Modelling Uncertainties in Porous Media Transport by the Stochastic Finite Element Method

Susanna Kube

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Introduction

Starting point:

- highly developed and very accurate discretization methods, but uncertainties in data

Goal:

- determination of size and distribution of uncertainties

What can be computed?

- moments of the solution (expected value, variance)
- probability of events (failure of material, expected flow rate across an interface)

Approaches

- Monte Carlo methods: sampling of coefficients, then approximation of corresponding realizations $\rightarrow$ high computational cost
- Wick product and Wiener chaos expansion: $E[a * u] = E[a]E[u]$ regardless of the correlation (Holden, Øksendal, Ubøe)
- Ghanem and Spanos: expansion of stochastic coefficients in terms of Hermite polynomials $\rightarrow$ deterministic parametric problem with higher dimension
- Babuška: close relation to the classical FEM approach (piecewise or global polynomials), theorems about existence and stability of the solution

Deterministic Problem

Transport of a substance in an incompressible fluid through a porous medium

$$\boxed{\frac{\partial u}{\partial t} + \nabla \cdot (\boldsymbol{V} u - \boldsymbol{D} \nabla u) = f, \quad x \in D, \ \ t \in [0, T]}$$

+ initial and boundary conditions

- $u(\boldsymbol{x}, t)$: concentration
- f: source or sink term
- $\boldsymbol{V}(\boldsymbol{x}, t)$: velocity field
- $\boldsymbol{D}(\boldsymbol{x}, \boldsymbol{V})$: diffusion-dispersions-tensor, $|\boldsymbol{D}| \ll |\boldsymbol{V}|$
- D: convex bounded polygonal domain in $\mathbb{R}^n$
- $[0, T]$: time interval
- in the following $\mathcal{D} = D \times [0, T]$

Stochastic Model Problem

Stochastic initial boundary value problem: Find a stochastic function $u : \overline{\mathcal{D}} \times \Omega \to \mathbb{R}$, such that P-almost everywhere in Ω (almost surely):

$$
\begin{aligned}
\frac{\partial u(\boldsymbol{x},t,\omega)}{\partial t} + \nabla \cdot (\boldsymbol{V}(\boldsymbol{x},t,\omega)u(\boldsymbol{x},t,\omega) - \boldsymbol{D}\nabla u(\boldsymbol{x},t,\omega)) &= f, \text{ on } \mathcal{D} \\
u(\boldsymbol{x},t=0,\omega) &= g(\boldsymbol{x}) \text{ on } D \\
u(\cdot,t,\omega) &= 0, \text{ on } \partial D \times [0,T]
\end{aligned}
$$

for simplicity: $f = f(\boldsymbol{x},t),\ \boldsymbol{D} = \boldsymbol{D}(\boldsymbol{x})$

Notation and Function Spaces

Define

$$\mathcal{V} = L^2\left([0,T], H_0^1(D)\right)$$

and

$$L_P^q(\Omega) = \left\{\xi : \Omega \mapsto \mathbb{R} | \int_\Omega \xi^q(\omega) dP(\omega) < \infty\right\}, \quad 1 \leq q < \infty.$$

Let $\boldsymbol{\xi}$ be a $\mathbb{R}^M$-valued random variable in $(\Omega, \mathcal{F}, P)$. If $\boldsymbol{\xi} \in L_P^1(\Omega)$ has a density function $\rho_{\boldsymbol{\xi}} : \mathbb{R}^M \to [0, \infty)$, its expected value is denoted by

$$E[\boldsymbol{\xi}] = \int_\Omega \boldsymbol{\xi}(\omega) dP(\omega) = \int_{\mathbb{R}^M} \boldsymbol{\xi} \rho_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}.$$

Whenever $\xi_i \in L^2_P(\Omega)$ for $i = 1, \ldots, M$, the covariance matrix $\mathrm{cov}[\boldsymbol{\xi}] \in \mathbb{R}^{M\times M}$ of $\boldsymbol{\xi}$ is defined by

$$\mathrm{cov}(\xi_i, \xi_j) = E[(\xi_i - E[\xi_i])(\xi_j - E[\xi_j])], \; i, j = 1, \ldots, M.$$

$\boldsymbol{V}$, $u : \mathcal{D} \times \Omega \to \mathbb{R}$ are stochastic functions. They are defined to be elements of the space

$$\tilde{\mathcal{V}} = \mathcal{V} \otimes L^2_P(\Omega).$$

Weak Formulation

Define the bilinear form $\mathcal{B} : \tilde{\mathcal{V}} \times \tilde{\mathcal{V}} \to \mathbb{R}$

$$\mathcal{B}(v, w) \equiv E\left[\int_0^T \int_D (v_t w - (\boldsymbol{V} v - \boldsymbol{D}\nabla v) \cdot \nabla w)\, d\boldsymbol{x}\, dt\right]$$

and the linear functional

$$\mathcal{L}(w) \equiv E\left[\int_0^T \int_D f w \, d\boldsymbol{x}\, dt\right] \qquad \forall\, w \in \tilde{\mathcal{V}}.$$

Then the weak formulation can be written as: Find $u \in \tilde{\mathcal{V}}$, such that

$$\mathcal{B}(u, w) = \mathcal{L}(w), \quad \forall\, w \in \tilde{\mathcal{V}}.$$

Finite Dimensional Approximation of Stochastic Coefficients

- $\{\xi_i\}_{i=1}^M$: real random variables with mean value zero and bounded variance, **mutually independent**
- images $\Gamma_i \equiv \xi_i(\Omega)$ are intervals in $\mathbb{R}$
- assume: each ξ_i has a density function $\rho_i : \Gamma_i \to \mathbb{R}^+$
- joint probability density of $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_M)$: $\quad \rho(\boldsymbol{\xi}) = \prod_{i=1}^M \rho_i(\xi_i) \quad \forall\, \boldsymbol{\xi} \in \Gamma$
- support of the density function: $\quad \Gamma \equiv \Gamma_1 \times \Gamma_2 \ldots \Gamma_M \subset \mathbb{R}^M$

- $\boldsymbol{V}$ can be approximated using just a small number of random variables $\{\xi_i\}_{i=1}^M$
- $\boldsymbol{V}$ depends (besides ω) either only on $\boldsymbol{x}$ or only on t

$$\boldsymbol{V}(\boldsymbol{x},\omega) = \boldsymbol{V}(\boldsymbol{x},\xi_1(\omega),\ldots,\xi_M(\omega))$$

- Example: representation of a scalar random function v by a truncated Karhunen-Loève expansion

$$v_M(\omega,\boldsymbol{x}) = E[v](\boldsymbol{x}) + \sum_{i=1}^{M} \sqrt{\lambda_i} b_i(\boldsymbol{x})\xi_i(\omega)$$

where $\{(\lambda_i, b_i(\boldsymbol{x}))\}_{i=1}^{\infty}$ is the sequence of eigenpairs associated with the covariance operator

$$\int_D \mathrm{cov}[v](\boldsymbol{x}_1,\boldsymbol{x}_2) b(\boldsymbol{x}_1) d\boldsymbol{x}_1 = \lambda b(\boldsymbol{x}_2)$$

Deterministic Parametric Problem

Find $u \in \mathcal{V} \otimes L^2_\rho(\Gamma)$ such that

$$\int_\Gamma \rho(\boldsymbol{\xi}) \int_0^T \int_D (u_t w + (\boldsymbol{V} u - \boldsymbol{D}\nabla u) \cdot \nabla w)(\boldsymbol{x}, t, \xi)\, d\boldsymbol{x}\, dt\, d\boldsymbol{\xi}$$
$$= \int_\Gamma \rho(\boldsymbol{\xi}) \int_0^T \int_D f(\boldsymbol{x}, t) w(\boldsymbol{x}, t, \boldsymbol{\xi})\, d\boldsymbol{x}\, dt\, d\boldsymbol{\xi}, \qquad \forall\, w \in \mathcal{V} \otimes L^2_\rho(\Gamma)$$

with

$$L^2_\rho(\Gamma) = \left\{ w : \Gamma \to \mathbb{R} | \int_\Gamma \rho(\boldsymbol{\xi}) w^2(\boldsymbol{\xi}) d\boldsymbol{\xi} < \infty \right\}.$$

Corresponding strong formulation: partial differential equation with an M-dimensional parameter $\boldsymbol{\xi}$, i.e.

$$\begin{aligned}\frac{\partial u(\cdot,\boldsymbol{\xi})}{\partial t} + \nabla\cdot\left(\boldsymbol{V}(\cdot,\boldsymbol{\xi})u(\cdot,\boldsymbol{\xi}) - D\nabla u(\cdot,\boldsymbol{\xi})\right) &= f(\cdot), \quad \forall\,(\boldsymbol{x},t,\boldsymbol{\xi})\in\mathcal{D}\times\Gamma\\ u(\boldsymbol{x},t=0,\boldsymbol{\xi}) &= g(\boldsymbol{x}), \quad \forall\,(\boldsymbol{x},\boldsymbol{\xi})\in D\times\Gamma\\ u(\cdot,t,\boldsymbol{\xi}) &= 0, \quad \forall\,(\boldsymbol{x},t,\boldsymbol{\xi})\in\partial D\times[0,T]\times\Gamma.\end{aligned}$$

$\rightarrow$ finite element techniques to approximate the solution of the deterministic problem.

Finite Element Spaces

Finite dimensional subspaces:

- $\mathcal{V}_h \subset \mathcal{V}$
- $Z^{\boldsymbol{p}} \subset L^2_\rho(\Gamma)$,

$$Z^{\boldsymbol{p}} = \bigotimes_{i=1}^{M} Z_i^{p_i}, \qquad \dim Z^{\boldsymbol{p}} = \prod_{i=1}^{M} (1 + p_i)$$

with

$$Z_i^{p_i} = \{v : \Gamma_i \to \mathbb{R} \mid v \in \mathscr{P}_{p_i}(\xi_i)\}, \quad i = 1, \dots, M.$$

For simplicity: $\boldsymbol{p} = \{p, \dots, p\}$, i.e. $\dim Z^{\boldsymbol{p}} = (p+1)^M := P$

Discrete Formulation

Find $u_h^p \in \mathcal{V}_h \otimes Z^p$, such that

$$\int_\Gamma \rho(\boldsymbol{\xi}) \int_0^T \int_D \left(\frac{\partial u_h^p}{\partial_t} w + (\boldsymbol{V} u_h^p - \boldsymbol{D} \nabla u_h^p) \nabla w(x,t,\xi) \right) d\boldsymbol{x}\, dt\, d\boldsymbol{\xi}$$
$$= \int_\Gamma \rho(\boldsymbol{\xi}) \int_0^T \int_D f(\boldsymbol{x},t) w(\boldsymbol{x},t,\boldsymbol{\xi})\, d\boldsymbol{x}\, dt\, d\boldsymbol{\xi}, \ \ \forall\ w \in \mathcal{V}_h \otimes Z^p.$$

Let $\{\psi_j(\boldsymbol{\xi})\}$ be a basis of Z^p and $\{\varphi_i(\boldsymbol{x},t)\}$ a basis of $\mathcal{V}_h$. The approximating solution can be written as

$$u_h^p(\boldsymbol{x},t,\boldsymbol{\xi}) = \sum_i \sum_j u_{ij} \psi_j(\boldsymbol{\xi}) \varphi_i(\boldsymbol{x},t).$$

With test functions $w(\boldsymbol{x}, t, \xi) = \psi_k(\boldsymbol{\xi})\varphi_l(\boldsymbol{x}, t)$ one obtains

$$\sum_{i,j} u_{ij} \Bigg[\int_\Gamma \rho(\boldsymbol{\xi})\psi_k(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi})$$

$$\underbrace{\Big(\int_0^T \int_D \frac{\partial \varphi_i(\cdot)}{\partial t} \varphi_l(\cdot) + (\boldsymbol{V}(\cdot, \boldsymbol{\xi})\varphi_i(\cdot) - \boldsymbol{D}\nabla\varphi_i(\cdot)) \cdot \nabla\varphi_l(\cdot)\, d\boldsymbol{x}\, dt \Big)}_{=:\, [K(\boldsymbol{\xi})]_{i,l}} d\boldsymbol{\xi} \Bigg]$$

$$= \int_\Gamma \rho(\boldsymbol{\xi})\psi_k(\boldsymbol{\xi}) \int_0^T \int_D f(\boldsymbol{x}, t)\varphi_l(\boldsymbol{x}, t)\, d\boldsymbol{x}\, dt\, d\boldsymbol{\xi}, \qquad \forall\, k, l.$$

Now insert the KL-decomposition of $\boldsymbol{V}$

$$\boldsymbol{V}(\boldsymbol{x},\boldsymbol{\xi}) = \overline{\boldsymbol{V}} + \sum_{s=1}^{M} \boldsymbol{b}_s(\boldsymbol{x})\xi_s.$$

This results in

$$[K(\boldsymbol{\xi})]_{i,l} := [K^{(0)}]_{i,l} + \sum_{s=1}^{M} \xi_s [K^{(s)}]_{i,l}$$

with

$$[K^{(0)}]_{i,l} := \int_0^T \int_D \frac{\partial \varphi_i(\boldsymbol{x},t)}{\partial t} \varphi_l(\boldsymbol{x},t) + (\overline{\boldsymbol{V}}\varphi_i(\boldsymbol{x},t) - \boldsymbol{D}\nabla\varphi_i(\boldsymbol{x},t)) \cdot \nabla\varphi_l(\boldsymbol{x},t)\, d\boldsymbol{x}\, dt,$$

$$[K^{(s)}]_{i,l} := \int_0^T \int_D \boldsymbol{b}_s(\boldsymbol{x})\varphi_i(\boldsymbol{x},t) \cdot \nabla\varphi_l(\boldsymbol{x},t)\, d\boldsymbol{x}\, dt.$$

Furthermore, we introduce the notations

$$[G^{(0)}]_{k,j} \quad := \quad \langle \psi_k \psi_j \rangle = E[\psi_k(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi})], \qquad k,j = 1,\dots,P = \prod_{s=1}^{M}(1+p_s)$$

$$[G^{(s)}]_{k,j} \quad := \quad \langle \xi_s \psi_k \psi_j \rangle = E[\xi_s \psi_k(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi})].$$

Then the global matrix in the linear system of equations $A\boldsymbol{u} = \boldsymbol{f}$ can be written as

$$\boxed{A = G^{(0)} \otimes K^{(0)} + \textstyle\sum_{s=1}^{M} G^{(s)} \otimes K^{(s)}.}$$

Numerical Examples

Advection Equation

$$\frac{\partial u}{\partial t} + V(x,t,\omega)\frac{\partial u}{\partial x} = 0, \quad \forall (t,x) \in [0,T] \times D = [-1,1]$$
$$u(t=0,x) = g(x) = \sin(\pi(x+1))$$
$$u(-1,t) = u(1,t) \quad \forall t \in [0,T]$$

Analytic Solution

- assume $V = V(t,\omega) > 0 \rightarrow$ change of variables: $d\tau = V(t)dt, \quad \tau(t=0) = 0$

$$\frac{\partial u}{\partial \tau} + \frac{\partial u}{\partial x} = 0, \quad u(x,0) = g(x).$$

- solution: $u(x,t) = g(x-\tau)$

- $V = \overline{V} + \sigma\xi,$

$$\tau(t) = \int_0^t V(s)ds := \overline{V}t + \sigma\xi t$$

- mean value of the solution $u(x,t) = g(x - \tau(t))$:

$$E[u(x,t)] = \int_{-\infty}^{\infty} \rho(\xi) g(x - \tau(t,\xi)) d\xi$$

Case 1:

- $\xi \sim N(0,1), \quad \rho(\xi) = \frac{1}{\sqrt{2\pi}} \exp(-\xi^2/2)$
- $E[u(x,t)] = \sin(\pi(x + 1 - \overline{V}t))e^{-\pi^2\sigma^2 t^2/2}$

Case 2:

- $\xi \sim U[-\sqrt{3}, \sqrt{3}], \quad \rho(\xi) = \frac{1}{2\sqrt{3}}$
- $E[u(x,t)] = \sin(\pi(x + 1 - \overline{V}t))\frac{\sin(\pi\sigma t\sqrt{3})}{\pi\sigma t\sqrt{3}}$

Numerical results

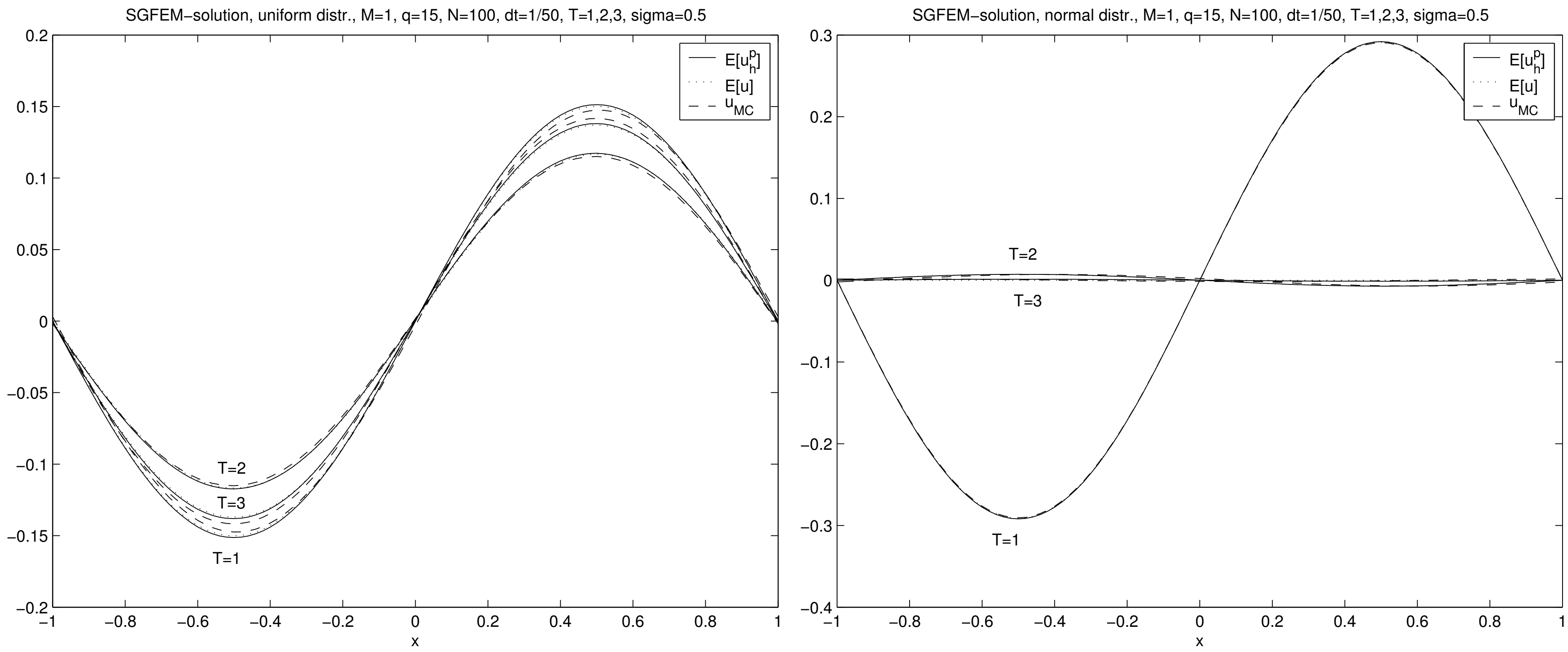


Figure 1: SGFEM solution with $\sigma = 0.5$ for a uniformly distributed ξ (left) and a normally distributed ξ (right)

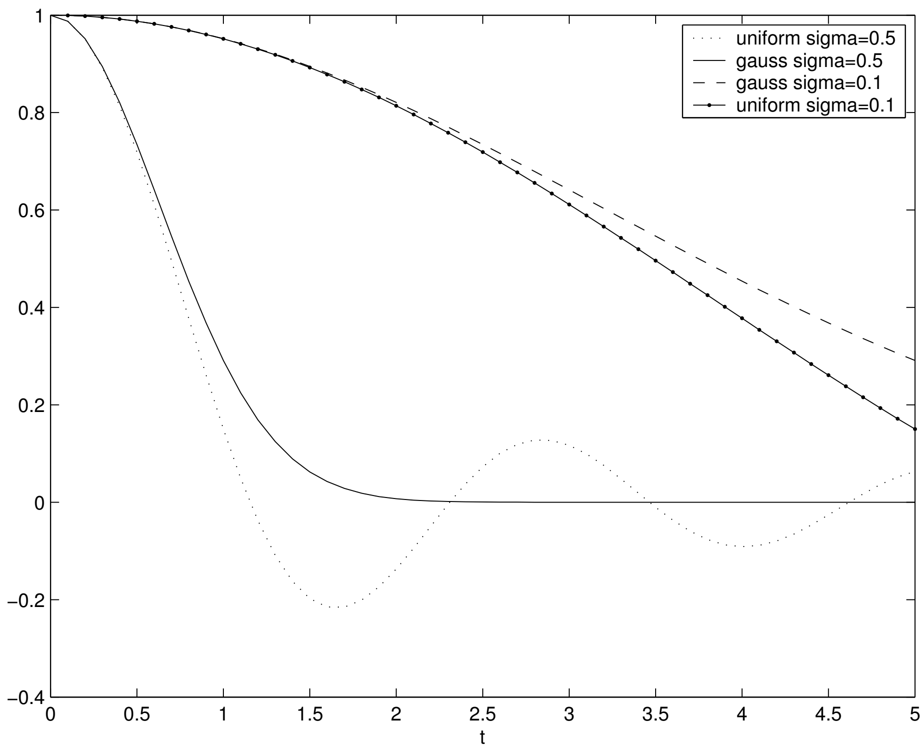


Figure 2: Damping factor for uniform and Gaussian distribution

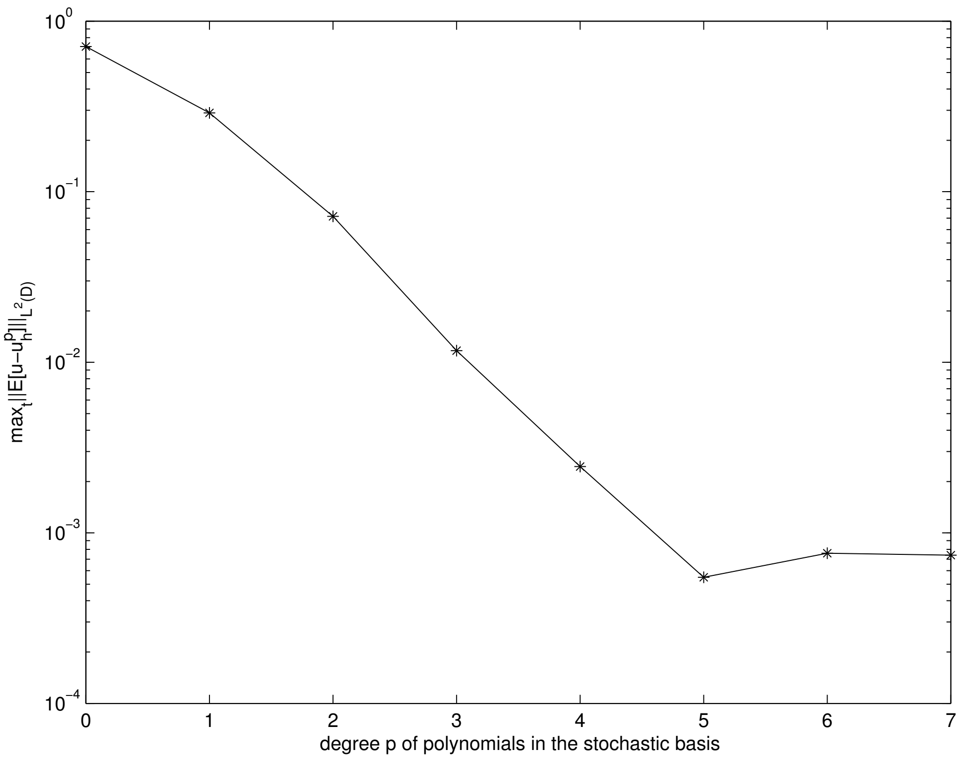


Figure 3: $\max_t ||E[u] - E[u_h^p]||_{L^2(D)}$ for $\xi \sim N(0,1)$, $\sigma = 0.5$

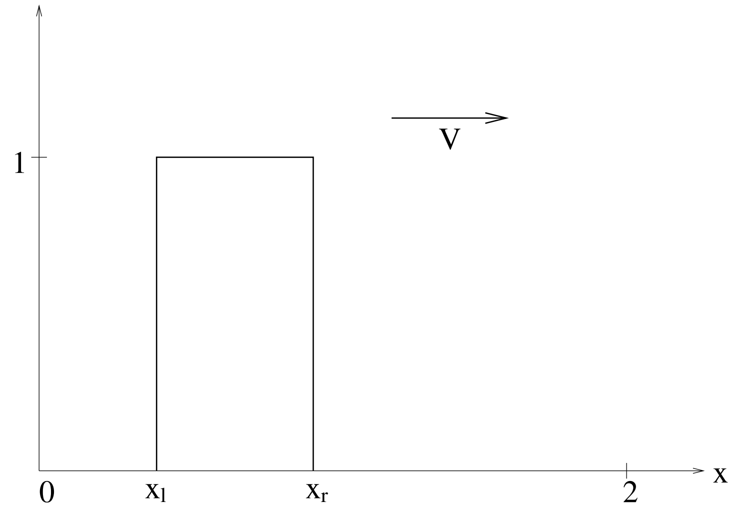
Advection-Diffusion Equation

$$u_t + V u_x - D u_{xx} = 0,$$

$$x \in (a,b), \quad t \in [0,T]$$

$$u_0(x) = \begin{cases} 1, & \text{if } x \in [x_l, x_r] \subset (a,b) \\ 0, & \text{otherwise} \end{cases}$$

$$u(x=a,t,\xi) = u(x=b,t,\xi) = 0$$



- $T = 0.8$, $x_l = 0.2$, $x_r = 0.7$
- analytic deterministic solution

$$u(x,t) = \frac{1}{2}\left[\operatorname{erf}\left(\frac{x - \overline{V}t - x_l}{\sqrt{4\overline{D}t}}\right) - \operatorname{erf}\left(\frac{x - \overline{V}t - x_r}{\sqrt{4\overline{D}t}}\right)\right].$$

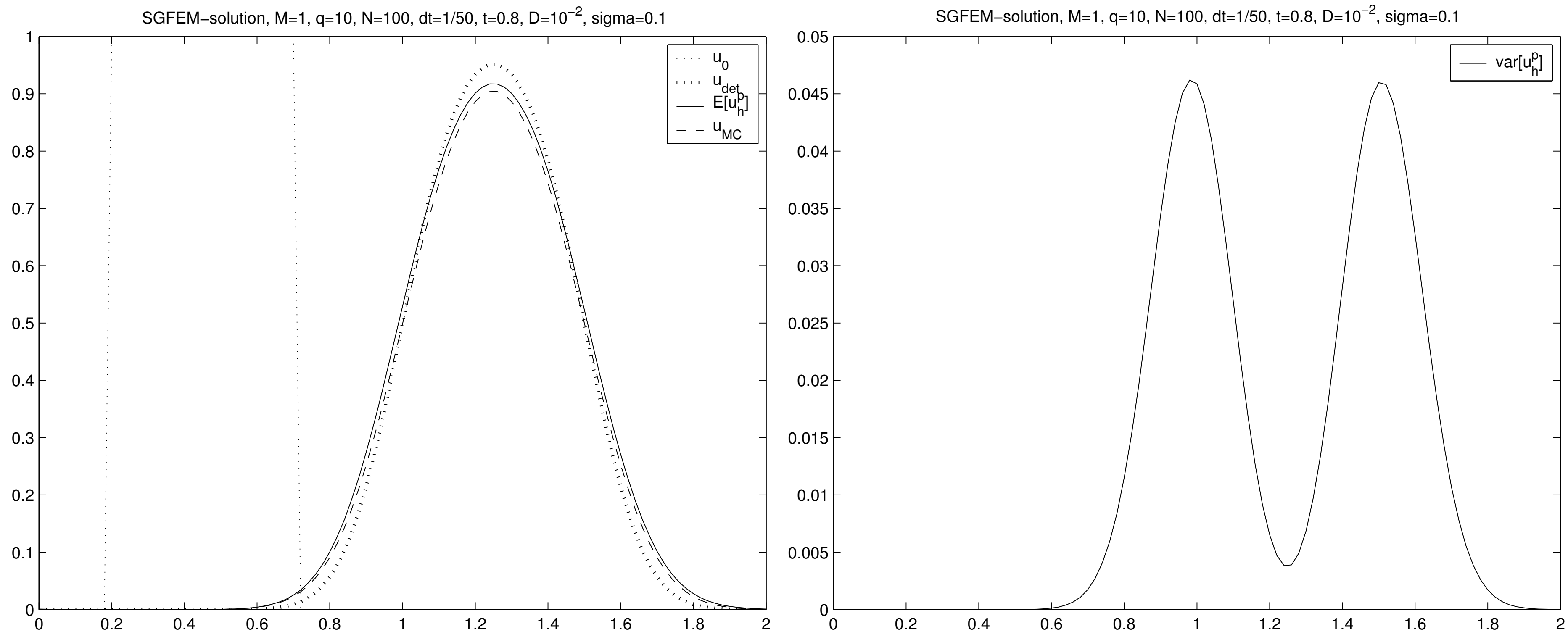


Figure 4: Mean value and variance for $V = \overline{V} + \xi$, $\xi \sim N[0, \sigma^2]$, $\overline{V} = 1$, $\sigma = 0.1$

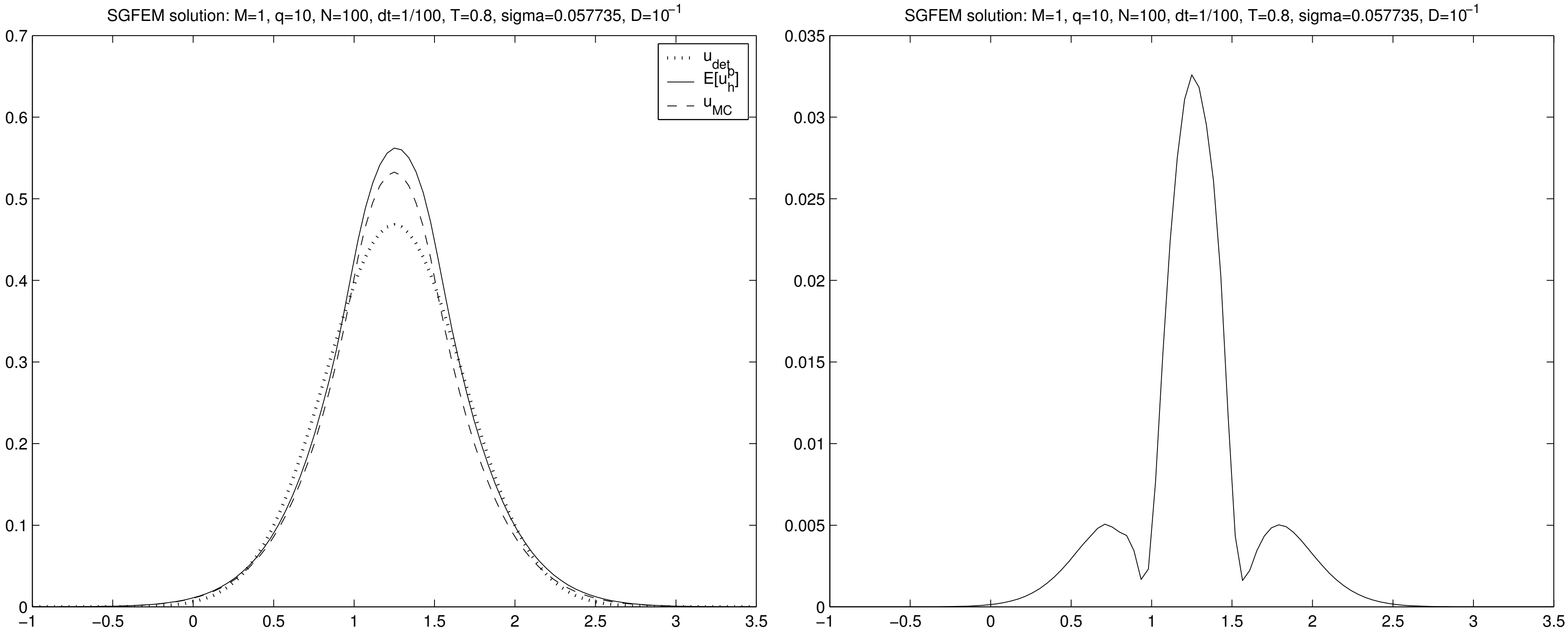


Figure 5: Mean value and variance for $D = \overline{D} + \xi$, $\xi \sim U[-\sqrt{3}\sigma, \sqrt{3}\sigma]$, $\overline{D} = 10^{-1}$, $\sigma = \overline{D}/\sqrt{3}$

Summary

- SFEM as a flexible tool not only for elliptic SPDEs
- the stochastic solution strongly depends on the distribution functions of the random variables
- exponential convergence with respect to the polynomial degree p of the stochastic discretization
- a stochastic velocity acts like additional diffusion while a stochastic diffusion leads to less damping

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For More Information

- Susanna Kube, kube_s@student.tu-freiberg.de

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