TECHNISCHE UNIVERSITÄT BERGAKADEMIE FREIBERG

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Solvers for large linear systems arising in the Stochastic Finite Element Method

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Outline

- Stochastic Finite Element Method (SFEM)
  - Variational formulation of elliptic SPDEs
  - Structure of Galerkin matrix
- Aspects of the stochastic discretization
  - Multivariate basis functions: complete/tensor polynomials
  - Structure and spectral properties of stochastic Galerkin matrices
- Solvers for the global Galerkin system
  - block-diagonal Galerkin system: Krylov subspace recycling method
  - fully-coupled Galerkin system: Mean-based preconditioner
- Numerical examples

1 Review of SFEM

[Ghanem & Spanos, 1991]

Stochastic elliptic boundary value problem

Given: bounded spatial domain $D \subset \mathbb{R}^2$ with boundary $\Gamma = \Gamma_D \cup \Gamma_N$ and a complete probability space $(\Omega, \mathscr{A}, P)$.

Task: solve the second order elliptic stochastic boundary value problem

$$-\nabla \cdot (T(\boldsymbol{x}, \omega) \nabla p(\boldsymbol{x}, \omega)) = F(\boldsymbol{x}), \qquad \boldsymbol{x} \in D,\ P.-a.s. \tag{1a}$$

$$p(\boldsymbol{x}) = p_D(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma_D, \tag{1b}$$

$$\boldsymbol{n} \cdot (T \nabla p)(\boldsymbol{x}) = p_N(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma_N. \tag{1c}$$

Note: T and therefore p are **random fields**.

Mixed formulation of stochastic elliptic bvp

$$\boldsymbol{u}(\boldsymbol{x},\omega) = -T(\boldsymbol{x},\omega)\nabla\, p(\boldsymbol{x},\omega), \qquad \boldsymbol{x} \in D,\ P. - a.s \tag{2a}$$

$$\nabla \cdot \boldsymbol{u}(\boldsymbol{x},\omega) = F(\boldsymbol{x}), \qquad \boldsymbol{x} \in D,\ P. - a.s. \tag{2b}$$

$$p(\boldsymbol{x}) = p_D(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma_D, \tag{2c}$$

$$\boldsymbol{n} \cdot \boldsymbol{u}(\boldsymbol{x}) = -p_N(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma_N. \tag{2d}$$

Mixed stochastic variational formulation

Find functions $\boldsymbol{u} \in H_{\Gamma_N}(\text{div}, D) \otimes L^2_P(\Omega)$ and $p \in L^2(D) \otimes L^2_P(\Omega)$ such that for all test functions $\boldsymbol{v} \in H_{\Gamma_N}(\text{div}, D) \otimes L^2_P(\Omega)$ and $q \in L^2(D) \otimes L^2_P(\Omega)$ there holds

$$\left\langle \int_D T^{-1}\boldsymbol{u} \cdot \boldsymbol{v}\, d\boldsymbol{x} \right\rangle - \left\langle \int_D p\, \nabla \cdot \boldsymbol{v}\, d\boldsymbol{x} \right\rangle = -\left\langle \int_{\Gamma_D} p_D\, \boldsymbol{n} \cdot \boldsymbol{v} \right\rangle \tag{3a}$$

$$\left\langle -\int_D \nabla \cdot \boldsymbol{u} q\, d\boldsymbol{x} \right\rangle = -\left\langle \int_D F q\, d\boldsymbol{x} \right\rangle . \tag{3b}$$

Notation:

$\langle \cdot \rangle$ denotes the expectation operator w.r.t. the measure P

$$\langle \xi \rangle := \int_\Omega \xi(\omega) dP(\omega),$$

$$L^2_P(\Omega) := \left\{ \xi(\omega) : \int_\Omega \xi^2(\omega) dP(\omega) < \infty \right\} = \left\{ \xi : \langle \xi^2 \rangle < \infty \right\}$$

Discretization steps of stochastic variational formulation

- Input random fields depend on M mutually independent random variables $\{\xi_m\}_{m=1}^M$ with given probability density functions $\rho_m : \Gamma_m \to [0, \infty)$.

$$\rho(\boldsymbol{\xi}) := \rho_1(\xi_1) \cdots \rho_M(\xi_M), \qquad \boldsymbol{\xi} \in \Gamma := \Gamma_1 \times \cdots \times \Gamma_M.$$

- Reformulation of (3): Identify $L^2_P(\Omega)$ with $L^2_\rho(\Gamma)$ and $\langle \cdot \rangle$ with $\int_\Gamma \rho(\boldsymbol{\xi}) \cdot d\boldsymbol{\xi}$.
- Deterministic discretization: choose finite dimensional spaces

$$X^h := \text{ span } \{\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_{N_{\boldsymbol{x}}^{\boldsymbol{u}}}\} \subset H_{\Gamma_N}(\text{div}, D)$$
$$Y^h := \text{ span } \{\pi_1, \pi_2, \ldots, \pi_{N_{\boldsymbol{x}}^p}\} \subset L^2(D)$$

- Stochastic discretization:

$$W^h := \text{ span } \{\psi_1(\boldsymbol{\xi}), \psi_2(\boldsymbol{\xi}), \ldots, \psi_{N_{\boldsymbol{\xi}}}(\boldsymbol{\xi})\} \subset L^2_\rho(\Gamma).$$

- Variational space:

$$(X^h \times Y^h) \otimes W^h \subset (H_{\Gamma_N}(\text{div}, D) \times L^2(D)) \otimes L^2_\rho(\Gamma)$$

Representation of input random field

$$T^{-1}(\boldsymbol{x}, \boldsymbol{\xi}) = \sum_{n=1}^{N_{\boldsymbol{\xi}}} T_n(\boldsymbol{x}) \psi_n(\boldsymbol{\xi})$$

Karhunen-Loève expansion	Wiener's polynomial chaos expansion
$T^{-1} = \langle T^{-1} \rangle + \sum_{m=1}^{M} T_m(\boldsymbol{x}) \xi_m$	$T^{-1} = \sum_{\alpha \in \mathscr{I}} T_\alpha(\boldsymbol{x}) H_\alpha(\boldsymbol{\xi})$
For details see O. Ernst's talk.	$\mathscr{I} := \{\alpha \in \mathbb{N}_0^M, \ \lvert\alpha\rvert \leq d\}$
linear in $\boldsymbol{\xi}$	**nonlinear** in $\boldsymbol{\xi}$ for $d > 1$
$M + 1$ terms	$\binom{M+d}{M}$ terms
Example: **Gaussian** random fields	Example: **lognormal** random fields

Structure of Galerkin matrix $(\psi_1 \equiv 1)$

$$A = \sum_{n=1}^{N_{\boldsymbol{\xi}}} G_n \otimes K_n$$

Stochastic part:

$$[G_n]_{\ell,j} = \langle \psi_n \psi_\ell \psi_j \rangle, \qquad n, j, \ell = 1, \dots, N_{\boldsymbol{\xi}}.$$

Deterministic part:

$$K_1 = \begin{bmatrix} A_1 & B^T \\ B & O \end{bmatrix} \quad K_n = \begin{bmatrix} A_n & O \\ O & O \end{bmatrix} \qquad n = 2, 3, \dots, N_{\boldsymbol{\xi}},$$

$$[B]_{i,k} = -\int_D \nabla \cdot \boldsymbol{\phi}_i(\boldsymbol{x}) \pi_k(\boldsymbol{x}) d\boldsymbol{x}, \qquad i = 1, 2, \dots, N_{\boldsymbol{x}}^{\boldsymbol{u}},\ k = 1, 2, \dots, N_{\boldsymbol{x}}^{p},$$

$$[A_n]_{i,k} = \int_D T_n(\boldsymbol{x}) \boldsymbol{\phi}_i(\boldsymbol{x}) \cdot \boldsymbol{\phi}_k(\boldsymbol{x}) d\boldsymbol{x}, \qquad i, k = 1, 2, \dots, N_{\boldsymbol{x}}^{\boldsymbol{u}}, n = 1, \dots, N_{\boldsymbol{\xi}}.$$

2 The stochastic discretization

Basis functions for $W_h \subset L^2_\rho(\Gamma)$: $\psi_\alpha(\boldsymbol{\xi}) = \prod_{m=1}^{M} p^{(m)}_{\alpha_m}(\xi_m)$

where $\left\langle p^{(m)}_i p^{(m)}_j \right\rangle = \delta_{ij}$ and $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_M) \in \mathbb{N}_0^M$ is a multi-index.

tensor polynomials (TP)	**complete polynomials** (CP)
$\deg\left(p^{(m)}_{\alpha_m}\right) \le d$, $m = 1, \ldots, M$	$\sum_{m=1}^{M} \deg\left(p^{(m)}_{\alpha_m}\right) \le d$
$W_h = \mathbb{Q}_d$	$W_h = \mathbb{P}_d$
$\dim(\mathbb{Q}_d) = (d+1)^M$	$\dim(\mathbb{P}_d) = \binom{M+d}{M}$

Numbering convention of basis polynomials: $n \leftrightarrow \alpha$, $G_n \leftrightarrow G_\alpha$

(TP) $\alpha_1 = 0, \alpha_1 = 1, \ldots, \alpha_1 = d, \alpha_2 = 0, \alpha_2 = 1, \ldots, \alpha_2 = d, \ldots, \alpha_M = d$

(CP) Same as for (TP), but drop multi-indices with $|\alpha| > d$.

α	ψ_α	In $\mathbb{P}_d$?
(0,0)	$p_0(\xi_1)p_0(\xi_2)$	✓
(1,0)	$p_1(\xi_1)p_0(\xi_2)$	✓
(2,0)	$p_2(\xi_1)p_0(\xi_2)$	✓
(0,1)	$p_0(\xi_1)p_1(\xi_2)$	✓
(1,1)	$p_1(\xi_1)p_1(\xi_2)$	✓
(2,1)	$p_2(\xi_1)p_1(\xi_2)$	x
(0,2)	$p_0(\xi_1)p_2(\xi_2)$	✓
(1,2)	$p_1(\xi_1)p_2(\xi_2)$	x
(2,2)	$p_2(\xi_1)p_2(\xi_2)$	x

Table 1: Dropping of basis polynomials for $M = 2$, $d = 2$.

Matrix structure and eigenvalue bounds

	G_α	$\lambda_{\max}(G_\alpha)$
$M = 1$	$\langle p_n p_i p_j \rangle = [U_n]_{ij}$	
$n = 0$	I_{d+1}	$= 1$
$n = 1$	$\langle \xi p_i p_j \rangle$	largest root of p_{d+1} [Golub, Welsch]
$n = 2$	$\langle p_2 p_i p_j \rangle$	$\mathscr{O}(d)$ [U.] for Gaussian ξ
$\mathbb{Q}_d$	$U^{(M)}_{\alpha_M} \otimes \cdots \otimes U^{(1)}_{\alpha_1}$	$= \max \left\{ \prod_{m=1}^{M} \lambda_m, \lambda_m \in \Lambda(U^{(m)}_{\alpha_m}) \right\}$
$\lvert\alpha\rvert = 1$	-	$= \lambda_{\max} \left(U^{(m)}_1 \right), \alpha_m = 1$
$\mathbb{P}_d$	-	$\leq \max \left\{ \prod_{m=1}^{M} \lambda_m, \lambda_m \in \Lambda(U^{(m)}_{\alpha_m}) \right\}$
$\lvert\alpha\rvert = 1$	-	$= \lambda_{\max} (U_1)$ [U.], [Elman, Powell] for $\{\xi_i\}_{i=1}^{M}$ iid

3 Solution strategies

The input random field T is

- **linear** $\Rightarrow G_\alpha, |\alpha| \leq 1.$ The stochastic basis functions are
  - complete polynomials: Solve system in $N_{\boldsymbol{x}} \cdot N_{\boldsymbol{\xi}}$ unknowns. [Ghanem & Pellissetti], [Ghanem & Kruger], [Le Maître et al.], [Matthies & Keese], [Seynaeve et al.], [Elman & Furnival], [Elman & Powell], [Rosseel et al.]

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  - tensor polynomials: Construct biorthogonal stochastic basis functions. Solve $N_{\boldsymbol{\xi}}$ systems in $N_{\boldsymbol{x}}$ unknowns in parallel or use Krylov subspace recycling techniques. [Eiermann, Ernst & U.], [Cai et al.], [Ernst, U. et al.]

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- **nonlinear** $\Rightarrow G_\alpha, |\alpha| > 1.$ The stochastic basis functions are
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  - ▶ tensor polynomials: Solve system in $N_{\boldsymbol{x}} \cdot N_{\boldsymbol{\xi}}$ unknowns. [?]

(A) Decoupled case

Task: Solution of $N_{\boldsymbol{\xi}}$ linear systems of size $N_{\boldsymbol{x}} \times N_{\boldsymbol{x}}$.

$$K_\ell = \begin{bmatrix} A_1 & B^T \\ B & O \end{bmatrix} + \sum_{n=2}^{N_{\boldsymbol{\xi}}} g_{n,\ell} \begin{bmatrix} A_n & O \\ O & O \end{bmatrix}, \quad \ell = 1, \ldots, N_{\boldsymbol{\xi}}.$$

Our approach: Sequential solution of systems by iterative methods.

- MINRES [Paige & Saunders]
- R-MINRES [De Sturler et al.]

(A) Decoupled case - preconditioning

$$P = \begin{bmatrix} D & O \\ O & S \end{bmatrix}, \quad D = \mathtt{diag}(A_1), \quad S = BD^{-1}B^T$$

(a) [Powell & Silvester, 2004]

$$P_{amg} = \begin{bmatrix} D & O \\ O & \mathtt{amg}(S) \end{bmatrix}$$

(b)

$$P_{chol} = \begin{bmatrix} D & O \\ O & \mathtt{cholinc}(S,0) \end{bmatrix}$$

(B) Coupled case

Task: Solution of **one** linear system of size $(N_{\boldsymbol{x}} \cdot N_{\boldsymbol{\xi}}) \times (N_{\boldsymbol{x}} \cdot N_{\boldsymbol{\xi}})$

Our approach: use MINRES together with a mean-based preconditioner

$$P = I_{N_{\boldsymbol{\xi}}} \otimes \begin{bmatrix} D & O \\ O & \texttt{amg}(S) \end{bmatrix}$$

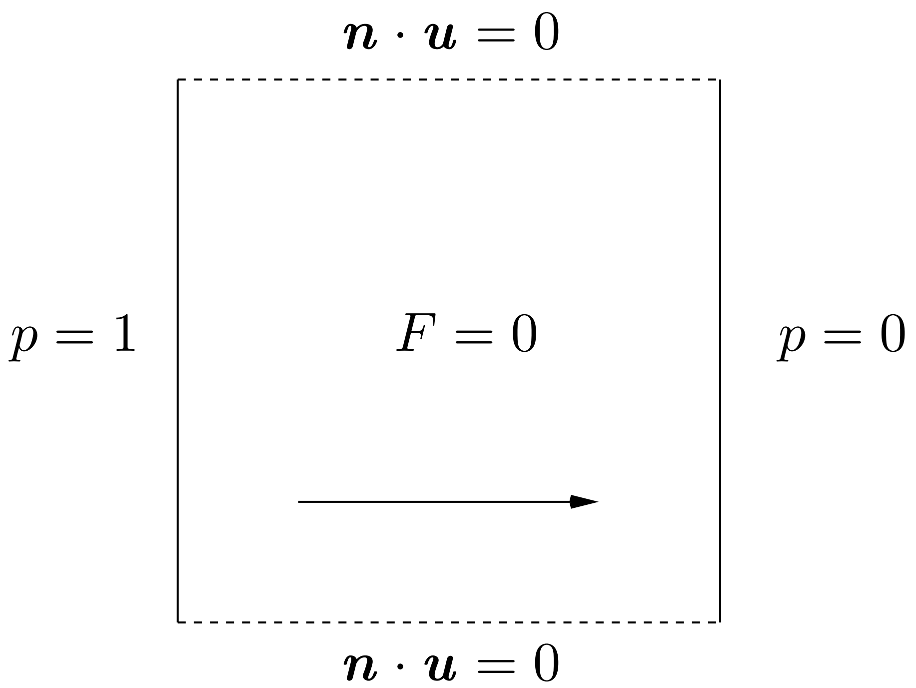
$$D = \texttt{diag}(A_1), \quad S = BD^{-1}B^T, \quad \text{[Powell \& Silvester, 2004]}$$

$$(A_1)_{i,k} = \int_D \langle T^{-1}(\boldsymbol{x}) \rangle \boldsymbol{\phi}_i(\boldsymbol{x}) \cdot \boldsymbol{\phi}_k(\boldsymbol{x}) d\boldsymbol{x}, \quad i,k = 1,2,\ldots,N_{\boldsymbol{x}}^{\boldsymbol{u}}.$$

4 Numerical examples

(A) Decoupled case - model problem

Flow from western to eastern boundary in unit square $D = (0,1) \times (0,1)$.



<u>Deterministic discretization</u>

- 32×32 mesh
- RT_0 square elements for $\boldsymbol{u}$
- Q_0 square elements for p

Random field model:

T^{-1} is a **Gaussian random field** with constant mean $\mu = \langle T^{-1} \rangle = 1$ and double exponential covariance function

$$\mathsf{Cov}_{T^{-1}}(\boldsymbol{x}, \boldsymbol{y}) = \sigma^2 \exp\left(-\frac{|x_1 - y_1|}{c_1} - \frac{|x_2 - y_2|}{c_2}\right), \quad c_1 = c_2 = 3.$$

- Truncated Karhunen-Loève (KL) expansion:

$$T^{-1}(\boldsymbol{x}, \boldsymbol{\xi}) = \mu + \sigma \sum_{m=1}^{M} T_m(\boldsymbol{x})\xi_m, \qquad \xi_m \sim N(0,1), \quad m = 1, \ldots, M.$$

- Use analytic expressions for KL expansion terms [Ghanem & Spanos].

- Mean problem has solution $\boldsymbol{u} = [1,\, 0]^T$, $p = 1 - x$.

Performance of preconditioners - no recycling

Average MINRES iterations, $\frac{||\boldsymbol{r}_k||_{P^{-1}}}{||\boldsymbol{r}_0||_{P^{-1}}} < 10^{-8}$, $N_{\boldsymbol{x}} = 3072$.

AMG version

σ	$M\backslash d$	2	3	4	5
0.1	3	39	40	40	40
	4	39	40	40	41
	5	39	40	41	41
0.2	3	42	44	45	48
	4	42	44	46	-
	5	43	45	48	-

CHOL version

σ	$M\backslash d$	2	3	4	5
0.1	3	159	161	162	163
	4	159	161	163	164
	5	160	162	164	165
0.2	3	166	172	175	182
	4	168	174	178	-
	5	169	175	182	-

Performance of R-MINRES(m,k)

Average iterations, $\frac{||\boldsymbol{r}_k||_{P^{-1}}}{||\boldsymbol{r}_0||_{P^{-1}}} < 10^{-8}$, $N_{\boldsymbol{x}} = 3072$, $M = 5$, $d = 3$, $N_{\boldsymbol{\xi}} = 1024$.

Store at most $m + k$ vectors, recycle k vectors.

AMG version

m	k	$\sigma = 0.1$	$\sigma = 0.2$
20	10	40	46
20	20	40	46
40	20	40	46
40	40	39	45
-	-	40	45

CHOL version

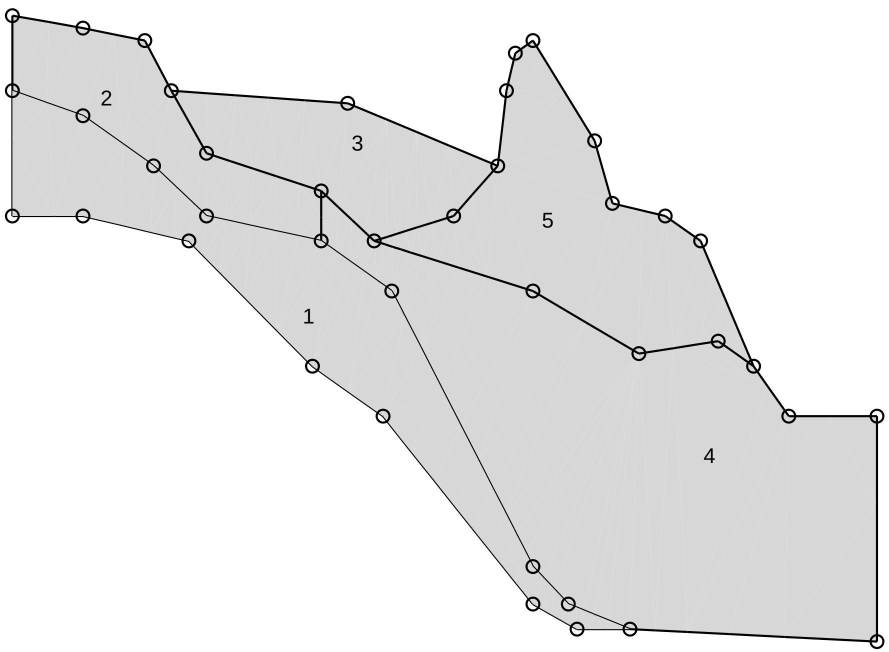
m	k	$\sigma = 0.1$	$\sigma = 0.2$
20	10	86	103
20	20	68	83
40	20	68	82
40	40	55	69
-	-	162	175

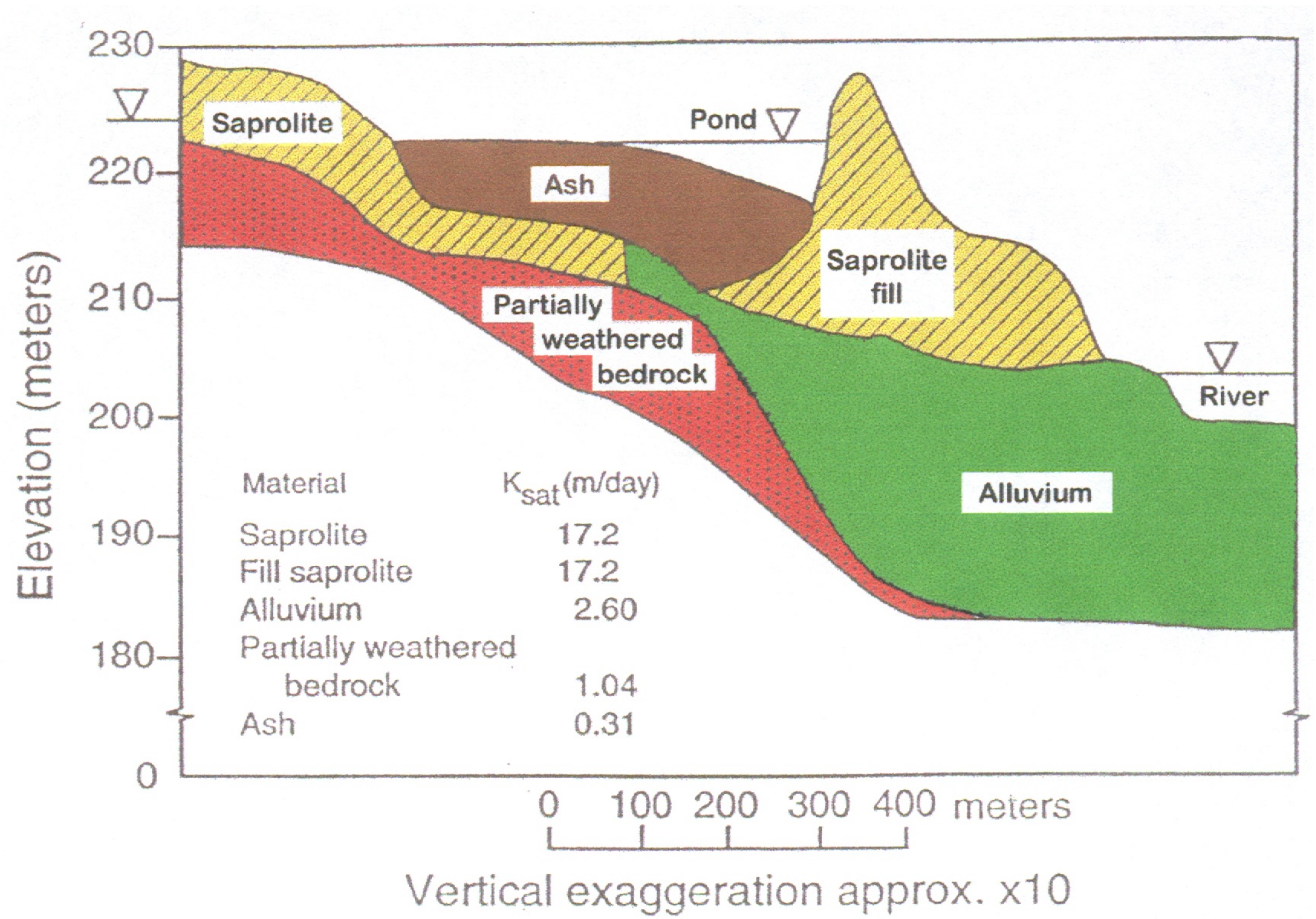
(B) Coupled case - model problem

Fluid flow in a geological site in the south-eastern United States.
(cf. Wheeler et al.)

Deterministic discretization:

- 1961 elemental triangular mesh
- RT_0 triangular elements for $\boldsymbol{u}$
- P_0 triangular elements for p




230
220
210
200
190
180
0
Elevation (meters)
Saprolite
Ash
Pond
Saprolite fill
Partially weathered bedrock
River
Alluvium
Material
K_{sat} (m/day)
Saprolite 17.2
Fill saprolite 17.2
Alluvium 2.60
Partially weathered bedrock 1.04
Ash 0.31
0 100 200 300 400 meters
Vertical exaggeration approx. x10

Random field model:

T^{-1} is a **lognormal random field**:

$$T^{-1}(\boldsymbol{x},\boldsymbol{\xi}) = \exp(-G(\boldsymbol{x},\boldsymbol{\xi})),$$

where G is a Gaussian field with mean μ_G and Bessel covariance function

$$\mathsf{Cov}_G(r) = \sigma_G^2 \left(\frac{r}{\ell}\right) K_1 \left(\frac{r}{\ell}\right).$$

Truncated KL expansion: $G(\boldsymbol{x},\boldsymbol{\xi}) = \mu_G + \sigma_G \sum_{m=1}^{M} \sqrt{\nu_m} g_m(\boldsymbol{x})\xi_m$.

Polynomial chaos expansion:

$$T^{-1}(\boldsymbol{x},\boldsymbol{\xi}) = \sum_{\alpha} T_\alpha(\boldsymbol{x}) H_\alpha(\boldsymbol{\xi})$$

$$T_\alpha(\boldsymbol{x}) = \mu_{T^{-1}} \frac{(-1)^{|\alpha|}\sigma_G^{|\alpha|}}{\sqrt{\alpha!}} \prod_{m=1}^{M} \left(\sqrt{\nu_m} g_m(\boldsymbol{x})\right)^{\alpha_m}$$

Performance of mean-based preconditioner

MINRES iterations, $\frac{||\boldsymbol{r}_k||_{P^{-1}}}{||\boldsymbol{r}_0||_{P^{-1}}} < 10^{-8}$, $N_{\boldsymbol{x}} = 4763$, $N_{\boldsymbol{\xi}} = 5, \ldots, 84$.

$\ell = 600, \quad M = 4$

σ_T/μ_T	$d=1$	$d=2$	$d=3$
0.01	81	99	100
0.1	106	124	143
0.2	117	159	190
0.3	135	190	250

$\ell = 400, \quad M = 6$

σ_T/μ_T	$d=1$	$d=2$	$d=3$
0.01	81	98	98
0.1	104	124	143
0.2	117	159	191
0.3	135	193	250

Summary

- Large linear systems arise from the Stochastic Finite Element Method.
- The structure of the global Galerkin matrix is mainly determined by the coefficient random field and the stochastic shape functions.
- In case the Galerkin matrix can be decoupled, R-MINRES reduces the average iteration count when applied together with a weak preconditioner. Recycling is less efficient when using a stronger preconditioner for R-MINRES.
- When solving the fully-coupled system, mean-based preconditioners work for lognormal random fields when σ_T/μ_T is not too large.