



Spline-Based Stochastic Collocation Methods for Uncertainty Quantification in Nonlinear Hyperbolic PDEs

Alina Chertock¹ , Arsen S. Iskhakov² , Safa Janajra¹ ,
and Alexander Kurganov³

¹ Department of Mathematics, North Carolina State University, Raleigh, NC, USA
chertock@math.ncsu.edu, sjanajr@ncsu.edu

² Department of Mechanical and Nuclear Engineering, Kansas State University,
Manhattan, KS, USA
aishhak@ksu.edu

³ Department of Mathematics, Shenzhen International Center for Mathematics, and
Guangdong Provincial Key Laboratory of Computational Science and Material
Design, Southern University of Science and Technology, Shenzhen, China
alexander@sustech.edu.cn

Abstract. In this paper, we study the stochastic collocation (SC) methods for uncertainty quantification (UQ) in hyperbolic systems of nonlinear partial differential equations (PDEs). In these methods, the underlying PDEs are numerically solved at a set of collocation points in random space. A standard SC approach is based on a generalized polynomial chaos (gPC) expansion, which relies on choosing the collocation points based on the prescribed probability distribution and approximating the computed solution by a linear combination of orthogonal polynomials in the random variable. We demonstrate that this approach struggles to accurately capture discontinuous solutions, often leading to oscillations (Gibbs phenomenon) that deviate significantly from the physical solutions. We explore alternative SC methods, in which one can choose an arbitrary set of collocation points and employ shape-preserving splines to interpolate the solution in a random space. Our study demonstrates the effectiveness of spline-based collocation in accurately capturing and assessing uncertainties while suppressing oscillations. We illustrate the superiority of the spline-based collocation on two numerical examples, including the inviscid Burgers and shallow water equations.

1 Introduction

Numerous scientific problems encompass inherent uncertainties arising from a variety of factors. Within the context of partial differential equations (PDEs), uncertainties can be characterized using random variables. This study focuses on hyperbolic systems of conservation and balance laws, examining their behavior under uncertain conditions. In the one-dimensional (1-D) case, the formulation of these systems is expressed as

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{S}(\mathbf{U}), \quad (1)$$

where x is the spatial variable, t is time, $\mathbf{U}(x, t; \xi) \in \mathbb{R}^m$ is an unknown vector-function, $\mathbf{F}(\mathbf{U}) : \mathbb{R}^m \rightarrow \mathbb{R}^m$ are the flux functions, and $\mathbf{S}(\mathbf{U})$ is a source term. Furthermore, we assume that $\xi \in \Xi \subset \mathbb{R}$ are real-valued random variable with (Ξ, \mathcal{F}, ν) being the underlying probability space. Here, Ξ is a set of events, $\mathcal{F}(\Xi)$ is the σ -algebra of Borel measurable sets, and $\nu(\xi) : \Xi \rightarrow \mathbb{R}_+$ is the probability density function (PDF), $\nu \in L^1(\Xi)$.

The system (1) emerges in various applications, such as fluid dynamics, geophysics, electromagnetism, meteorology, and astrophysics. It is crucial to assess uncertainties inherent in input quantities, as well as in the initial and boundary conditions resulting from empirical approximations or measurement errors. This quantification is vital for performing the sensitivity analysis and offers valuable insight to improve the accuracy of the studied model.

This paper focuses on developing accurate and robust numerical techniques for quantifying uncertainties in (1). Among the various existing methods, Monte Carlo-type methods (see, e.g., [1, 13]) are reliable but computationally intensive due to the substantial number of realizations required to approximate statistical moments accurately. Another commonly used approach is based on generalized polynomial chaos (gPC) methods, in which the solution is expressed as a series of orthogonal polynomials with respect to the probability density in ξ [11, 14]. There are two types of gPC methods: intrusive and non-intrusive. Intrusive approaches, such as gPC stochastic Galerkin (gPC-SG) methods, substitute gPC expansions into the governing equations. These expansions are then projected using a Galerkin approximation to derive a system of deterministic PDEs for the expansion coefficients; see, e.g., [17, 18]. Solving these coefficient equations provides the statistical moments of the original solution of the uncertain problem. On the other hand, non-intrusive algorithms, such as gPC stochastic collocation (gPC-SC) methods, aim to satisfy the governing equations at discrete nodes, called collocation points, in the random space. They employ a deterministic numerical solver, utilizing interpolation and quadrature rules to numerically evaluate the PDF and/or statistical moments [16, 19].

The application of gPC-SG and gPC-SC methods to nonlinear hyperbolic systems (1) poses several challenges. Although spectral-type gPC-based methods exhibit rapid convergence for solutions that depend smoothly on random parameters, a significant issue arises when solutions contain shock waves and other nonsmooth structures, which is a generic case for nonlinear hyperbolic PDEs (even if initial data are smooth). Despite the discontinuities manifesting in the spatial variable, their propagation speed can be influenced by uncertainty, introducing discontinuities in the random variable and causing Gibbs-type phenomena [12]. Another unresolved matter involves representing strictly positive quantities, such as water depth in shallow water equations, and imposing discrete bound-preserving constraints [5, 6, 15].

In this paper, we concentrate on alternative spline-based stochastic collocation (SC) methods, which are positivity-preserving and do not suffer from Gibbs-type oscillations. The proposed methods utilize a solution obtained by a deterministic numerical solver implemented repeatedly on an arbitrarily selected set of collocation points in the random variable ξ . Specifically, at each collocation point, we solve the corresponding deterministic PDEs by a semi-discrete second-order central-upwind scheme from [9, 10]. As a result, at the final computational time, for each discrete value of the spatial variable x , we obtain an approximation of \mathbf{U} as a discrete function of ξ . Equipped with these point values, we employ spline-based interpolations in random space and use the obtained global (in ξ) solution to calculate the stochastic moments. In order to enforce the non-oscillatory and positivity-preserving properties of the interpolated solution, we use shape-preserving (SP) rational quartic splines from [21]. We conduct a comparative numerical study of the gPC-based and spline-based SC approaches to quantify uncertainties in (1). Our findings demonstrate the superior efficacy of the proposed spline-based SC methods when applied to the inviscid Burgers and shallow water equations.

2 Methodology

In this section, we describe the gPC- and spline-based SC approaches applied to (1).

We start by selecting a set of collocation points ξ_ℓ , $\ell = 1, \dots, L$ and numerically solving the following deterministic systems:

$$\mathbf{U}_t(x, t; \xi_\ell) + \mathbf{F}(\mathbf{U}(x, t; \xi_\ell))_x = \mathbf{S}(\mathbf{U}(x, t; \xi_\ell)), \quad \ell = 1, \dots, L, \quad (2)$$

until the final time T (one can use one's favorite numerical method for solving (2)). Then, for each discrete node of the spatial variable denoted below by \tilde{x} , we use either the gPC (§2.1) or spline (§2.2) interpolation to approximate the numerical solution and its stochastic moments, that is, the mean and variance or standard deviation for each component U of \mathbf{U} :

$$\begin{aligned} \mathbb{E}_\xi[U] &:= \int_{\Xi} U(\tilde{x}, T; \xi) \nu(\xi) d\xi, \\ \text{Var}[U] &:= \mathbb{E}_\xi[U^2] - \mathbb{E}_\xi[U]^2, \quad \sigma[U] := \sqrt{\text{Var}[U]}. \end{aligned} \quad (3)$$

2.1 gPC Interpolation

The gPC interpolation in random space represents the solution as a generalized discrete Fourier series in terms of orthonormal polynomials, $\{\Phi_i(\xi)\}_{i=0}^N$, selected based on the PDF:

$$U(\tilde{x}, T; \xi) \approx \mathbf{U}^N(\tilde{x}, T; \xi) := \sum_{i=0}^N \widehat{U}_i(\tilde{x}, T) \Phi_i(\xi), \quad (4)$$

where $\widehat{U}_i(\tilde{x}, T)$ are deterministic Fourier coefficients.

It is well-known that for large values of N , the polynomial interpolation (4) may be very oscillatory. To minimize the oscillations, one needs to choose the roots of $\Phi_{N+1}(\xi)$ as collocation points ξ_ℓ , $\ell = 1, \dots, L$ with $L = N + 1$. In this case, the Fourier coefficients can be computed with the help of the discrete Fourier transform:

$$\widehat{U}_i(\tilde{x}, T) = \sum_{\ell=1}^{N+1} U_\ell \Phi_i(\xi_\ell) \omega_\ell, \quad i = 0, \dots, N, \quad (5)$$

where $U_\ell := U(\tilde{x}, T; \xi_\ell)$ and ω_ℓ are the Gauss quadrature weights corresponding to the PDF $\nu(\xi)$. These coefficients are also used to calculate the stochastic moments of for each component U of the computed solution \mathbf{U} :

$$\mathbb{E}_\xi[U^N] = \widehat{U}_0, \quad \text{Var}[U^N] = \sum_{i=1}^N \widehat{U}_i^2.$$

It should be observed that the gPC interpolation (4) is exponentially accurate for smooth solutions but suffers from the Gibbs-type phenomenon when discontinuities appear in the numerical solution, which is a generic case for nonlinear hyperbolic PDEs. Therefore, in the next two sections, we turn our attention to alternative interpolation methods that lead to non-oscillatory approximation of $U(\tilde{x}, T; \xi)$.

2.2 Shape-Preserving (SP) Spline Interpolation

In order to suppress Gibbs-type oscillations, one can use cubic B-splines (see, e.g., [2–4, 20]), which also retain the positivity of the interpolated data, but as we demonstrate in our numerical experiments below, B-spline approximations may oversmear shock discontinuities. Moreover, B-splines do not necessarily maintain the monotonicity and/or convexity of the interpolated data.

Therefore, in this paper, we use (provably) SP rational quartic interpolation splines from [21], specifically designed to preserve the shape of positive, monotonic, and convex solutions. These SP splines also ensure C^2 continuity of the constructed interpolant.

Let us describe the SP spline for a certain component U of \mathbf{U} . We denote by $\Delta\xi_\ell := \xi_{\ell+1} - \xi_\ell$, $\ell = 1, \dots, L - 1$, and introduce the following quantities:

$$\begin{aligned} \delta_\ell &:= \frac{1}{\Delta\xi_\ell + \Delta\xi_{\ell-1}} \left(\frac{U_{\ell+1} - U_\ell}{\Delta\xi_\ell} - \frac{U_\ell - U_{\ell-1}}{\Delta\xi_{\ell-1}} \right), \\ A_1 &:= \Delta\xi_1 \delta_2, \quad A_\ell := \Delta\xi_\ell \delta_\ell, \\ B_{\ell-1} &:= \Delta\xi_{\ell-1} \delta_\ell, \quad B_{L-1} := \Delta\xi_{L-1} \delta_{L-1}, \end{aligned} \quad \ell = 2, \dots, L - 1.$$

For each subinterval $[\xi_\ell, \xi_{\ell+1}]$, $\ell = 1, 2, \dots, L-1$, the computed solution is interpolated by the spline given by

$$U(\tilde{x}, T; \xi) \approx S(\tilde{x}, T; \xi) := (1 - \tau_\ell)U_\ell + \tau_\ell U_{\ell+1} - \frac{\Delta\xi_\ell(1 - \tau_\ell)\tau_\ell [(1 - \tau_\ell)^2 A_\ell + \lambda_\ell(1 - \tau_\ell)\tau_\ell A_\ell B_\ell + \tau_\ell^2 B_\ell]}{Q_\ell},$$

where

$$Q_\ell = 1 + (1 - \tau_\ell)\tau_\ell [(1 - \tau_\ell)(B_\ell\lambda_\ell + \mu_\ell) + \tau_\ell(A_\ell\lambda_\ell + \mu_{\ell+1})],$$

where $\tau_\ell := (\xi - \xi_\ell)/\Delta\xi_\ell$, and λ_ℓ and μ_ℓ are two local tension shape parameters. Note that specific choices of λ_ℓ and μ_ℓ guarantee the preservation of monotonicity, positivity, and convexity of the interpolation spline; see [21].

Once the spline function is constructed, one can use one's favorite quadrature rule to numerically approximate the stochastic moments in (3).

3 Numerical Examples

In this section, we illustrate the performance of the gPC and spline-based SC approaches on numerical examples for the inviscid Burgers and shallow water equations. We consider a random variable ξ uniformly distributed on the interval $[-1, 1]$ ($\xi \in \mathcal{U}[-1, 1]$), which induces the usage of the Legendre polynomials $\Phi_i(\xi)$ in the generalized Fourier expansion (4) and Gauss-Legendre quadratures for computing the gPC coefficients in (5). For the spline interpolation, we take equally-spaced collocation nodes ξ_ℓ , but note that in principle, they can be chosen arbitrarily since, unlike the gPC interpolation, the spline one can be efficiently conducted on any set of nodes. Recall that the SP splines require a specific choice of the local tension parameters λ_ℓ and μ_ℓ to guarantee the shape-preserving properties of the constructed interpolant; see [21, Formulae (12), (19), (24), and (28)] for details.

In this work, we use semi-discrete second-order central-upwind schemes from [9, 10] to numerically solve the deterministic systems (2). The semi-discretization results in the system of ODEs, which is integrated in time using the three-stage third-order strong stability preserving (SSP) Runge-Kutta method (see, e.g., [7, 8]) with the time step chosen according to the CFL number 0.45. The central-upwind scheme employs the generalized minmod limiter with parameter $\theta = 1.3$; see [9, 10] for details.

Example 1—Burgers Equation

We start with the inviscid Burgers equation,

$$U_t + \left(\frac{U^2}{2}\right)_x = 0, \tag{6}$$

considered subject to the following stochastic initial data:

$$U(x, 0; \xi) = \begin{cases} 2, & x > 0.1\xi, \\ 1, & x < 0.1\xi. \end{cases} \quad (7)$$

The problem is numerically solved in the physical domain $x \in [-1, 1]$ with free boundary conditions.

To numerically solve the problem (6)–(7), we choose $L = 16$ collocation points and perform deterministic simulations on a uniform spatial mesh consisting of cells of size $\Delta x = 1/800$ until the final time $T = 0.5$. In Fig. 1, we plot the solution $U(x, 0.5; \xi)$ obtained by interpolating the computed data in the random variable ξ by the gPC and spline-based approaches. For the latter, we present results produced by both the B-splines and SP splines. As one can see, the gPC approach exhibits Gibbs-type oscillations near the discontinuity, whereas both spline-based approximations are oscillation-free. Figure 2a additionally shows the profile of $U(0.734, 0.5; \xi)$ to provide more evidence that the shock propagates from the physical space to the random space. From this figure, one can also observe that B-splines smear the discontinuity compared to the SP splines. The mean and variance values obtained with all three approaches appear similar, as demonstrated in Fig. 2b and 2c.

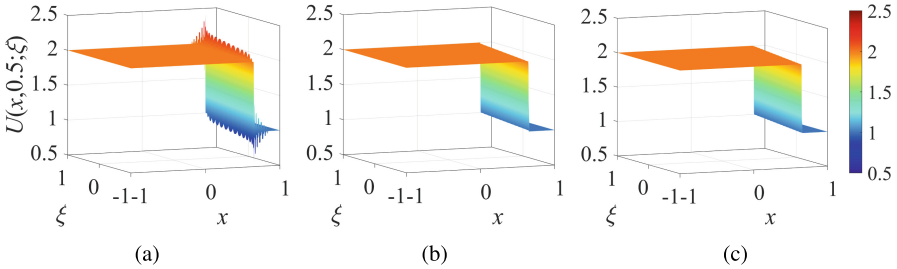


Fig. 1. Example 1: $U(x, 0.5; \xi)$ obtained using (a) gPC expansion, (b) B-splines, and (c) SP splines.

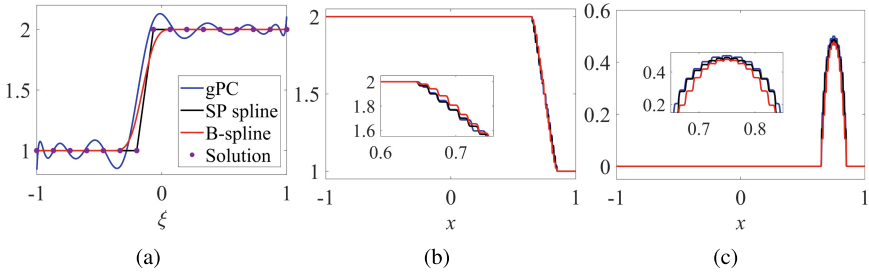


Fig. 2. Example 1: $U(0.734, 0.5; \xi)$, (a) mean, and (b) standard deviation obtained using the gPC expansion and splines. Panels (b) and (c) contain a zoom at the areas of interest.

Example 2—Shallow Water Equations

In this example, we consider the Saint-Venant system of shallow water equations given by (1) with

$$\mathbf{U} = (h, hu)^\top, \quad \mathbf{F}(\mathbf{U}) = \left(hu, hu^2 + \frac{g}{2}h^2\right)^\top, \quad \mathbf{S} = (0, -ghZ_x)^\top,$$

where $h(x, t; \xi)$ is the water depth, $u(x, t; \xi)$ is the velocity, $Z(x; \xi)$ is the bottom topography, and g is the constant acceleration due to gravity (we take $g = 1$).

The Saint-Venant system is considered in the physical domain $x \in [-1, 1]$ subject to free boundary condition, deterministic initial data for the water surface $w = h + Z$ and velocity u ,

$$w(x, 0; \xi) = \begin{cases} 1, & x < 0, \\ 0.5, & x > 0, \end{cases} \quad u(x, 0; \xi) \equiv 0,$$

and stochastic bottom topography

$$Z(x) = \begin{cases} 0.125\xi + 0.125(\cos(5\pi x) + 2), & |x| < 0.2, \\ 0.125\xi + 0.125, & \text{otherwise.} \end{cases}$$

We numerically solve the deterministic systems (2) on a uniform mesh consisting of cells of size $\Delta x = 1/400$ until the final time $T = 0.8$ on a set of collocation points. Here, we examine the performance of the proposed methods with the number of collocation points set to either $L = 16$ or $L = 32$.

In Fig. 3, we plot the water surface $w(x, 0.8; \xi)$. It is evident that the gPC solution exhibits oscillations near the discontinuity location ($x \approx 0.694$). These oscillations become less pronounced as the number of collocation points increases, indicating an improvement in capturing of the stochastic behavior with increased resolution. When a spline interpolation is employed, these oscillations are suppressed. Note that the oscillations visible near $x \approx 0$ in Fig. 3b and 3c appear in the solution (not a feature of the interpolation). Similar results are obtained

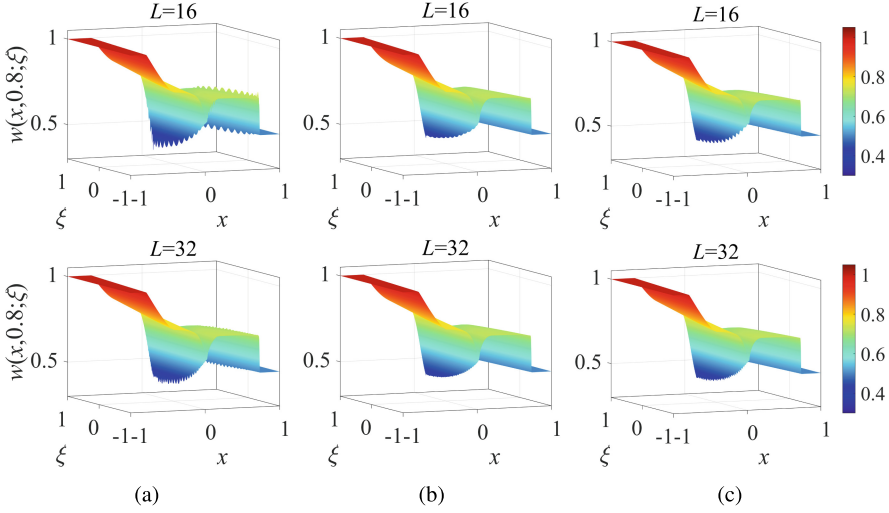


Fig. 3. Example 2: $w(x, 0.8; \xi)$ obtained using (a) gPC expansion, (b) B-splines, and (c) SP splines with different number of collocation points L .

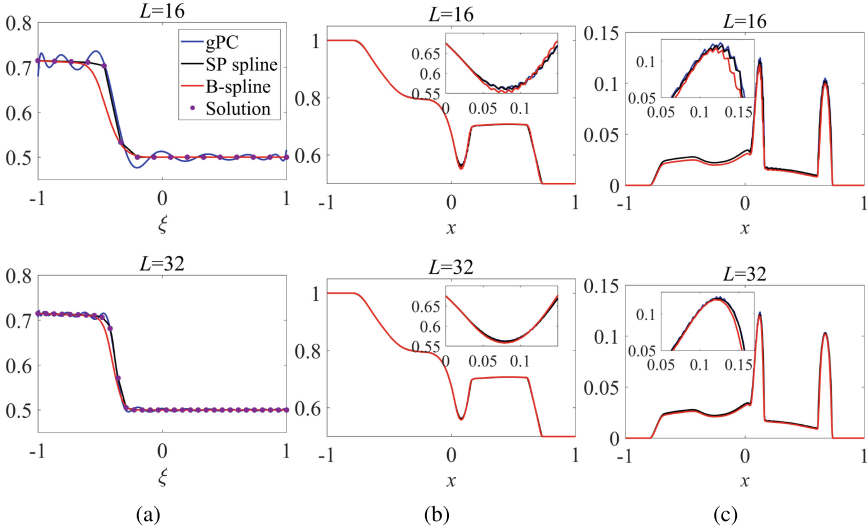


Fig. 4. Example 2: (a) $w(0.694, 0.8; \xi)$, (b) mean, and (c) standard deviation obtained using the gPC expansion and splines. Panels in columns (b) and (c) contain a zoom at the areas of interest.

for water discharge hu (not shown for the sake of brevity). We additionally plot $w(0.694, 0.8; \xi)$ in Fig. 4 to provide a more clear picture. The expected value and standard deviation are also shown in Fig. 4: for all approaches, similar results are observed.

4 Conclusions

In this paper, we have studied the stochastic collocation (SC) methods for uncertainty quantification (UQ) in hyperbolic systems of nonlinear PDEs. We have numerically solved the underlying PDEs at a set of collocation points in random space. Then, we have used a standard SC approach based on a gPC expansion, which relied on choosing the collocation points based on the prescribed probability distribution and approximating the computed solution by a linear combination of orthogonal polynomials. We have illustrated that this approach struggles to accurately capture discontinuous solutions, leading to oscillations (Gibbs-type phenomenon) that significantly deviate from the exact solutions. We have explored alternative SC methods using uniformly distributed collocation points and employing spline interpolations in a random space. Our study has demonstrated the effectiveness of spline-based collocation in accurately capturing and assessing uncertainties while suppressing oscillations. We have illustrated the superiority of the spline-based collocation on two numerical examples, including the inviscid Burgers and shallow water equations. The future work will include higher-dimensional extensions of spline-based SC methods.

Acknowledgements.. The work of A. Chertock and S. Janajra were supported in part by NSF grant DMS-2208438. The work of A. Kurganov was supported in part by NSFC grant 12171226 and the fund of the Guangdong Provincial Key Laboratory of Computational Science and Material Design (No. 2019B030301001).

References

1. Abgrall, R., Mishra, S.: Chapter 19 - Uncertainty quantification for hyperbolic systems of conservation laws. In: Abgrall, R., Shu, C.W. (eds.) *Handbook of Numerical Methods for Hyperbolic Problems*, *Handbook of Numerical Analysis*, vol. 18, pp. 507–544. Elsevier (2017)
2. de Boor, C.: On calculating with B-splines. *J. Approximation Theory* **6**, 50–62 (1972)
3. de Boor, C., Pinkus, A.: The B-spline recurrence relations of Chakalov and of Popoviciu. *J. Approx. Theory* **124**(1), 115–123 (2003)
4. Cox, M.G.: The numerical evaluation of B-splines. *J. Inst. Math. Appl.* **10**, 134–149 (1972)
5. Dai, D., Epshteyn, Y., Narayan, A.: Hyperbolicity-preserving and well-balanced stochastic Galerkin method for shallow water equations. *SIAM J. Sci. Comput.* **43**(2), A929–A952 (2021)
6. Gerster, S., Herty, M., Sikstel, A.: Hyperbolic stochastic Galerkin formulation for the p -system. *J. Comput. Phys.* **395**, 186–204 (2019)
7. Gottlieb, S., Ketcheson, D., Shu, C.W.: *Strong stability preserving Runge-Kutta and multistep time discretizations*. World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ (2011)
8. Gottlieb, S., Shu, C.W., Tadmor, E.: Strong stability-preserving high-order time discretization methods. *SIAM Rev.* **43**(1), 89–112 (2001)

9. Kurganov, A., Noelle, S., Petrova, G.: Semidiscrete central-upwind schemes for hyperbolic conservation laws and Hamilton-Jacobi equations. *SIAM J. Sci. Comput.* **23**(3), 707–740 (2001)
10. Kurganov, A., Petrova, G.: A second-order well-balanced positivity preserving central-upwind scheme for the Saint-Venant system. *Commun. Math. Sci.* **5**(1), 133–160 (2007)
11. Le Maître, O.P., Knio, O.M.: *Spectral Methods for Uncertainty Quantification*. Scientific Computation, Springer, New York (2010)
12. Le Maître, O.P., Knio, O.M., Najm, H.N., Ghanem, R.G.: Uncertainty propagation using Wiener-Haar expansions. *J. Comput. Phys.* **197**(1), 28–57 (2004)
13. Mishra, S., Schwab, C., Šukys, J.: Multi-level Monte Carlo finite volume methods for uncertainty quantification in nonlinear systems of balance laws. In: *Uncertainty quantification in computational fluid dynamics, LNCSE.*, vol. 92, pp. 225–294. Springer, Heidelberg (2013)
14. Pettersson, M.P., Iaccarino, G., Nordström, J.: *Polynomial Chaos Methods for Hyperbolic Partial Differential Equations*. Mathematical Engineering, Springer, Cham (2015)
15. Schlachter, L., Schneider, F.: A hyperbolicity-preserving stochastic Galerkin approximation for uncertain hyperbolic systems of equations. *J. Comput. Phys.* **375**, 80–98 (2018)
16. Šukys, J., Mishra, S., Schwab, C.: Multi-level Monte Carlo finite difference and finite volume methods for stochastic linear hyperbolic systems. In: *Monte Carlo and quasi-Monte Carlo methods 2012*, Springer Proc. Math. Stat., vol. 65, pp. 649–666. Springer, Heidelberg (2013)
17. Tryoen, J., Le Maître, O., Ndjinga, M., Ern, A.: Intrusive Galerkin methods with upwinding for uncertain nonlinear hyperbolic systems. *J. Comput. Phys.* **229**(18), 6485–6511 (2010)
18. Tryoen, J., Le Maître, O., Ndjinga, M., Ern, A.: Roe solver with entropy corrector for uncertain hyperbolic systems. *J. Comput. Appl. Math.* **235**(2), 491–506 (2010)
19. Xiu, D.: Fast numerical methods for stochastic computations: a review. *Commun. Comput. Phys.* **5**(2–4), 242–272 (2009)
20. Zhang, Z., Martin, C.F.: Convergence and Gibbs’ phenomenon in cubic spline interpolation of discontinuous functions. *J. Comput. Appl. Math.* **87**(2), 359–371 (1997)
21. Zhu, Y., Han, X.: Shape preserving C2 rational quartic interpolation spline with two parameters. *Int. J. Comput. Math.* **92**(10), 2160–2177 (2015)