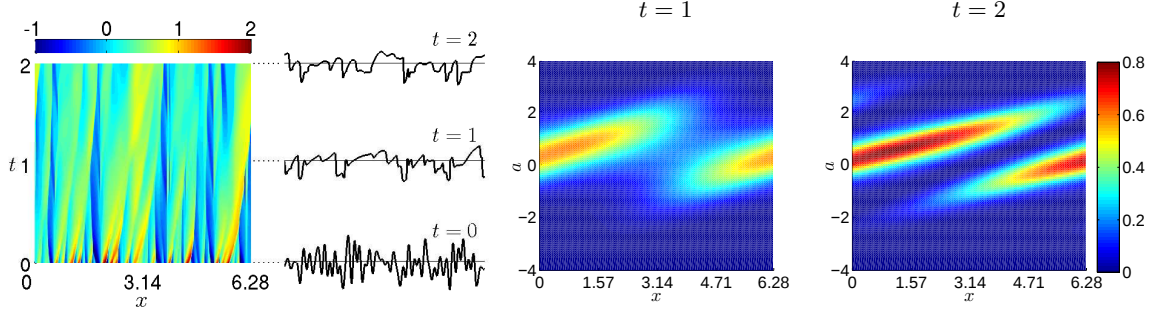


Figure 1: Stochastic Burgers equation. One realization of the velocity field computed by using adaptive discontinuous Galerkin methods (left). Time snapshots of the one-point PDF obtained by solving the MZ-PDF equation (1).

1.2 Research Accomplishments

In this section we would like to summarize some of the research accomplishment we have published in the papers listed above, in particular in Ref. [3] and Ref. [4]

1.2.1 Mori-Zwanzig Equations for Burgers Turbulence

The MZ-PDF approach allows us to systematically eliminate degrees of freedom from nonlinear random system, to obtain formally exact equations for quantities of interest. In the context of randomly forced Burgers turbulence, this allows us to derive exact equations for the one-point PDF of the velocity field by formally integrating out random noise of small amplitude or small correlation length. The result of such integration can be represented as a perturbation expansion in powers of a suitable coupling constant, e.g., noise amplitude. The result is

$$\begin{aligned} \frac{\partial p_u(t)}{\partial t} = & L_0 p_u(t) + \sigma \langle f(x, t) \rangle \frac{\partial p_u(t)}{\partial a} + \\ & \sigma^2 \left[\int_0^t \left\langle f(x, t) \frac{\partial}{\partial a} e^{(t-s)L_0} f(x, s) \right\rangle \frac{\partial}{\partial a} e^{-(t-s)L_0} ds \right] p_u(t) + \dots, \end{aligned} \quad (1)$$

where $p_u(t) = p(x, t, a)$ is the one-point one-time PDF of the velocity field (a is the phase-space coordinate associated with u), and L_0 is the linear operator

$$L_0 = - \int_{-\infty}^a da \frac{\partial}{\partial x} - a \frac{\partial}{\partial x}. \quad (2)$$

In Figure 2 we compare the PDF dynamics obtained by solving Eq. (1) with Monte Carlo simulation. It is seen that, as we increase the amplitude σ of the forcing term, the first- and second-order truncations of equation (1) lose accuracy. However, if we include more terms in the perturbation series we can get as close as we like to the MC results - provided we re-normalize the perturbation series.

In summary, the MZ-PDF framework allows us to study the statistical properties of the solution to the stochastic Burgers equation subject to random space-time perturbations and random initial conditions. This includes random shock waves in both physical and probability spaces (see the results in Ref. [4]). The mathematical methods and algorithms we developed for the Burgers equation can be applied to other randomly forced conservation laws, potentially leading to new insights in high-dimensional stochastic dynamics and more efficient computational techniques.

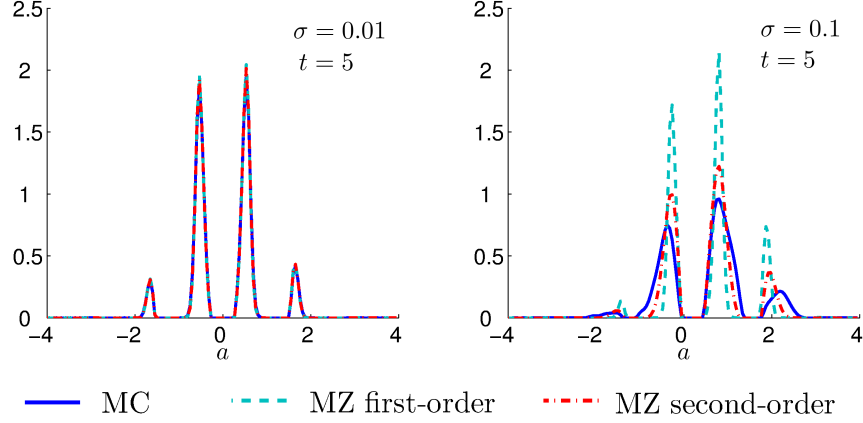


Figure 2: Stochastic Burgers equation. One-point PDF of the velocity field at $x = \pi$ for exponentially correlated, homogeneous (in space) random forcing processes with correlation time 0.01 and amplitude $\sigma = 0.01$ (left plot) and $\sigma = 0.1$ (right plot). Shown are results obtained from MC, and from two different truncations of the MZ-PDF equation (1).

1.2.2 Numerical Methods for High-Dimensional PDF equations

In this section I would like to briefly discuss the research accomplishments in the context of numerical methods for high-dimensional probability density function equations. In particular, I would like to highlight a new class of adaptive algorithms based on separated series expansions (SSE) which yield a sequence of low-dimensional problems that can be solved recursively and in parallel by using alternating direction methods. The mathematical details of the new algorithms are described in Ref. [3] above. Given a high-dimensional PDF evolution equation

$$\frac{\partial p}{\partial t} = Lp, \quad (3)$$

where L is a linear differential operator, we look for a representation of the solution $p = p(x_1, \dots, x_n, t)$ as a summation of separable functions, i.e.,

$$p(x_1, \dots, x_n, t) = \sum_{r=1}^R p_t^{(r)}(t) \prod_{j=1}^n p_i^{(r)}(x_i) \quad (4)$$

In this way, we can determine the unknown functions $p_t^{(r)}$ and $p_i^{(r)}$ ($1, \dots, n$) by using an alternating-direction weighted residual formulation, - in particular an alternating direction Galerkin method. In this way, the computational cost of solving high-dimensional PDF equations scales *linearly* with the dimension of the PDF and the algorithm can be parallelized with asynchronous updates - we are currently working on this. We applied the alternating-direction Galerkin method to a variety of PDF equations, including prototype equations in high-dimensional parameter spaces, e.g.

$$\frac{\partial p}{\partial x} = - \left(\sin(t) \sum_{k=1}^m \frac{1}{5(k+1)} \sin((k+1)x)b_k \right) \frac{\partial p}{\partial a}. \quad (5)$$

This equation involves two phase variables (x and a), and m parameters (b_k). Equation (5) represents the one-point PDF formulation of a randomly forced advection problem in one spatial dimension. To compute

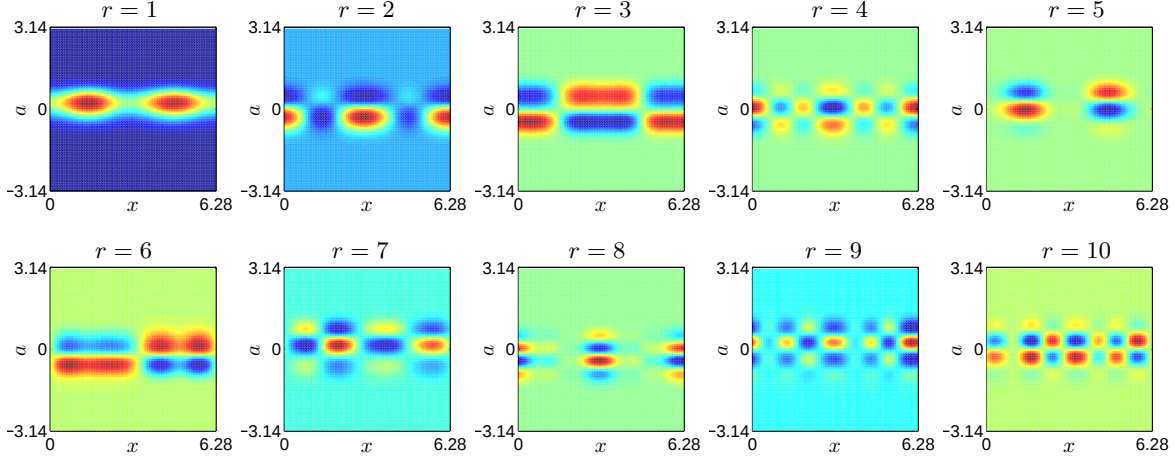


Figure 3: PDF equation (5): series expansion modes $p^{(r)}(x, t, a)$ at $t = 2$.

the solution to such equation we look for a series expansion in terms of separated functions

$$p(x, t, a, b_1, \dots, b_m) = \sum_{r=1}^R p^{(r)}(x, t, a) \prod_{j=1}^m h_j^{(r)}(b_j), \quad (6)$$

and determine the unknowns $p^{(r)}(x, t)$ and $h_j^{(r)}$ by solving at most two-dimensional linear problems at each time step. In Figure 3 we show the modes $p^{(r)}(x, t)$ ($r = 1, \dots, 10$) we obtain at $t = 2$. The L2 error of the separated solution (6) relative to an analytical solution is shown in Figure 4 versus the number of parameters and for different separation ranks R . The main feature of the numerical methods we developed for high-dimensional PDF equations is that they allow us to compute their solution by solving a sequence of low-dimensional problems. This will find its way in many different applications, ranging from the Boltzmann equation to the Fokker-Plank and Liouville equations. In particular, we are currently using the separated series expansion method for *optimal control* of the Liouville equation, i.e., optimal control under uncertainty of nonlinear dynamical systems.

1.3 International Collaborations

During the reporting period of grant I invited Lucia Parussini, a young assistant professor from the department of Mechanical Engineering at University of Trieste, to join the Division of Applied Mathematics at Brown University from September 8 to October 4, 2014 and from May 13 to June 14, 2015. Lucia's visit was funded by Italy/US science and technology exchange program sponsored by AFOSR. For technical reason those fundings were added to the AFOSR grant I am reporting on. Lucia collaborated with me, Prof. Karniadakis and other members of the research group at Brown in developing new methods addressing the curse of dimensionality forward uncertainty quantification (UQ) problems. Specifically, she studied a multivariate Gaussian process regression approach that allows us to infer quantities of interest, including random functions and fields, in physical models governed by stochastic partial differential equations (SPDEs). We have results on stochastic Burgers, and Navier-Stokes equations indicating that the new method is accurate and can achieve speed-up factors of up to several orders of magnitude relative to classical UQ approaches. This was made possible by combining the output of variable-fidelity stochastic simulations (variable-fidelity in both models and probability space) in a Bayesian inference process that relies on recursive co-kriging. Lucia brought to the Division of Applied Math at Brown the expertise and the mathematical tools developed by the research group on optimization of Prof. Carlo Poloni at University of Trieste. Carlo is the owner of the

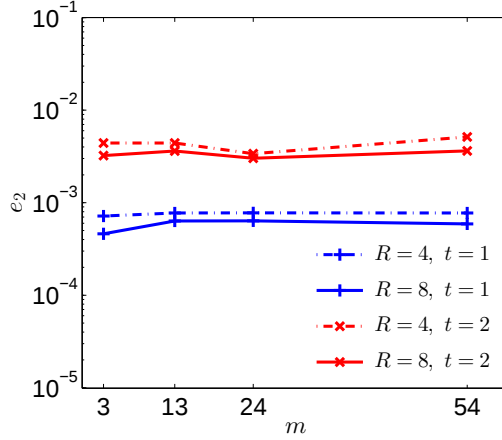


Figure 4: PDF equation (5): Relative L_2 errors of the separated series expansion of the solution relative to a benchmark solution. Shown are results for different number of parameters m and different separation ranks R in (6). It is seen that the accuracy of the separated expansion method mainly depends on the separation rank rather than on the number of random variables.

ESTECO company that developed the multi-objective and multi-disciplinary optimization software package *modeFrontier*. The collaboration with Lucia triggered AFOSR in the context of the Italy/US international initiative is still active and will continue in the years to come.

1.4 Invited Lectures, Conferences and Workshops

Hereafter, I provide a list of all invited lectures and talks I gave from the tentative start date of the project (Nov 1, 2013) to the final date (July 31, 2015). Note: not all lectures and conferences listed here were financially supported by AFOSR (see the cost breakdown section 1.5), but all of them involve the research work I performed in the context of the AFOSR project. I acknowledged support from AFOSR in all of them.

Invited Lectures in Universities

1. D. Venturi, “Information fusion in stochastic models of physical systems”, *Stanford University*, Palo Alto (CA), June 8, 2015.
2. D. Venturi, “Multi-fidelity stochastic modeling, simulation and information fusion in physical systems”, *Arizona State University*, Tempe (AZ), Mar. 25-27, 2015.
3. D. Venturi, “Coarse-graining high-dimensional random systems: the probability density function approach”, *University of Massachusetts Dartmouth*, Dartmouth (MA), Mar. 24, 2015.
4. D. Venturi, “A new paradigm for variable-fidelity stochastic modeling and information fusion in physical systems”, *University of California Santa Cruz*, Santa Cruz (CA), Feb. 2nd, 2015.
5. D. Venturi, “Spectral properties of random correlation operators”, *University of Massachusetts Amherst*, Amherst (MA), Dec. 10th, 2014.
6. D. Venturi, “Computing with uncertainty: coarse-graining stochastic dynamical models and PDF equations”, *University of California Santa Cruz*, Santa Cruz (CA), Nov. 24th, 2014.

7. D. Venturi, "Reduced-order methods for probability density function equations", *University of Massachusetts Amherst*, Amherst (MA), Nov. 4th, 2014.
8. D. Venturi, "Recent developments on reduced-order methods for high-dimensional kinetic equations", *North Carolina State University*, Raleigh (NC), Sep. 16th, 2014.
9. D. Venturi, "State variable versus probability density function methods in the stochastic modeling of nonlinear dynamical systems", *University of Delaware*, Delaware, Apr. 17th, 2015
10. D. Venturi, "Statistical analysis and simulation of random shock waves in Burgers turbulence", *George Washington University*, Washington DC, Apr. 7th, 2014.
11. D. Venturi, "A new framework for stochastic analysis in large scale simulations based on convolutionless Nakajima-Zwanzig PDF equations", *EPFL*, Lausanne (Switzerland), Dec. 19th, 2013.
12. D. Venturi, "Convolutionless Nakajima-Zwanzig PDF equations for stochastic analysis in large scale simulations", *Massachusetts Institute of Technology*, Boston (MA), Dec. 3rd, 2013.

Invited Talks in Conferences and Workshops

1. D. Venturi, Dimension reduction in kinetic equations: Mori-Zwanzig formulation, BBGKY hierarchies and effective propagators, *Houghton Conference on Non-Equilibrium Statistical Mechanics*, ICERM, Providence (RI), May 4-5th, 2015.
2. D. Venturi, Dimension reduction through the Mori-Zwanzig formulation, *SIAM Workshop on Dimension Reduction*, Penn State University, State College (PA), Mar. 21-24, 2015.
3. D. Venturi, A multi-fidelity data-driven paradigm for information fusion in physical and biological systems, *Pacific Northwest National Laboratory*, Richland (WA), March 13, 2015.
4. D. Venturi, Variable-fidelity stochastic modeling and calibration of multi-physics systems, *Schlumberger-Doll research center*, Boston (MA), Dec. 1, 2014.
5. D. Venturi, Statistical analysis and simulation of random shock waves in scalar conservation laws, *APS-DFD 2014*, San Francisco (CA), Nov. 23-25, 2014.
6. D. Venturi, MZ-PDF methods for UQ, *AFOSR Program Review in Computational Math.*, Arlington (VA), July 29-31, 2014.
7. D. Venturi, A new framework for stochastic analysis in large scale simulations based on goal-oriented probability density function methods, (Keynote Lecture) *WCCM/ECCOMAS*, Barcelona, July 20-25, 2014.
8. D. Venturi, MZ-PDF methods for stochastic analysis in nonlinear dynamical systems, *SIAM AN14*, Chicago, July 7-11, 2014
9. D. Venturi, Goal-oriented probability density function methods for uncertainty quantification, 2014 SIAM conference on uncertainty quantification *SIAM UQ14*, Savannah (GE), Mar. 31-Apr. 3, 2014.

1.5 Cost Breakdown

Hereafter, I provide a cost breakdown of the grant during the period of performance (8/1/2014 - 7/31/2015)

- PI effort - 3.19 months - \$17,311.94
- PI benefits - \$5,228.20
- International collaborations (**section 1.3**) - \$9,500
- Domestic Conferences, Workshops and Invited Talks (**section 1.4**) - \$3,382.19
 1. 11/4/14 - Invited talk at the University of Massachusetts Amherst - \$89.63
 2. 12/4/14 - APS-DFD and invited talk at UCSD - \$367.81
 3. 2/5/15 - Invited talk at UCSC - \$329.87
 4. 6/7/15 - Invited talk at Stanford University and UCSC - \$2,445.65
 5. 6/26/15 - Workshop at Woods Hole Oceanographic Institute - \$149.23
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1.

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Principal Investigator Name**The full name of the principal investigator on the grant or contract.**

Daniele Venturi

Program Manager**The AFOSR Program Manager currently assigned to the award**

Jean-Luc Cambier

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Abstract

During the performance period of the grant we developed the proposed goal-oriented probability density function method based on the Mori-Zwanzig formulation and applied it to stochastic PDEs such as advection-reaction and Burgers equations. We also developed new algorithms to solve high-dimensional probability density function (PDF) equations and stochastic domain decomposition techniques to propagate uncertainty across heterogeneous domains.

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equation. In the context of the Burgers equation, we studied numerically one- and two-point MZ-PDF equations and computed the statistical properties of random shock waves generated by high dimensional random initial conditions and random additive forcing terms. We also addressed the problem of computing the numerical solution to high-dimensional PDF equations. To this end, we developed three different classes of new algorithms: 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 (ADI) methods. The second class of algorithms relies on a truncation the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of coupled probability density function equations. The third class of algorithms is based on high-dimensional model representations, e.g., ANOVA and probabilistic collocation methods. A common feature of all these approaches is that allow us to compute the solution of high-dimensional PDF equations via a sequence of low-dimensional problems. This is a very important question which will find its way in many related works. For instance, we are currently using the alternating direction Galerkin method we developed for high-dimensional PDF equations in the context of stochastic optimal control. i.e., optimal control under uncertainty of nonlinear dynamical systems, and plasma dynamics (numerical solution to the full Boltzmann equation).

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Funding Summary by Cost Category (by FY, \$K)

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Supplies			
Total			

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