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Fast Numerical Methods for Stochastic Partial Differential Equations

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Fast Numerical Methods for Stochastic Partial Differential Equations

FA9550-12-1-0281

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Abstract

Uncertainty quantification has been an active research area in the past 15 years because of its potential of significant applications ranging from signal processing to aircraft wing designs. It is well understood that effective numerical methods for stochastic partial differential equations (SPDES) are essential for uncertainty quantification. In the last decade much progress has been made in the construction of numerical algorithms to efficiently solve SPDES with random coefficients and white noise perturbations. However, high dimensionality and low regularity are still the bottleneck in solving real world applicable SPDES with efficient numerical methods. This project is intended to address the numerical analysis as well as algorithm aspects of SPDES. Three major contributions are made in this project: i) Construction and convergence analysis of Quasi Monte Carlo based Particle Swarm Optimization (PSO) method; ii) Efficient adaptive domain sparse grid method for SPDES; iii) High order methods of SPDES via systems of forward backward stochastic differential equations. Our work contains algorithm constructions, rigorous error analysis, and extensive numerical experiments to demonstrate our algorithm efficiency and validity of our theoretical analysis.

1 Introduction

The overall goal of our AFOSR sponsored research program is to construct fast and efficient numerical algorithms for solving stochastic partial differential equations and apply them to solve nonlinear filtering problems and optimal control problems under SPDE constraints.

Uncertainty quantification has been an active research area in the past 15 years with many significant application potentials ranging from signal processing to aircraft wing designs. It is well understood that effective numerical methods for stochastic partial differential equations (SPDES) are essential for uncertainty quantification. In the last decade much progress has been made in the construction of numerical algorithms to efficiently solve SPDES with random coefficients and white noise perturbations. However, high dimensionality and low regularity are still the bottleneck in solving real world applicable SPDES with efficient numerical methods. This project is intended to address the numerical analysis as well as algorithm aspects of SPDES. The following are our main contributions during the funding period.

(i). *Quasi Monte Carlo based Particle Swarm Optimization (PSO) method.* Inspired by the social behavior of the bird flocking or fish schooling, the particle swarm optimization (PSO) is a population based stochastic optimization method developed by Eberhart and Kennedy in 1995. It has been used across a wide range of applications. Faure, Halton and Vander Corput sequences have been used for initializing the swarm in PSO. Quasirandom(or

low-discrepancy) sequences such as Faure, Halton, Vander Corput etc are deterministic and suffers from correlations between radical inverse functions with different bases used for different dimensions. In this paper, we investigate the effect of initializing the swarm with scrambled optimal Halton sequence, which is a randomized quasirandom sequence. This ensures that we still have the uniformity properties of quasirandom sequences while preserving the stochastic behavior for particles in the swarm. Numerical experiments are conducted with benchmark objective functions with high dimensions to verify the convergence and effectiveness of the proposed initialization of PSO.

(ii). *Efficient adaptive domain sparse grid method for SPDES* The key of constructing efficient numerical algorithms for SPDES is to overcome the obstacles of low regularity and high dimensionality, and the associated unbounded domain problem. In our construction, we used the importance sampling method to construct bounded domains for the Zakai equation with a very small number of sample points. Then we used the split up scheme to construct higher order numerical algorithm on sparse grid, which reduced the computing cost from $\mathrm{O}(n^d)$ to $\mathrm{O}(n \ln^d n)$.

(iii). *High order methods of SPDES via systems of forward backward stochastic differential equations.* ln this subproject, we overcome the problem of low regularity, by using a class of high order numerical methods. In this approach, instead of solving SPDEs, we solved an equivalent coupled system of forward and backward stochastic differential equations (BSDEs). A special class of Itô-Taylor formulas provides a high order solution to the system of BSDEs. This approach, which solves a system of stochastic *ordinary* differential equations, is fundamentally different and more powerful than existing methods. To the best of our knowledge, our proposed approach represents a first attempt to design high order numerical algorithms for SPDES.

2 Detailed description of our accomplishments

2.1 Quasi Monte Carlo based Particle Swarm Optimization (PSO) method

A PSO algorithm maintains a population of M particles, and places them in the search space of the objective function which may involved the solution of a SPDE. PSO defines each particle's position as a potential solution to the function to be optimized, and then searches for the optima by updating its position in every iterative step. Each particle is associated with a velocity which directs the flying of the particle toward a new, presumably better, position/solution. The particles fly through the problem space by following the current optimum particles. In every iteration, each particle's velocity is updated by following two "best" values. The first one is current best solution it has achieved so far. This value is called *pbest*. Another "best" value that is tracked by the particle swarm optimizer is the best value, obtained so far by any particle in the population. This best value is a global best and called *gbest*.

After finding the two best values, the particle updates its velocity and positions with following equations.

$$\vec{v}_{t+1} = w\vec{v_t} + c_1 r_{1,t+1}(\vec{pbest}_t - \vec{a_t}) + c_2 r_{2,t+1}(\vec{gbest}_t - \vec{a_t}).$$

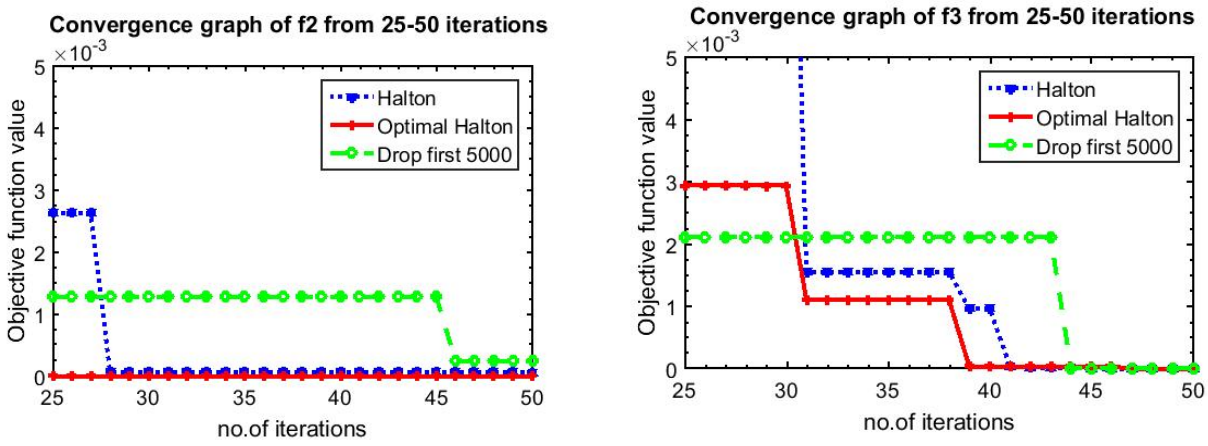

Figure 1: Convergence graph for function f2

$$\vec{a}_{t+1} = \vec{a_t} + \vec{v}_{t+1}.$$

The key to the success of the PSO is choosing the initial particles effectively. Traditional PSO methods use Monte Carlo samples for the initialization purpose, which may inherit the slow convergence feature of Monte Carlo methods. In our work, we use the quasi Monte Carlo methods to choose these initial particles [2]. A classical family of low-discrepancy sequences are Halton sequences which are bases on the radical inverse function defined as follows:

$$\phi_p(n) \equiv \frac{b_0}{p} + \frac{b_1}{p^2} + ... + \frac{b_m}{p^{m+1}}, \tag{1}$$

where p is a prime number and expansion of n in base b is given as $n = b_0 + b_1 p + ... + b_m p^m$, with integers $0 \leq b_j < p$.
Since Halton sequence X_n in $(0,1]^s$ is defined as

$$X_n = (\phi_{p_1}(n), \phi_{p_2}(n), ..., \phi_{p_s}(n)), \tag{2}$$

where $p_1, p_2, ..., p_s$ are pairwise co-primes. In practice, we always use the first s primes as the bases.

Comparison to other low-discrepancy sequences, Halton sequences are easier to implement. However, a problem with Halton sequence comes from the correlations between the radical inverse functions for different dimensions. The correlations cause the Halton sequence to have poor 2-D projection for some pairing coordinates. In order to improve the quality of Halton sequence, we use the scrambled Halton sequence tobreak the cycle and correlation among dimensions. Scrambled Halton sequence can help us to ignore the number of points and obtain good quality of Halton sequence. In Figure 1 we can see that the optimal Halton sequence significantly speed up the convergence of PSO.

2.2 Efficient adaptive domain sparse grid method for SPDES

In this project we are concerned with efficient numerical solutions of the Zakai equation, a parabolic SPDE, as follows.

$$\begin{cases} du(t,x) &= Lu(t,x)dt + \sum_{k=1}^{r} h_k^*(x)u(t,x)dY_t, \\ u(0,x) &= u_0(x), \quad x \in R^d, \end{cases} \tag{3}$$

where L is the infinitesimal generator associated with the state process X_t given by

$$Lu = \frac{1}{2}\sum_{i,j}^{d} \frac{\partial^2(\sigma\sigma^*)_{i,j}u}{\partial x_i \partial x_j} - \sum_{i=1}^{d} \frac{\partial b_i u}{\partial x_i}.$$

Zakai equation is a major tool of solving nonlinear filtering problems. One of the most effective methods of solving the Zakai equation is the split-up approximation scheme where the original Zakai equation is split into a second order deterministic partial differential equation in the prediction step, and a degenerate second order stochastic PDE in the update step. In the numerical simulation process of the split-up scheme, a prior PDF is obtained by solving the deterministic PDE at the prediction step; then this prior PDF is updated at the update step following an a posteriori criterion. The strength of the split-up is that it is a first order algorithm as opposed to most standard finite difference and finite element approximations which are half order, thus it alleviates the low regularity problem. However, high dimensionality and the unbounded domain are still the main obstacles for the Zakai filter to be an effective method of solving nonlinear filtering problems.

In this project, we constructed a fast split-up finite difference scheme for the Zakai equation using sparse grid and on adaptively chosen computational domains. Specifically, we use the importance sampling method to adaptively construct a bounded domain at each time step of the temporal discretization. This is a key novelty of our algorithm. Then we use the split-up finite difference scheme to solve the Zakai equation on sparse grids over these bounded adaptive domains. The hierarchical sparse grid method, which was originally created to approximate multi-variable functions, uses only $O(n\log^{d-1} n)$ number of grid points instead of $O(n^d)$ number of grid points for the standard full-grid approximation. Thus it has the potential of significantly alleviating the "curse of dimensionality" problem for moderately high dimensional problems.

To elaborate the basic idea of our proposed algorithm, we first create a partition $\mathcal{R}_t$ on $[0,T]$:

$$\mathcal{R}_t = \{t_n | t_n \in [0,T], t_n < t_{n+1}, n = 0,1,\cdots,N_T-1, t_0 = 0, t_{N_T} = T\}$$

and denote $\Delta t_n = t_{n+1} - t_n$, $n = 0,1,\cdots,N_T-1$. For $n = 0,1,\cdots N_T-1$, assume that u_n is the numerical solution of the Zakai equation at t_n. We will use the importance sampling method to draw M sample points, denoted by $\{p_n^m\}_{m=1,\cdots,M}$, according to the conditional PDF u_n of the state X_n. Then we propagate each of these samples from time step t_n to t_{n+1} using the *State Equation* in the nonlinear filtering problem (**??**) to get M updated sample points, denoted by $\{p_{n+1}^m\}_{m=1,\cdots,M}$. Let

$$\mathcal{D}_{n+\frac{1}{2}} = [a_{n+\frac{1}{2}}, b_{n+\frac{1}{2}}] \subset R^d$$

be the smallest box domain containing all the samples $\{p_{n+1}^m\}_{m=1}^M$ and $\Sigma = (\Sigma^1,\ldots,\Sigma^d)$ be the vector of marginal standard deviations of these samples. Then, for a user-defined positive

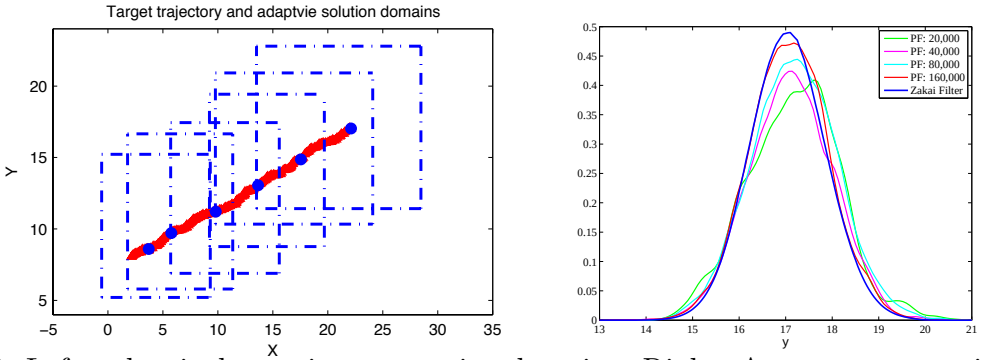

Figure 2: Left: adaptively moving computing domains. Right: Accuracy comparison between our method and the particle filter

constant λ we let

$$\begin{aligned} a_{n+1} &\doteq a_{n+\frac{1}{2}} - \lambda\Sigma \\ b_{n+1} &\doteq b_{n+\frac{1}{2}} + \lambda\Sigma \end{aligned} \tag{4}$$

and choose

$$\mathcal{D}_{n+1} = [a_{n+1}, b_{n+1}] \tag{5}$$

as the solution domain for u_{n+1}, which is the approximation of the support of u_{n+1}.

The idea of the adaptive selection of the solution domain $\mathcal{D}_n$ is similar to that in the prediction step of the particle filter method. As such the region $\mathcal{D}_{n+\frac{1}{2}}$ which includes all the updated samples is the support where the particle filter method builds the prior PDF of the target state. In our method, we choose a confidence region surrounding $\mathcal{D}_{n+\frac{1}{2}}$ as our solution domain. In this way, we can use a much smaller number of samples than the particle filter method and still maintain the accuracy of our algorithm.

In the next step, we use the split-up finite difference scheme on a sparse grid to approximate the Zakai equation on each adapted domain $\mathcal{D}_n$.

We conducted several numerical experiments to demonstrate our methodology in solving nonlinear filtering problems. The left subfigure of Figure 1 is the sketch of the moving domains at several different time steps. One can see that the size and location of the computing domain vary adaptively at different time steps. The right subfigure of Figure 1 are the graphs of marginal conditional PDFs at time $T = 1$ on the x coordinate using our algorithm for the Zakai filter as well as those obtained by the particle filter. From the graph we can see the convergence trend of the particle filter toward the one obtained by our algorithm. When the particle size is 160000, the solution generated by the particle filter is very close to our result while the results obtained by smaller sizes of particles are not quite accurate. In Table 1 we list the computing costs of the particle filter with different sizes of particles, the standard Zakai filter, and the Zakai filter with our algorithm.

We can conclude hat our adaptive Zakai filter algorithm has clear advantages over the particle filter: it is more accurate with the same computing cost and it is far more computationally efficient with the same accuracy.

2.3 Efficient and high order methods for SPDES through BSDES

One naturally asks if there is any way to systematically construct higher order numerical algorithms for nonlinear filtering problems. In this subproject, we answered this question by

Table 1: CPU time comparison

Method	CPU time (seconds)
Particle filter: 20,000 particles	554
Particle filter: 40,000 particles	1976
Particle filter: 80,000 particles	7703
Particle filter: 160,000 particles	32380
Standard Zakai filter	270954
Our adaptive Zakai filter	587

taking a completely different approach from existing methods: instead of solving the Zakai equation, we solve equivalent coupled forward–backward SDES. Then we construct a class of efficient and higher order numerical schemes for this coupled forward-backward system.

To describe the basic idea of our approach, we briefly describe the theoretical results we obtained in [**?**]. These results lay the foundation of our BSDE methods for solving SPDES. Through rigorous stochastic analysis we first derived a system of forward and backward SDEs (BSDEs) for (X_t, Q_t, Z_t)

$$\begin{cases} dX_s &= b(X_s)dt + \sigma_s dW_s, \qquad X_t = x, t < s < T, \quad \text{(SDE)} \\ dQ_s &= Z_s dW_s - g(X_s)Q_s dV_s, \quad Q_T = \Phi(X_T). \quad \text{(BSDE)} \end{cases} \tag{6}$$

Here W_t and V_t are two independent Brownian motions. The first equation in (6) is a forward SDE while the second equation is a backward SDE. One may suspect that (6) is under-determined because it has two equations but three unknown stochastic processes X_t, U_t and Z_t. However, under the constraint that X_t, U_t and Z_t are adapted to some filtrations generated by B_t and W_t, they can be uniquely determined.

We have a constructed a number of numerical algorithms to demonstrate efficient of our BSDE approach of solving SPDES. Here we outline the derivation of the first order scheme for a general coupled system of forward-backward SDEs [1]:

$$\begin{cases} dX_s &= b(X_s)ds + \sigma(X_s)dW_s, \quad t \le s \le T, \\ dY_s &= +f(s, X_s, Y_s)ds \\ & \quad +g(s, X_s, Y_s)\overleftarrow{dB_s} - Z_s dW_s, \quad t \le s \le T, \\ X_t &= x, \\ Y_T &= h(X_T). \end{cases} \tag{7}$$

For simplicity we assume that $b = 0$, $\sigma = I$, and g depends on t and Y only. For this simple case, the two sided Itô-Taylor expansion for g is given by

$$\begin{aligned} g(t, y_t) &= g(0, y_0) - \int_0^t g'_y(s, y_s) \cdot g d\overleftarrow{B}_s \\ &\quad + \textstyle\int_0^t g'_y(s, y_s) \cdot z_s dW_s - \int_0^t g'_y(s, y_s) \cdot f_s ds \\ &\quad - \frac{1}{2}\int_0^t g''_{yy}(s, y_s \cdot g^2)ds + \frac{1}{2}\int_0^t + g''_{yy}(s, y_s) \cdot z_s^2 ds. \end{aligned} \tag{8}$$

So for a first order algorithm, the last three terms are the "higher order" terms and can be dropped in the numerical algorithm. Specifically, if $t_i = i\Delta t$, $i = 0, \cdots, N$ is a uniform

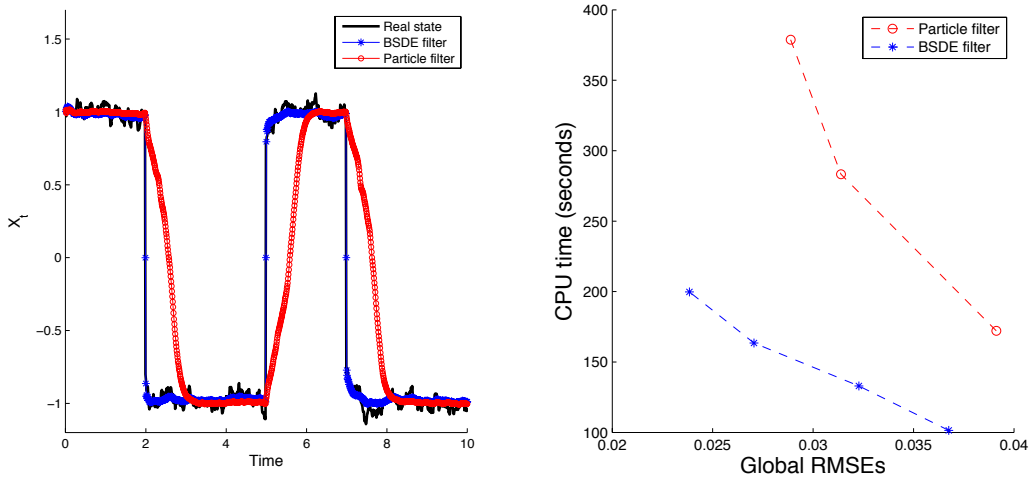

Figure 3: Comparison between the particle filter and BSDE filter: Left: accuracy comparison in simulating the wells. Right: computing complexity comparison

partition of $[0, T]$, then

$$\begin{aligned} g(t_n, Y(t_n)) &= g(t_{n+1}, Y(t_{n+1})) - g'_y(t_{n+1}, Y(t_{n+1})) \cdot Z(t_{n+1}) \Delta W_{n+1} \\ &\quad + g'_y(t_{n+1}, Y(t_{n+1})) \cdot g(t_{n+1}, Y(t_{n+1})) \Delta B_{t_{n+1}} + O(\Delta t). \end{aligned}$$

To complete the construction of the algorithm we need to eliminate the Z term in the above equation. This can be done by taking the conditional expectation $E(\cdot|\mathcal{F}^x_{t,s})$ where $\mathcal{F}^x_{s,t} := \sigma(x + W_r; t \le r \le s) \vee \sigma(W_t) \vee \sigma(B_t; 0 \le t \le T)$. Then after some manipulations of the noise terms we derived the algorithm for the approximate solution Y_n and Z_n as follows.

$$\begin{aligned} Y_n &= Y_{n+1} + \Delta t E[f(t_{n+1}, Y_{n+1}) - \frac{1}{2} g'_y(t_{n+1}, Y_{n+1}) \cdot g(t_{n+1}, Y_{n+1})] \\ &\quad + \tfrac{1}{2} E[g(t_{n+1}, Y_{n+1}) + g'_y(t_{n+1}, Y_{n+1}) \cdot g(t_{n+1}, Y_{n+1})] \Delta B_{t_{n+1}} \\ \Delta t_n Z_n &= E[Y_{n+1} \Delta W_{t_{n+1}}] + \Delta t_n \cdot E[f(t_{n+1}, Y_{n+1}) \Delta W_{t_{n+1}}] \\ &\quad + \Delta B_{t_{n+1}} \cdot (E[g(t_{n+1}, Y_{n+1}) \Delta W_{t_{n+1}}]. \end{aligned}$$

We proved in [1] that the mean square error is $O(\Delta t)$ for Y_n.

Theorem (*Bao, Cao, Meir, Zhao, SIAM J.U.Q. 2015*) Under some regularity condition of functions f and g, the convergence rate of above algorithm is first order:

$$\max_{0 \le n \le N-1} E[(Y^n - Y_{t_n})^2] \le C(\Delta t)^2.$$

In our numerical experiments, we apply our BSDE method to solve nonlinear filtering problem. As can be seen from the left subfigure of Figure 3, our BSDE filter simulate the switch much better than the particle filter. From the right subfigure of Figure 3, we can see that with the same root mean square error, our BSDE based PDF filter requires far less CPU time than the particle filter. More importantly, our BSDE filter requires far few steps than that in the particle filter to complete the switch, which makes our method far more efficient than the particle filter.

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[2] Ganesha Weerasinghe, Hongmei Chi and Yanzhao Cao, Particle Swarm Optimization Simulation via Optimal Halton Sequences, accepted by ***Procedia Computer Science*** (2016).

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4 Publications

1. Ganesha Weerasinghe, Hongmei Chi and Yanzhao Cao, Particle Swarm Optimization Simulation via Optimal Halton Sequences, accepted by ***Procedia Computer Science*** (2016).

2. Haiyan Tian, Hongmei Chi and Yanzhao Cao, Comparing two types of bases for solving elliptic boundary value problems, **Neural, Parallel, and Scientific Computations**, Vol. 23, 411–420 (2015).

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Principal Investigator Name

The full name of the principal investigator on the grant or contract.

Hongmei Chi

Program Manager

The AFOSR Program Manager currently assigned to the award

Farina Fahroo

Reporting Period Start Date

07/01/2012

Reporting Period End Date

12/31/2015

Abstract

Uncertainty quantification has been an active research area in the past 15 years because of its potential of significant applications ranging from signal processing to aircraft wing designs. It is well understood that effective numerical methods for stochastic partial differential equations (SPDES) are essential for uncertainty quantification. In the last decade much progress has been made in the construction of numerical algorithms to efficiently solve SPDES with random coefficients and white noise perturbations. However, high dimensionality
and low regularity are still the bottleneck in solving real world applicable SPDES with efficient numerical methods. This project is intended to address the numerical analysis as well as algorithm aspects of SPDES. Three major contributions are made in this project: i) Construction and convergence analysis of Quasi Monte Carlo based Particle Swarm Optimization (PSO) method; ii) Efficient adaptive domain sparse grid method for SPDES; iii) High order methods of SPDES via systems of forward backward stochastic differential equations. Our work contains algorithm constructions, rigorous error analysis, and extensive numerical experiments to demonstrate our algorithm efficiency and validity of our theoretical analysis.

Distribution Statement

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Archival Publications (published) during reporting period:

Haiyan Tian, Hongmei Chi and Yanzhao Cao, Comparing two types of bases for solving elliptic boundary value problems, Neural, Parallel, and Scientific Computations, Vol. 23, 411–420 (2015).

Hongmei Chi, Peter Beerli: Quasi-Monte Carlo method in population genetics param- eter estimation. Mathematics and Computers in Simulation 103: 33-38 (2014).

Hongmei Chi, Generation of parallel modified Kronecker sequences. Monte Carlo Meth. and Appl. 19(4): 261-271 (2013).

Cao, Yanzhao; Zhang, Ran; A stochastic collocation method for stochastic Volterra equations of the second kind. J. Integral Equations Appl. 27 (2015), no. 1, 1–25.

Bao, Feng; Cao, Yanzhao; Webster, Clayton; Zhang, Guannan A hybrid sparse-grid ap- proach for nonlinear filtering problems based on adaptive-domain of the Zakai equation approximations. SIAM/ASA J. Uncertain. Quantif. 2 (2014), no. 1, 784–804.

Cao, Yanzhao; Wang, Peng; Wang, Xiaoshen Homotopy continuation methods for stochastic two-point boundary value problems driven by additive noises. J. Comput. Math. 32 (2014), no. 6, 630–642.

Bao, Feng; Cao, Yanzhao; Han, Xiaoying An implicit algorithm of solving nonlinear filtering problems. Commun. Comput. Phys. 16 (2014), no. 2, 382–402.

Changes in research objectives (if any):

Change in AFOSR Program Manager, if any:

The Program Manager has been changed from Dr. Fariba Fahroo to Dr. Jean-Luc Cambier

Extensions granted or milestones slipped, if any:

Extension was granted from June 30, 2015 to December 31, 2015.

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

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

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

Report Document - Text Analysis

Appendix Documents

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