

University of Stuttgart

Computational Methods for Uncertainty Quantification Institute for Applied Analysis und Numerical Simulation Pfaffenwaldring 57, D-70569 Stuttgart, Germany andreas.stein@ians.uni-stuttgart.de

Motivation

The modeling of time-dependent/stationary subsurface and fractured porous media flows by parabolic/elliptic equations, where:

- Random advection- and diffusion coefficients account for uncertain permeability and insufficient measurements.
- Random discontinuities in the coefficients are incorporated to model heterogeneous media and fractures in ground layers.

Advection-Diffusion Equations with Random Jump Coefficients MLMC-FEM Simulation

Andreas Stein

Approximation of *a* **and Finite Element Method**

In order to draw approximate samples of u, it is in general necessary to approximate the coefficients a and b. First, the Gaussian random field W is replaced by W_N , where $N \in \mathbb{N}$ represents the cutoff-index of the Karhúnen-Loève expansion of W. In addition, only biased samples \tilde{P}_i of the jump heights P_i might be generated such that

 $||\widetilde{P}_i - P_i||_{L^2(\Omega;\mathbb{R})} \leq \sqrt{\epsilon}, \text{ for some } \epsilon > 0.$

For example, if P_i follows a non-standard distribution, this error may stem

Advection-Diffusion Problem with Jump Coefficients

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space, $\mathcal{D} \subset \mathbb{R}^d$ a bounded, connected Lipschitz domain for some $d \in \mathbb{N}$ and $\mathbb{T} = [0, T]$ with T > 0 be a finite time interval. We consider the random parabolic problem

 $-\nabla \cdot (a(\omega, x, t)\nabla u(\omega, x, t)) + b(\omega, x, t)\nabla u(\omega, x, t) = f(\omega, x, t)$

in $\Omega \times \mathcal{D} \times \mathbb{T}$, subject to the initial-boundary conditions

$$\begin{split} u(\omega, x, 0) &= u_0(\omega, x) \quad \text{in } \Omega \times \mathcal{D}, \\ u(\omega, x, t) &= 0 \quad \text{on } \Omega \times \Gamma_1 \times \mathbb{T}, \\ a(\omega, x, t) \vec{n} \cdot \nabla u(\omega, x, t) &= g(\omega, x, t) \quad \text{on } \Omega \times \Gamma_2 \times \mathbb{T}, \end{split}$$

where

- $a, b : \Omega \times \mathcal{D} \times \mathbb{T} \to \mathbb{R}$ are the stochastic jump diffusion resp. jump advection coefficients,
- $f: \Omega \times \mathcal{D} \times \mathbb{T} \to \mathbb{R}$ is a random source function,
- $u_0: \Omega \times \mathcal{D} \to \mathbb{R}$ is the stochastic initial condition,
- $\partial \mathcal{D} = \Gamma_1 \cup \Gamma_2$ with $|\Gamma_1| > 0$ and Γ_2 are such that the exterior normal derivative $\vec{n} \cdot \nabla u$ is well-defined for any $u \in C^1(\overline{\mathcal{D}})$ and
- $g: \Omega \times \Gamma_2 \times \mathbb{T} \to \mathbb{R}$ is the Neumann part of the boundary conditions.

We consider the following structure for the diffusion coefficient:

 $a(\omega, x, t) := \overline{a}(x, t) + \Phi(W(\omega, x)) + P(\omega, x),$

where $H := L^2(\mathcal{D})$ and $\overline{D} = \Phi \subset C^1(\mathcal{D}) \subset \mathbb{T} \setminus \mathbb{D}$ from Fourier Inversion sampling, see [1].

This yields approximations $a_{N,\epsilon}$ of a and $b_{N,\epsilon} = \Psi(a_{N,\epsilon}, \cdot, \cdot)$ of b, which are utilized to simulate pathwise FEM solutions $u_{N,\epsilon,h,\Delta}(\omega, \cdot) \approx u(\omega, \cdot)$. The parameter h > 0 refers to the mesh width of the FEM triangulation and $\Delta t > 0$ to the stepsize of the employed Backward Euler scheme.

 \implies Given that $u \in L^2(\Omega; L^2(\mathbb{T}, H^m(\mathcal{D})))$ for some $m \in (1, 2]$,

$$||\boldsymbol{u}-\boldsymbol{u}_{N,\epsilon,h,\Delta}||_{L^2(\Omega;H^1(\mathcal{D}))} \leq C_1\left(\sqrt{\sum_{i>N}\eta_i} + \sqrt{\epsilon} + \boldsymbol{h}^{m-1} + \Delta\right),$$

where $(\eta_i)_{i \in \mathbb{N}}$ are the eigenvalues of Q and $C_1 > 0$ a constant. \implies To increase the order of convergence with respect to h in the finite dimensional approximation, the FEM triangulation should be chosen pathwise accordingly to the sampled diffusion coefficient, see Fig. 1.

Multilevel Monte Carlo Moment Estimation

The moments of u (expected value, variance etc.) are estimated using the *Multilevel Monte Carlo* (MLMC) method: Let $L \in \mathbb{N}$ and consider the sequences of approximation parameters $h_0 > \cdots > h_L$, $\Delta_0 > \cdots > \Delta_L$, $\epsilon_0 > \cdots > \epsilon_L$ and $N_0 < \cdots < N_L$. The MLMC estimator of $\mathbb{E}(u)$ is then defined as

$$\mathsf{E}^{L}(\boldsymbol{u}_{N_{L},\epsilon_{L},h_{L},\Delta_{L}}):=\sum^{L}\frac{1}{M_{I}}\sum^{M_{I}}\boldsymbol{u}_{N_{I},\epsilon_{I},h_{I},\Delta_{I}}^{(i)}-\boldsymbol{u}_{N_{I-1},\epsilon_{I-1},h_{I-1},\Delta_{I-1}}^{(i)},$$

- $\overline{a}, \Phi \in C^1(\mathcal{D} \times \mathbb{T}; \mathbb{R}_{>0})$ (i.e. $\Phi(w) = \exp(w)$).
- W is a (zero-mean) Gaussian random field associated to a non-negative, symmetric trace class operator $Q: H \rightarrow H$.
- *T* : Ω → B(D), ω ↦ {*T*₁,...,*T*_τ} is a random partition of D, where the number *τ* of elements in *T* is a N-valued random variable *τ* : Ω → N on (Ω, A, P).
- (P_i)_{i∈ℕ} is a sequence of random variables on (Ω, A, ℙ) with arbitrary non-negative distribution(s) and

$$m{P}: \Omega imes \mathcal{D} o \mathbb{R}_{\geq 0}, \quad (\omega, m{x}) \mapsto \sum_{i=1}^{ au(\omega)} \mathbf{1}_{\{\mathcal{T}_i\}}(m{x}) m{P}_i(\omega).$$

The sequence $(P_i)_{i \in \mathbb{N}}$ is independent of τ (but not necessarily i.i.d.). The advection coefficient depends on a and is given by

 $b(\omega, \mathbf{x}, t) = \Psi(a(\omega, \mathbf{x}, t), \mathbf{x}, t),$

where the mapping $\Psi : \mathbb{R}_{>0} \times \mathcal{D} \times \mathbb{T} \to \mathbb{R}$ is affine linear with respect to the diffusion coefficient a.

⇒ Under natural assumptions on a, f, Ψ and the initial-boundary data, there exists \mathbb{P} -a.s. a unique weak solution $u \in L^2(\Omega; L^2(\mathbb{T}, H^1(\mathcal{D})))$. ⇒ In general, this solution is not available in closed form and it is not possible to draw unbiased samples from u.

Example of Jump Diffusion and Advection coefficients

l=0 *i*=1

where $M_0 > \cdots > M_L$ are the decreasing numbers of sampled differences and $u_{N_l,\epsilon_l,h_l,\Delta_l}^{(i)} - u_{N_{l-1},\epsilon_{l-1},h_{l-1},\Delta_{l-1}}^{(i)}$ are generated independently in *i* on each level *I*. It is possible to adjust the truncation indices N_l , the sampling bias ϵ_l and the number of samples M_l throughout the levels to obtain an overall error of

 $||\mathbb{E}(u) - E^{L}(u_{N_{L},\epsilon_{L},h_{L},\Delta_{L}})||_{L^{2}(\Omega;L^{2}(\mathbb{T},H^{1}(\mathcal{D})))} \leq C_{2}h_{L}^{m-1},$ where $C_{2} > 0$ is independent of $N_{L}, \epsilon_{L}, h_{L}, \Delta_{L}$ and M_{L} .

Numerical Results

 \implies Combining the MLMC estimator with an adaptive pathwise triangulation leads to faster convergence to the expected value $\mathbb{E}(u)$ and produces a lower error for any computational budget, see Fig. 2.

 \implies The algorithm can be further enhanced by *bootstrapping* (BS), meaning the simulated quantities $u_{N_l,\epsilon_l,h_l}^{(i)}$ are "recycled" on the next level l + 1.





The specific structure of *a* allows for a very flexible modeling of the random diffusion coefficient. For instance, changes in permeability may be modeled by a log-Gaussian diffusion coefficient with incorporated jumps. The discontinuities are random with respect to their spatial position and magnitude and the corresponding pathwise solution reflects the behavior of the coefficients, see Figure 1.



Figure 1: Sample of a time-independent log-Gaussian diffusion coefficient a (left) and corresponding sample of u with $b(\omega, x, t) := -2a(\omega, x, t)$.

nverse spatial/temporal refinement $h^{-1} = \Delta t^{-1}$

Mean simulation time in seconds

Figure 2: Convergence of different error norms (left), Time-to-error plot (right).

References

[1] A. Barth and A. Stein.

Approximation and simulation of infinite-dimensional Lévy processes. *Stochastics and Partial Differential Equations*, 2017.

[2] A. Barth and A. Stein.

A study of elliptic partial differential equations with jump diffusion coefficients.

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