uncertainty quantification for kinetic equations with random imputs

Shi Jin
University of Wisconsin-Madison, USA
& Shanghai Jiao Tong University, China
Dongbin Xiu and Xueyu Zhu
University of Utah
Jingwei Hu
Purdue University

Uncertainty in kinetic equations

- Collision kernels are often expirical
- Initial and boundary data contain uncertainties due to measurement errors or modelling errors
- While UQ has been popular in solid mechanics, CFD, elliptic equations, etc. there has been little activities for kinetic equation
- Neutron transport: Fichtl-Prinja-Warsa

Outlines in this talk

- how can UQ methods handle the asymptotic transition from microscopic to macroscopic scales, and long-time (steady state solution)

- UQ for the Boltzmann equation

Example 1: linear random Goldstein-Taylor model

$$
\begin{aligned}
u_t + v_x &= 0, \\
v_t + \frac{a(z)}{\epsilon} u_x &= -\frac{1}{\epsilon} v.
\end{aligned}
$$

a(z)>0, z random (random wave speed)

Diffusion limit: $\epsilon \to 0^+$

Fourier law

$$
\begin{aligned}
v &= -a(z) u_x, \\
u_t &= a(z) \partial_{xx} u.
\end{aligned}
$$

Example 2: nonlinear random Carleman model

$$u_t + v_x = 0,$$
$$v_t + \frac{1}{\epsilon} u_x = -\frac{\kappa(x,z)}{\epsilon} uv.$$

$\kappa(x,z)$ is random (random forcing)

- Diffusion limit: as $\epsilon \to 0^+$

Darcy's law
$$v = -\frac{1}{\kappa(x,z)u} \partial_x u,$$

Porous media equations
$$u_t = \partial_x \left(\frac{1}{\kappa(x,z)u} \partial_x u \right)$$

Deterministic limit: Kurtz, McKean, Lions-Toscani

Example 3: linear transport with random cross-sections

$$\epsilon \partial_t f(v) + v \partial_x f(v) = \frac{\sigma(x,z)}{\epsilon} \left[\frac{1}{2} \int_{-1}^{1} f(v')\, dv' - f(v) \right],$$

$\sigma(x,z)$ the scattering cross-section, is random

Diffusion limit: Larsen-Keller, Bardos-Santos-Sentis,
Bensoussan-Lions-Papanicolaou (for each z)

as $\epsilon \to 0^+$ f→ $\rho(t,x) = \frac{1}{2} \int_{-1}^{1} f(v')\, dv'$

$$\rho_t = \partial_x \left[\frac{1}{3\sigma(x,z)} \partial_x \rho \right]$$

Numerical challenges (small or multiple scales)

- The problems become computational challenging (even for deterministic problems) when ε is small, or varies from O(1) to <<1
- Numerical stiffness; does underresolved computations give the correct (physical) solutions?

Asymptotic-preserving schemes

- Since the 90s the Asymptotic-preserving (AP) schemes have been found to be effective to bridge the transitions from the microscopic (kinetic) to the macroscopic (hydrodynamic) scales;
- they are microscopic solvers. When ε is not numerically resolved

$$\Delta x, \Delta t \gg \varepsilon$$

they automatically become macroscopic solvers.

No need to glue two different solvers

AP diagram

$$\begin{tikzcd}
\mathcal{F}_\delta^\varepsilon \arrow[rrr, "\varepsilon \to 0"] \arrow[d, "\delta \to 0"] & & & \mathcal{F}_\delta^0 \arrow[d, "\delta \to 0"] \\
\mathcal{F}^\varepsilon \arrow[rrr, "\varepsilon \to 0"] & & & \mathcal{F}^0
\end{tikzcd}$$

Deterministic AP schemes for kinetic equations with Euler or diffusive scalings

- Larsen-Morel-Miller; Coron-Perthame, J-Levemore, Golse-J-Levermore, Klar, J-Pareschi-Toscani, Gosse-Toscani, Degond, Lemou-Miusseuns, Filbet-J, …

- How about problems with random coefficients or forcing or IC/BC?

Polynomial Chaos (PC) approximation

- The PC or generalized PC (gPC) approach first introduced by Wiener, followed by Cameron-Martin, and generalized by Ghanem and Spanos, Xiu and Karniadakis etc. has been shown to be very efficient in many UQ applications when the solution has enough regularity in the random variable
- Let z be a random variable with pdf $\rho(z) > 0$
- Let $\Phi_m(z)$ be the orthonormal polynomials of degree m corresponding to the weight $\rho(z) > 0$

$$\int \Phi_i(z)\Phi_j(z)\rho(z)\,dz = \delta_{ij}$$

The Wiener-Askey polynomial chaos for random variables (table from Xiu-Karniadakis SISC 2002)

	Random variables ζ	Wiener-Askey chaos $\{\Phi(\zeta)\}$	Support
Continuous	Gaussian	Hermite-Chaos	$(-\infty, \infty)$
	Gamma	Laguerre-Chaos	$[0, \infty)$
	Beta	Jacobi-Chaos	$[a, b]$
	Uniform	Legendre-Chaos	$[a, b]$
Discrete	Poisson	Charlier-Chaos	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk-Chaos	$\{0, 1, \dots, N\}$
	Negative Binomial	Meixner-Chaos	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn-Chaos	$\{0, 1, \dots, N\}$

TABLE 4.1

The correspondence of the type of Wiener-Askey polynomial chaos and their underlying random variables ($N \geq 0$ is a finite integer).

Intrusive vs non-intrusive approaches

- Intrusive: stochastic Galerkin, change the equations and solvers, nice mathematical formulation, better accuracy, and efficiency in higher dimension

  (Xiu 2009, Elman, Miller, Phipps and Tuminaro 2011; Aleksev,etc. 2011)
- Non-intrusive stochastic collocation methods: running deterministic solvers, for samplings chosen to be the zeroes of the orthogonal polynomials rather than the Monte-Carlo samplings; using interpolations/quadrature rules to get information at non-sampling points and other quantities of interests

Accuracy and efficiency

- We will consider the gPC Galerkin method

- Under suitable regularity assumptions this method has a spectral accuracy
- Much more efficient than Monte-Carlo samplings

Stochastic AP schemes (s-AP)

2.1. Stochastic asymptotic preserving scheme. We now consider the same problem subject to random inputs.

$$\partial_t u^\epsilon = \mathcal{L}^\epsilon(t, x, z, u^\epsilon; \epsilon), \tag{2.3}$$

where $z \in I_z \subseteq \mathbb{R}^d$, $d \geq 1$, are a set of random variables equipped with probability density function ρ. These random variables characterize the random inputs into the system. As $\epsilon \to 0$, the diffusive limit becomes

$$\partial_t u = \mathcal{L}(t, x, z, u). \tag{2.4}$$

We now extend the concept of deterministic AP to the stochastic case. To avoid the cluttering of notations, let us now focus on the discretization in the random space I_z.

DEFINITION 2.1 (Stochastic AP). *Let $\mathcal{S}$ be a numerical scheme for* (2.3), *which results in a solution $v^\epsilon(z) \in V_z$ in a finite dimensional linear function space V_z. Let $v(z) = \lim_{\epsilon \to 0} v^\epsilon(z)$ be its asymptotic limit. We say that the scheme $\mathcal{S}$ is* strongly asymptotic perserving *if the limiting solution $v(z)$ satisfies the limiting equation* (2.4) *for almost every $z \in I_z$; and it is* weakly asymptotic perserving *if the limiting solution $v(z)$ satisfies the limiting equation* (2.4) *in a weak form.*

gPC Galerkin method

- For diffusion equation (Shen-Xiu):

$$u_t = \partial_x [a(x,z)\partial_x u]$$

- Galerkin approximation:

$$u(x,z,t) = \sum_{m=0}^{M} \hat{u}_m(t,x)\Phi_m(z)$$

- moments: $\mathbb{E}[u] = \hat{u}_0 \,,\qquad \mathrm{Var}[u] = \sum_{m=0}^{M} \hat{u}_m^2$
- Let $\hat{\mathbf{u}} = (\hat{u}_1, \cdots, \hat{u}_M)^T$ then

$$\partial_t \hat{\mathbf{u}} = \partial_x \left(\mathbf{A}\partial_x \hat{\mathbf{u}}\right) \qquad \mathbf{A} = (a_{ij})_{M\times M}$$ symm. pos. def

$$a_{ij}(x) = \int a(x,z)\Phi_i(z)\Phi_j(z)\rho(z)dz.$$

gPC for random G-T model

gPC Approximation:

$$u(x,z,t)=\sum_{m=0}^{M}\hat{u}_m(t,x)\Phi_m(z), \qquad v(x,z,t)=\sum_{m=0}^{M}\hat{v}_m(t,x)\Phi_m(z).$$

- Let $\mathbf{u}=(\hat{u}_1,\cdots,\hat{u}_M)^T, \quad \mathbf{v}=(\hat{v}_1,\cdots,\hat{v}_M)^T$
- Then

$$\hat{\mathbf{u}}_t+\hat{\mathbf{v}}_x=0,$$
$$\hat{\mathbf{v}}_t+\frac{1}{\epsilon}\mathbf{A}\hat{\mathbf{u}}_x=-\frac{1}{\epsilon}\hat{\mathbf{v}}$$

- Clearly, if $\epsilon\to 0$ then $\hat{\mathbf{v}}=-\mathbf{A}\hat{\mathbf{u}}_x$

$$\hat{\mathbf{u}}_t=(\mathbf{A}\hat{\mathbf{u}}_x)_x.$$

thus the gPC is s-AP !

AP time and spatial discretizations

- For (deterministic) hyperbolic and transport equations in diffusive regime

  (J, J-Levermore, Caflisch-J-Russo, J-Pareschi-Toscani, Klar, Pareschi-Russo, Lemou-Musseun, Carrillo-Goudon, etc.)
- We take the time-splitting of J-Pareschi-Toscani

Implicit Relaxation:

$$\hat{\mathbf{u}}_t = 0,$$
$$\hat{\mathbf{v}}_t = -\frac{1}{\epsilon}[\hat{\mathbf{v}} + (\mathbf{A} - \epsilon\alpha\mathbf{I}_M)\hat{\mathbf{u}}_x]$$

Explicit Convection:

$$\hat{\mathbf{u}}_t + \hat{\mathbf{v}}_x = 0,$$
$$\hat{\mathbf{v}}_t + \alpha\hat{\mathbf{u}}_x = 0.$$

choose α so $\mathbf{A} - \epsilon\alpha\mathbf{I}_M$ is positive

Fully discrete scheme

- Implicit relaxation (center difference in space)

$$\hat{\mathbf{u}}_i^* = \hat{\mathbf{u}}_i^n$$
$$\frac{\hat{\mathbf{v}}_i^* - \hat{\mathbf{v}}_i^n}{\Delta t} = -\frac{1}{\epsilon}\left[\hat{\mathbf{v}}_i^* + (\mathbf{A} - \epsilon\alpha\mathbf{I}_M)\frac{\hat{\mathbf{u}}_{i+1}^n - \hat{\mathbf{u}}_{i-1}^n}{2\Delta x}\right]$$

- Explicit convection (upwind in space)

$$\hat{\mathbf{u}}_i^{n+1} = \hat{\mathbf{u}}_i^* - \frac{\Delta t}{2\Delta x}(\hat{\mathbf{v}}_{i+1}^* - \hat{\mathbf{v}}_{i+1}^*) + \frac{\sqrt{\alpha}\Delta t}{2\Delta x}(\hat{\mathbf{u}}_{i+1}^* - 2\hat{\mathbf{u}}_i^* + \hat{\mathbf{u}}_{i-1}^*),$$
$$\hat{\mathbf{v}}_i^{n+1} = \hat{\mathbf{v}}_i^* - \alpha\frac{\Delta t}{2\Delta x}(\hat{\mathbf{u}}_{i+1}^* - \hat{\mathbf{u}}_{i+1}^*) + \frac{\sqrt{\alpha}\Delta t}{2\Delta x}(\hat{\mathbf{v}}_{i+1}^* - 2\hat{\mathbf{v}}_i^* + \hat{\mathbf{v}}_{i-1}^*),$$

s-AP for fully discrete scheme

- When $\epsilon \to 0$, time step constraints bounded from below by the CFL condition of the limiting diffusion equation; the limiting scheme is

$$\hat{\mathbf{v}}_i^* = -\mathbf{A}\frac{\hat{\mathbf{u}}_{i+1}^n - \hat{\mathbf{u}}_{i-1}^n}{2\Delta x}$$

$$\hat{\mathbf{u}}_i^{n+1} = \hat{\mathbf{u}}_i^n - \Delta t\mathbf{A}\frac{\hat{\mathbf{u}}_{i+2}^n - 2\hat{\mathbf{u}}_i^n + \hat{\mathbf{u}}_{i-2}^n}{(2\Delta x)^2} + \frac{\sqrt{\alpha}\Delta t}{2\Delta x}(\hat{\mathbf{u}}_{i+1}^n - 2\hat{\mathbf{u}}_i^n + \hat{\mathbf{u}}_{i-1}^n)$$

which is the standard scheme for the diffusion equation + spatial discretization error: s-AP !

Numerical stability: time step not smaller than that required by the diffusive CFL condition required by solving the diffusion equation

The random (nonlinear) Carleman model

$$\partial_t u + \partial_x v = 0,$$
$$\partial_t v + \frac{1}{\epsilon}\partial_x u = -\frac{1}{\epsilon}\kappa(x,z)uv.$$

Very similar except: nonlinearity and the position of $\kappa(x,z)$

gPC expansion:

$$\kappa(x,z) \approx \sum_{m=0}^{M} \hat{\eta}_m(x)\Phi_m(z)\,.$$

gPC equations:

$$\partial_t \hat{\mathbf{u}} + \partial_x \hat{\mathbf{v}} = 0,$$
$$\partial_t \hat{\mathbf{v}} + \frac{1}{\epsilon}\partial_x \hat{\mathbf{u}} = -\frac{1}{\epsilon}\mathbf{B}(x,t)\hat{\mathbf{v}},$$

$$\mathbf{B}(x,t) = (b_{ij}(x,t))_{1\le i,j\le M}$$

$$b_{ij}(x,t) = \int \kappa(x,z)u_N(x,t,z)\Phi_i(z)\Phi_j(z)\rho(z)dz$$
$$= \sum_{\ell=1}^{M} \hat{u}_\ell \int \kappa(x,z)\Phi_\ell(z)\Phi_i(z)\Phi_j(z)\rho(z)dz\,.$$

S-AP?

The diffusion limit:

$$\begin{cases} v = -\dfrac{1}{\kappa(x,z)u}\partial_x u, \\ \partial_t u = \partial_x \left[\dfrac{1}{\kappa(x,z)u}\partial_x u\right]. \end{cases}$$

As $\epsilon \to 0^+$ the second gPC equation implies

$$\hat{\mathrm{v}} = \mathrm{B}^{-1}(x,t)\partial_x \hat{\mathrm{u}}.$$

This gives rise to the gPC approximation to the diffusion equation.

The method is s-AP

Linear transport equation with random coefficients

$$\epsilon f_t + v f_x = \frac{\sigma(x,z)}{\epsilon}\left[\int_{-1}^{1} f(v')\,dv' - f\right]$$

Introduce parities for v->υ.

$$r(t,x,v) = \frac{1}{2}[f(t,x,v) + f(t,x,-v)],$$

$$j(t,x,v) = \frac{1}{2\epsilon}[f(t,x,v) - f(t,x,-v)].$$

then

$$r_t + v j_x = \frac{\sigma(x,z)}{\epsilon^2}(\rho - r),$$

$$j_t + \frac{v}{\epsilon^2} r_x = -\frac{\sigma(x,z)}{\epsilon^2} j.$$

this is similar to to G-T model upon velocity discreitzation which does not destroy the AP property)…

The rest of the story is the same

How about stochastic collocation method

- Non-intrusive: take one random sample and run deterministic code. And then average
- Strongly AP for each sample; for other random points use interpolation

$$v^\epsilon(x,t,z) = \sum_{j=1}^{N_s} v_j^\epsilon(x,t)\ell_j(z), \qquad \text{e.g.} \qquad \ell_j(z^{(i)}) = \delta_{ij}$$

  or least square, discrete projection etc.
- good for expectation, variance but not s-AP due to interpolation errors

Numerical example 1: G-T model

- $a(x,z) = 2 + z, \qquad z \in [-1,1].$ uniform distribution
- Initial data

$$\begin{aligned} u(x,z,0) &= 2.0, \quad v(x,z,0) = 0, \qquad x \in [-1,0], \\ u(x,z,0) &= 1.0, \quad v(x,z,0) = 0, \qquad x \in (0,1], \end{aligned}$$

- Reference solution: stochastic collocation method with 20 quadrature points

$$\epsilon = 0.49$$

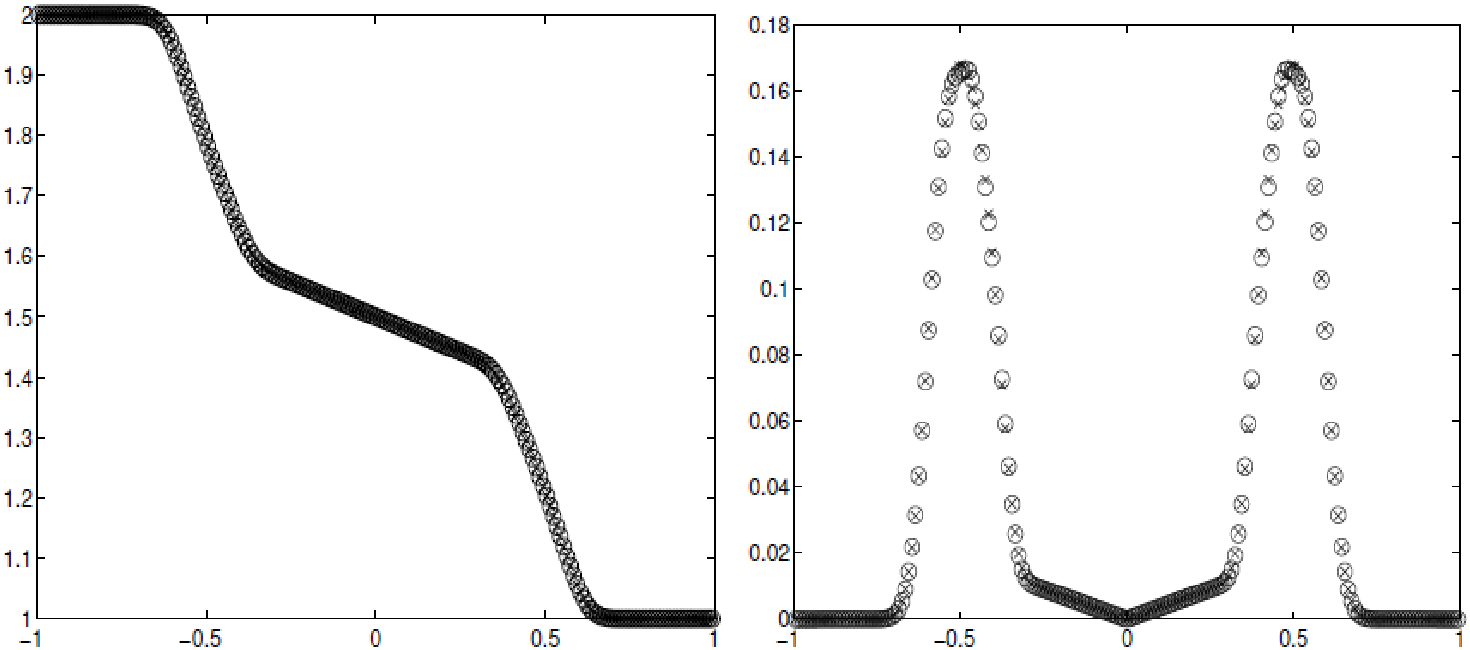

FIG. 8.1. *The mean (left) and standard deviation (right) of u with $\epsilon = 0.49$, obtained by 4th-order gPC Galerkin (circles) and stochastic collocation (crosses).*

$$\epsilon = 10^{-12}$$

- Analytic solution to the limiting diffusion equation

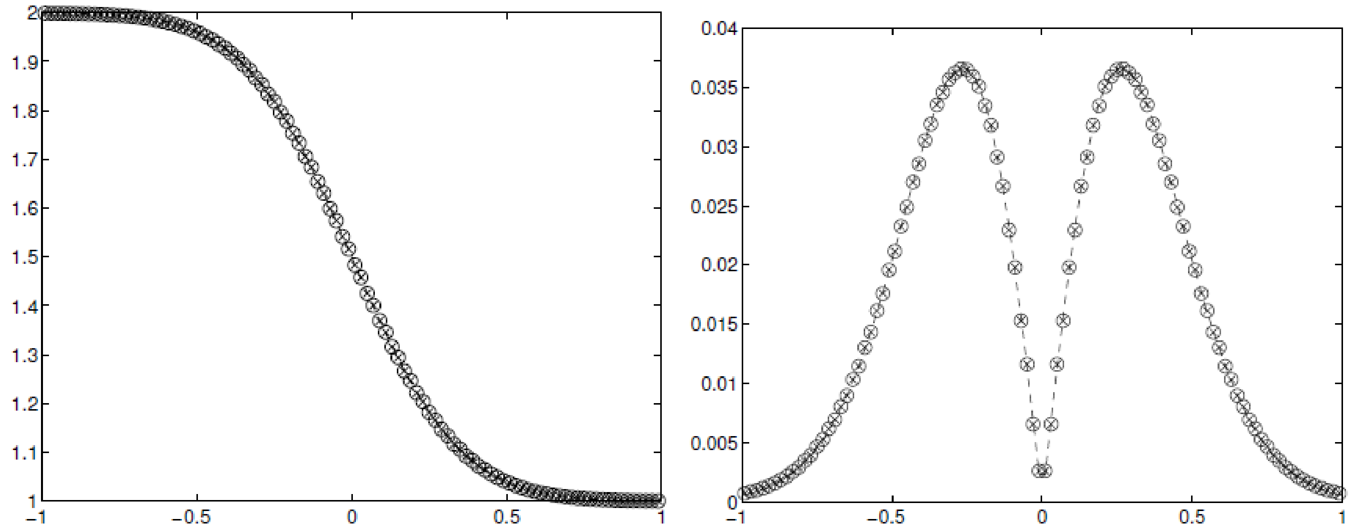

FIG. 8.2. *The mean (left) and standard deviation (right) of u with $\epsilon = 10^{-12}$, obtained by 4th-order gPC Galerkin (circles) and stochastic collocation (crosses), along with the analytical solution* (8.2) *(dashed lines) of the limiting diffusion equation* (2.2).

$$\Delta x = 0.02 \text{ (circles), and } \Delta x = 0.01 \text{ (stars)}.$$

The random Carleman model

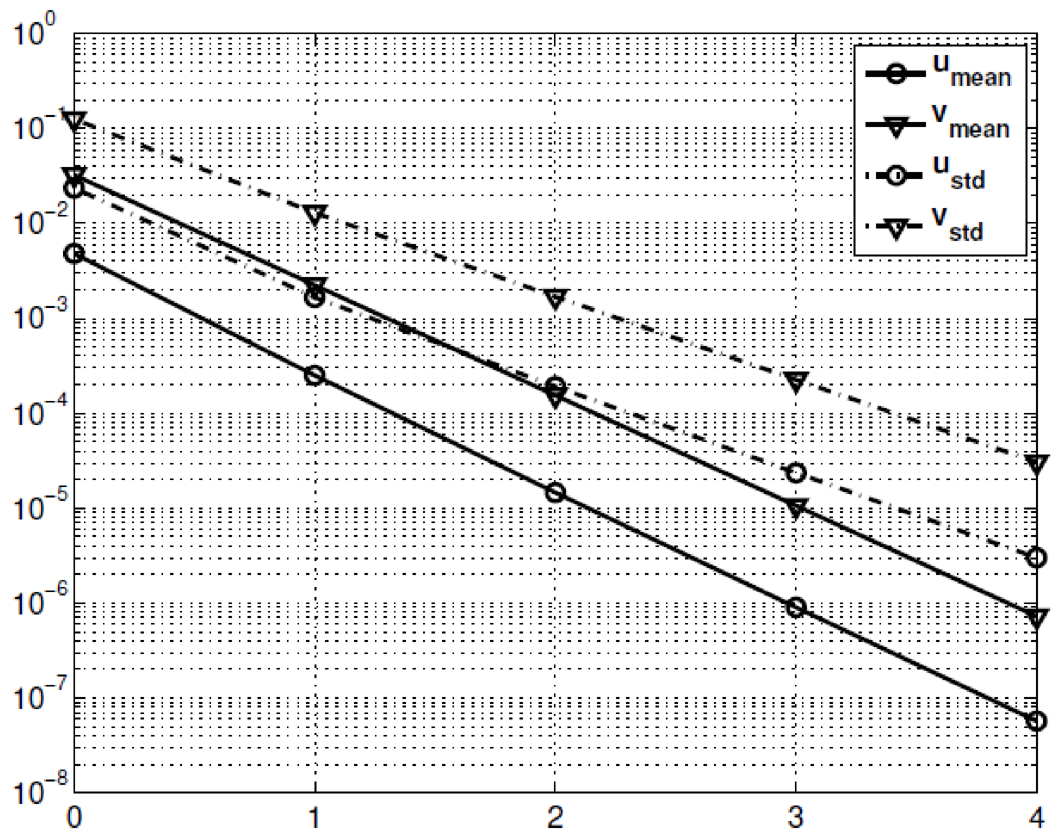

FIG. 8.5. *Error convergence with respect to gPC order for* $\epsilon = 10^{-12}$.

$$\Delta x = 0.02 \text{ and } \Delta t = \frac{1}{12}\Delta x^2$$

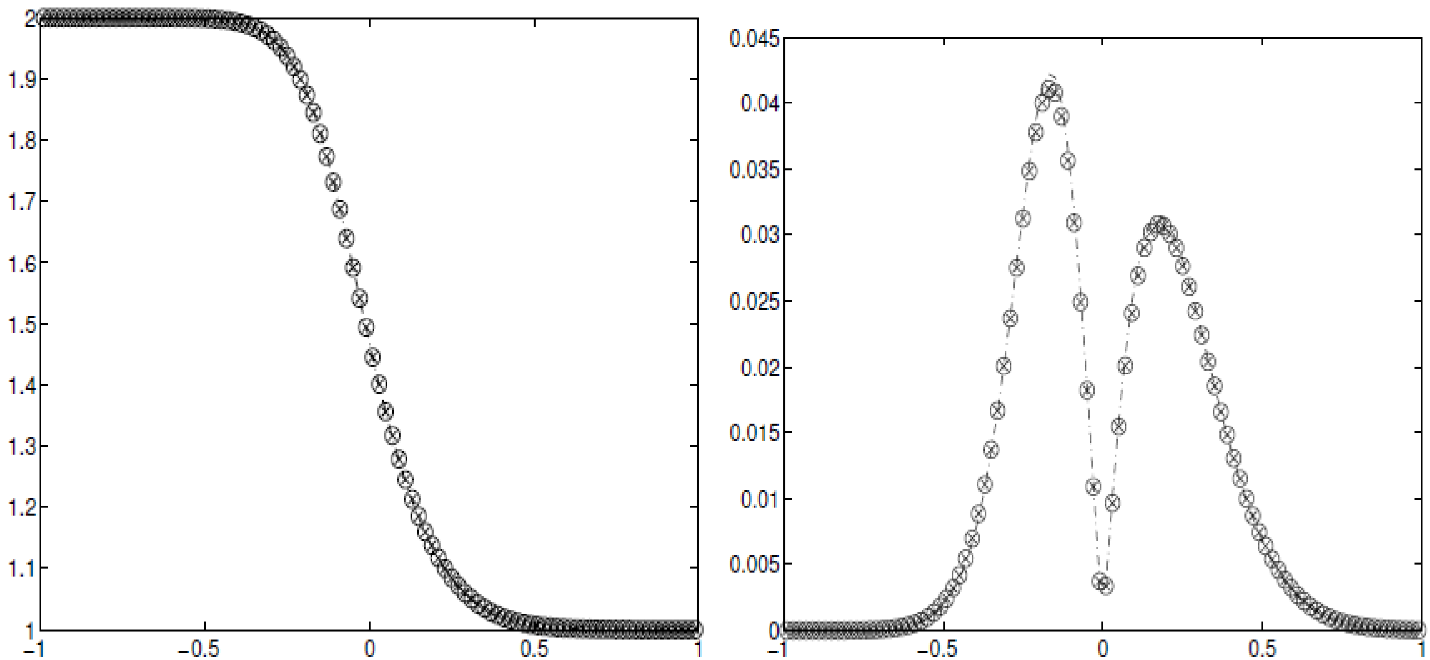

FIG. 8.6. *The mean (left) and standard deviation (right) of* u *at* $\epsilon = 10^{-12}$, *obtained by* $N = 4$ *order gPC Galerkin (circles), the stochastic collocation method (crosses), and the limiting random diffusion equation* (2.4) *(dashed line).*

Convergence in ϵ

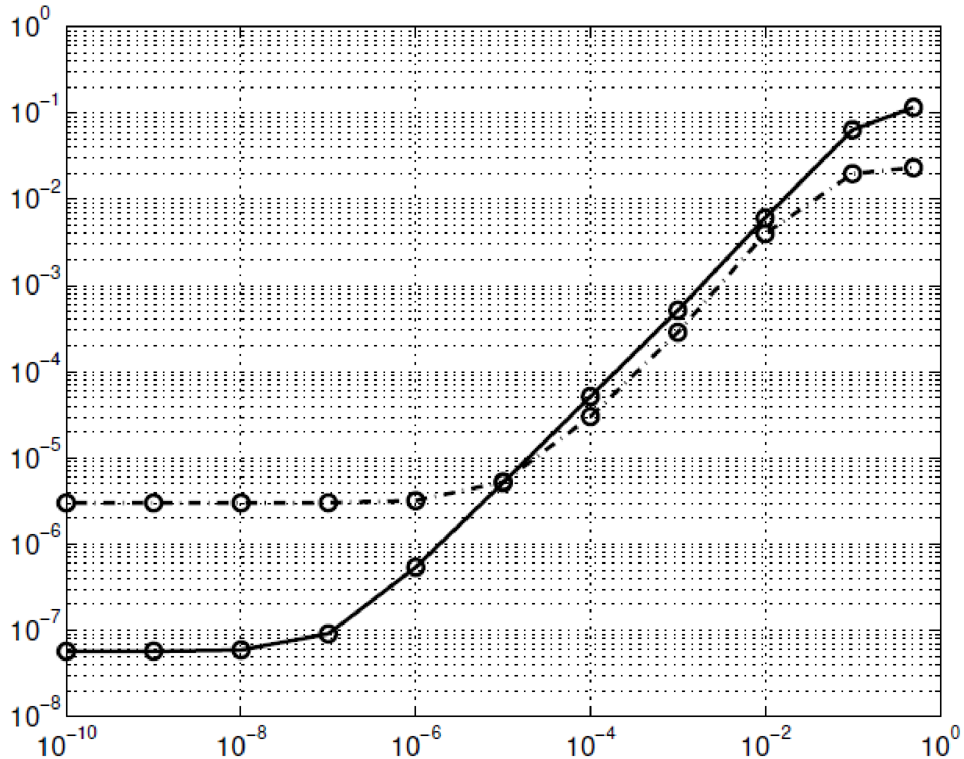

FIG. 8.7. *Errors in the mean (solid line) and standard deviation (dash line) of u by the gPC solution with order $N = 4$ at varying ϵ values. The reference solution is obtained by solving the limiting random diffusion equation (2.4).*

Karhunen-Loeve expansion

$$\kappa(x,z) = 1 + \sigma \sum_{i=1}^{d} \frac{1}{i\pi} \cos(2\pi i x) z_i. \qquad \sigma = 2,\ d = 2.$$

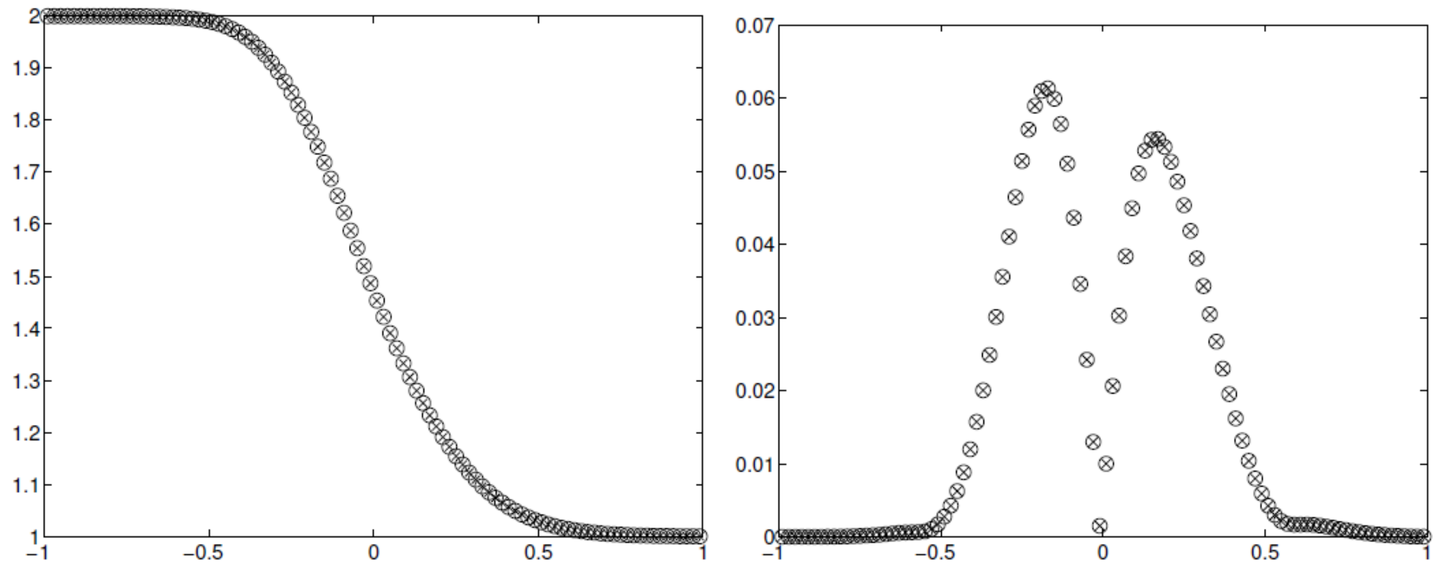

FIG. 8.8. *Mean (left) and standard deviation (right) of u by gPC Galerkin with order $N = 5$ (circles) and the stochastic collocation method (crosses) for $\epsilon = 10^{-12}$.*