Part 1: Stochastic Galerkin Approximation for PDEs with Uncertain Inputs

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June 3, 2019
Uncertainty Quantification (UQ)

Forward UQ: PDEs + Uncertain Inputs

Stochastic Galerkin (Mixed) FEM Approximation

Matrix Properties & Linear Algebra Challenges
Uncertainty Quantification (UQ) is a phrase used to describe methodologies for taking account of uncertainties when mathematical and computer models are used to describe real-world phenomena and make predictions.
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Standard applied mathematics goes like this:

- Choose a model (e.g., a system of ODEs, PDEs etc).
- Choose inputs for the model.
- Find/approximate the solution (outputs).
What is Uncertainty Quantification?

But when we want to model **real-world processes** and predict quantities of interest (QoIs), the situation is more like this:
Types of Uncertainty

- **Model Uncertainty**
  Uncertainty in form of the model (scales of the physical process, missing physics etc).

- **Parameter/Input Uncertainty**
  Uncertainty in coefficients, material parameters, boundary conditions, initial conditions, geometry etc.

- **Numerical Error**
  Uncertainty (error) stemming from choice of discretisation, numerical approximation etc.

- ...
In **forward UQ**, we are concerned with the propagation of uncertainty from model inputs to outputs.
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In **inverse UQ**, given (possibly, noisy) measurements (data) related to the output of a model, estimate statistical properties of the *inputs* of the model.
Temperature Sensor Data (Copper)

Measured Temperature Rise (Copper)

Time (ms)

Temperature Rise (K)
Find $u(x)$ (the velocity) and $p(x)$ (the pressure) such that,

$$\begin{align*}
-\nu \nabla^2 u + u \cdot \nabla u + \nabla p &= f \quad \text{in } D, \\
\nabla \cdot u &= 0 \quad \text{in } D, \\
u \frac{\partial u}{\partial n} - n p &= 0 \quad \text{on } \partial D_N.
\end{align*}$$
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\[- \nu \nabla^2 u + u \cdot \nabla u + \nabla p = f \quad \text{in } D, \]
\[\nabla \cdot u = 0 \quad \text{in } D, \]
\[u = g \quad \text{on } \partial D_D, \]
\[\nu \frac{\partial u}{\partial n} - np = 0 \quad \text{on } \partial D_N. \]

If the viscosity is uncertain, we could model it as a random variable $\nu : \Omega \rightarrow \mathbb{R}$. For example, a uniform random variable with

\[\mathbb{E}[\nu] = \mu, \quad \text{Var}[\nu] = \sigma^2. \]
Example: Flow over a step

$\mu = 1/50$ and $\sigma = 1/500$. Streamlines of the **mean** flow (top) and **mean** pressure (bottom) computed with a **stochastic Galerkin mixed FEM**.
**Example: Flow over a step**

**Variance** of the magnitude of velocity (top) and **variance** of the pressure (bottom) computed with a **stochastic Galerkin mixed FEM**.
A simple model for groundwater flow is

\[ a^{-1} \mathbf{v} + \nabla u = 0, \quad \nabla \cdot \mathbf{v} = f. \]

If the diffusion coefficient \( a \) is spatially varying in an uncertain way, we typically model it as a random field (RF) \( a(x, \omega) : D \times \Omega \to \mathbb{R} \).

**Aim:** Estimate statistical QoIs associated with \( u = u(x, \omega) \) and \( \mathbf{v} = \mathbf{v}(x, \omega) \).
Methods for Forward UQ in PDEs

- Monte Carlo methods (also MLMC, ...)
- **Stochastic Galerkin FEMs (SGFEMs)**
- Stochastic collocation FEMs
- Reduced basis FEMs
- ...  

SGFEMs are not sampling methods.
Monte Carlo methods (also MLMC, …)

**Stochastic Galerkin FEMs (SGFEMs)**

Stochastic collocation FEMs

Reduced basis FEMs

…

**SGFEMs are not sampling methods.**

\[
\begin{align*}
   u(x, y) &\approx \hat{u}(x, y) = \sum_{i=1}^{n_x} \sum_{j=1}^{n_P} u_{ij} \phi_i(x) \psi_j(y) \\
\end{align*}
\]

Common complaints include:

- ‘intrusive’ method
- Black-box linear algebra tools don’t work (well)!
Express/approximate uncertain inputs as functions of a finite no. of independent random variables $\xi = (\xi_1, \ldots, \xi_m)$.

(Optimal) Reformulate stochastic PDE(s) as a parametric PDE(s).

$$y_i := \xi_i(\omega) \in \Gamma_i, \quad y = (y_1, \ldots, y_m) \in \Gamma,$$

where $\Gamma := \Gamma_1 \times \Gamma_2 \times \cdots \times \Gamma_m$. 

Write down a weak/variational form on $D \times \Gamma$.

Choose a FEM space $X = \text{span} \{\varphi_1, \ldots, \varphi_n\}$ on $D$.

Choose a set of polynomials $P = \text{span} \{\psi_1, \ldots, \psi_n\}$ on $\Gamma$.

Discretise the weak formulation by finding a Galerkin approximation $\hat{u} \in \hat{V} = X \otimes P$. 

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Scalar Problem: Elliptic PDE

Find $u : D \times \Omega \to \mathbb{R}$ such that $\mathbb{P}$-a.s.,

$$-\nabla \cdot (a(x, \omega) \nabla u(x, \omega)) = f(x), \quad x \in D \subset \mathbb{R}^d.$$
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$$-\nabla \cdot (a(x, \omega) \nabla u(x, \omega)) = f(x), \quad x \in D \subset \mathbb{R}^d.$$ 

Key assumption (in this talk):

$$a(x, \xi(\omega)) = a_0(x) + \sum_{i=1}^{m} a_i(x) \xi_i(\omega)$$

where $\xi_i : \Omega \to \Gamma_i$ are independent (iid) and bounded random variables.
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Parametric PDE: Find \( u : D \times \Gamma \to \mathbb{R} \) such that

\[
-\nabla \cdot (a(x, y) \nabla u(x, y)) = f(x), \quad x \in D, y \in \Gamma.
\]
Diffusion coefficient defined **piecewise** (on subdomains):

\[ a(x, y) = \sum_{i=1}^{5} a_i(x) y_i, \quad x \in D, \quad y \in \Gamma, \]

where \( y_i \in \Gamma_i \) and \( \Gamma := \Gamma_1 \times \Gamma_2 \times \cdots \times \Gamma_5 \).
Second-order RFs \( a(x, \omega) \in L^2(\Omega, L^2(D)) \) can be decomposed using the Karhunen-Loève (KL) expansion:

\[
a(x, \omega) = \mu(x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \phi_i(x) \xi_i(\omega)
\]

\( \mu(x) \) is the mean, \( \phi_i(x) \) are the eigenfunctions, and \( \xi_i(\omega) \) are the random variables with zero mean and unit variance. Truncating after \( m \) terms,

\[
a(x, \omega) \approx a_m(x, \xi(\omega)) = \mu(x) + \sum_{i=1}^{m} \sqrt{\lambda_i} \phi_i(x) \xi_i(\omega)
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The Karhunen–Loève Expansion

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a(x, \omega) = \mu(x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \phi_i(x) \xi_i(\omega)
\]

\( \lambda_i, \phi_i(x) \) are the eigenvalues and eigenfunctions of \( C(x, x') \).

\( \xi_1, \xi_2, \ldots \) are **uncorrelated** with mean zero and unit variance.

Truncating after \( m \) terms,

\[
a(x, \omega) \approx a_m(x, \xi(\omega)) = \mu(x) + \sum_{i=1}^{m} \sqrt{\lambda_i} \phi_i(x) \xi_i(\omega).
\]
Example: Gaussian Random Field

Let $\mu(x) = 0$ and consider the covariance function

$$C(x, x') = \exp\left(-\|x - x'|_1\right), \quad x, x' \in D = [0, 1] \times [0, 1].$$

Realisations of truncated RF $a_m(x, \xi)$ with $m = 5, 20, 50$. 
Find \( u(x, y) : D \times \Gamma \to \mathbb{R} \) such that

\[
-\nabla \cdot a(x, y) \nabla u(x, y) = f(x) \quad (x, y) \in D \times \Gamma,
\]

(+ zero boundary conditions) where

\[
a(x, y) = a_0(x) + \sum_{i=1}^{m} a_i(x) y_i.
\]

with \( 0 < a_{\text{min}} \leq a(x, y) \leq a_{\text{max}} < \infty \) a.e. in \( D \times \Gamma \).
Find \( u(x, y) : D \times \Gamma \rightarrow \mathbb{R} \) such that

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Now define the *(Bochner)* space:

\[V := L^2_\pi(\Gamma, H^1_0(D)) = \left\{ v : D \times \Gamma \rightarrow \mathbb{R} \mid \int_{\Gamma} \| v \|^2_{H^1_0(D)} \, d\pi(y) < \infty \right\}\]

where \( \pi \) is *prob. measure* associated with input random variables.
Find \( u \in V = L^2_\pi(\Gamma, H^1_0(D)) \) satisfying:

\[
\int_\Gamma \int_D a(x, y) \nabla u(x, y) \cdot \nabla v(x, y) \, dx \, d\pi(y) = \int_\Gamma \int_D f(x) v(x, y) \, dx \, d\pi(y)
\]

\( \forall v \in V. \)
Find $u \in V = L^2_\pi(\Gamma, H^1_0(D))$ satisfying:

$$
\mathbb{E} \left[ \int_D a(x, y) \nabla u(x, y) \cdot \nabla v(x, y) \, dx \right] = \mathbb{E} \left[ \int_D f(x) v(x, y) \, dx \right]
$$

$\forall v \in V$. 
Weak Formulation (3)

Find $u \in V = L^2(\Gamma, H_0^1(D))$ satisfying:

$$B(u, v) = F(v) \quad \forall v \in V.$$
Find \( u \in V = L^2_\pi(\Gamma, H^1_0(D)) \) satisfying:

\[
B(u, v) = F(v) \quad \forall v \in V.
\]

Here, we have

\[
B(u, v) = B_0(u, v) + \sum_{i=1}^{m} B_i(u, v)
\]

where

\[
B_0(u, v) = \mathbb{E} \left[ \int_D a_0(x) \nabla u(x, y) \cdot \nabla v(x, y) \, dx \right]
\]

\[
B_i(u, v) = \mathbb{E} \left[ \int_D a_i(x)y_i \nabla u(x, y) \cdot \nabla v(x, y) \, dx \right]
\]
Find $u \in X = L^2_\pi(\Gamma, H^1_0(D))$ such that

$Au = F$

with a (here, symmetric) operator

$A : X \to X^*$

and if

$0 < a_{min} \leq a(x, y) \leq a_{max} < \infty \quad \text{a.e. in } D \times \Gamma,$

then we have that $A$ is bounded and invertible.
Find $u \in V$ satisfying:

$$B(u, v) = F(v) \quad \forall v \in V.$$
Find \( u \in V \) satisfying:

\[
B(u, v) = F(v) \quad \forall v \in V.
\]

Choose a \textbf{finite-dimensional} set \( \hat{V} \subset V \) and find \( \hat{u} \in \hat{V} \subset V \) satisfying:

\[
B(\hat{u}, v) = F(v) \quad \forall v \in \hat{V}.
\]

Standard approach: use a \textbf{tensor product} approximation space

\[
\hat{u} \in \hat{V} = X \otimes \mathcal{P}
\]
\[ V = L^2_\pi(\Gamma, H^1_0(D)) \cong L^2_\pi(\Gamma) \otimes H^1_0(D), \quad \hat{V} = X \otimes \mathcal{P} \]

▷ \( X = \text{span} \{ \phi_i(x), i = 1: n_X \} \subset H^1_0(D) \) is a \textbf{finite element} space on \( D \).
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- \( X = \text{span} \{ \phi_i(x), i = 1 : n_X \} \subset H^1_0(D) \) is a finite element space on \( D \).
- \( \mathcal{P} = \text{span} \{ \psi_\alpha(y), \alpha \in J_P \} \subset L^2_\pi(\Gamma) \) is a set of polynomials on \( \Gamma \) associated with a finite set of multi-indices

\[ J_P \subset J = \{ \alpha = (\alpha_1, \ldots, \alpha_m) \in \mathbb{N}_0^m \}. \]
\[ V = L^2_\pi(\Gamma, H^1_0(D)) \cong L^2_\pi(\Gamma) \otimes H^1_0(D), \quad \hat{V} = X \otimes \mathcal{P} \]

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\[ J_P \subset J = \{ \alpha = (\alpha_1, \ldots, \alpha_m) \in \mathbb{N}_0^m \} \]

**Example:** Let \( m = 5 \) and choose \( \alpha = (1, 0, 2, 0, 10) \). If \( \psi_0(y_i) = 1 \), then

\[ \psi_\alpha(y) = \prod_{i=1}^{m} \psi_{\alpha_i}(y_i) = \psi_1(y_1)\psi_2(y_3)\psi_{10}(y_5). \]
Find $\hat{u} \in \hat{V} \subset V$ satisfying: $B(\hat{u}, v) = F(v)$, $\forall v \in \hat{V} \Rightarrow A\mathbf{u} = \mathbf{f}$.

Solving $A\mathbf{u} = \mathbf{f}$ gives the coefficients $u_{i,\alpha}$ that represent $\hat{u}$

$$\hat{u}(x, y) = \sum_{\alpha \in J_P} \sum_{i=1}^{n_X} u_{i,\alpha} \phi_i(x) \psi_\alpha(y)$$

$$= \sum_{\alpha \in J_P} u_\alpha(x) \psi_\alpha(y).$$

Also known as a (intrusive) polynomial chaos approximation.
Mean & Variance of SGFEM Approximation

Max expectation = 7.5814e-02.

Max variance = 5.0305e-05.
Given $A \in \mathbb{R}^{n \times m}$ and $B \in \mathbb{R}^{r \times s}$, the matrix **Kronecker product** is the matrix

$$A \otimes B := \begin{pmatrix}
  a_{11}B & a_{12}B & \ldots & a_{1m}B \\
  a_{21}B & a_{22}B & \ldots & a_{2m}B \\
  \vdots & \vdots & \ddots & \vdots \\
  a_{n1}B & a_{n2}B & \ldots & a_{nm}B
\end{pmatrix} \in \mathbb{R}^{nr \times ms}.$$ 

For example, for any matrix $B \in \mathbb{R}^{r \times s}$, 

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes B = \begin{pmatrix} B & 0 \\ 0 & B \end{pmatrix}.$$
We have a symmetric and positive definite coefficient matrix:

\[ A = G_0 \otimes K_0 + \sum_{i=1}^{m} G_i \otimes K_i, \]

and the number of equations is

\[ n_X n_P = \dim(X) \times \dim(P). \]
We have a \textbf{symmetric} and \textbf{positive definite} coefficient matrix:

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n_X n_P = \dim(X) \times \dim(P).
\]

- $K_0, K_i$ associated with $X$ (FEM space) and are typically \textit{sparse}.

\[
[K_0]_{r,s} = \int_{D} a_0(x) \nabla \phi_r(x) \cdot \nabla \phi_s(x) \, dx
\]

\[
[K_i]_{r,s} = \int_{D} a_i(x) \nabla \phi_r(x) \cdot \nabla \phi_s(x) \, dx.
\]
G-Matrices

- $G_0$, $G_i$ are associated with $\mathcal{P}$ (the polynomial space). If the basis polynomials $\psi_\alpha(y)$ are orthonormal (polynomial chaos)

\[
\mathbb{E}[\psi_\alpha(y)\psi_\beta(y)] = \int_\Gamma \psi_\alpha(y)\psi_\beta(y) d\pi(y) = \delta_{\alpha,\beta},
\]

then $G_0 = I$ and $G_i$ are also sparse.
G-Matrices

- \( G_0, G_i \) are associated with \( \mathcal{P} \) (the polynomial space). If the basis polynomials \( \psi_\alpha(y) \) are \textbf{orthonormal} (polynomial chaos)

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\]

then \( G_0 = I \) and \( G_i \) are also \textbf{sparse}.

- Since \( a(x,y) \) is a \textbf{linear} function of \( y_1, \ldots, y_m \),

\[
[G_i]_{r,s} = \mathbb{E} [y_i \psi_\alpha(y)\psi_\beta(y)] = \int_\Gamma y_i \psi_\alpha(y)\psi_\beta(y) \, \rho(y) \, dy
\]

\[
= \mathbb{E} [y_i \psi_\alpha(y_i)\psi_\beta(y_i)] \times \prod_{\ell=1,\ell\neq i}^m \mathbb{E} [\psi_\alpha_\ell(y_\ell)\psi_\beta_\ell(y_\ell)]
\]

= 0 if \( \alpha_\ell \neq \beta_\ell \).
1. Polynomials of total degree $\leq k$.

$$n_P = \frac{(m + k)!}{m!k!}$$

2. Polynomials of degree $\leq k$ in each variable.

$$n_P = (k + 1)^m$$

<table>
<thead>
<tr>
<th></th>
<th>$m = 5$</th>
<th>$m = 10$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$k = 1$</td>
<td>$k = 2$</td>
</tr>
<tr>
<td>1.</td>
<td>6</td>
<td>21</td>
</tr>
<tr>
<td>2.</td>
<td>32</td>
<td>243</td>
</tr>
</tbody>
</table>
\[ A = G_0 \otimes K_0 + \sum_{i=1}^{m} G_i \otimes K_i. \]

\( m = 4 \) random variables and polynomials of total degree \( k = 1, 2, 3 \).

Each \( \square \) is a matrix of the same size as the deterministic FEM problem.
For example, when \( a(x, y) = a_0(x) + \sum_{i=1}^{m} a_i(x) \psi_i(y) \).

\( G \)-matrices less sparse & matrix vector products more expensive.
For the elliptic PDE with KL-type coefficients

\[-\nabla \cdot (a(x, y)\nabla u(x, y)) = f(x), \quad a(x, y) = a_0(x) + \sum_{i=1}^{m} a_i(x)y_i,\]

we have

\[A = G_0 \otimes K_0 + \sum_{i=1}^{m} G_i \otimes K_i.\]

Problem-specific features:

- \(A\) is \textbf{symmetric} and \textbf{positive definite}.
- \(K_0, K_1, K_2, \ldots\) are \textbf{symmetric} and \textbf{sparse}
- \(K_0\) is \textbf{positive definite} (if \(a_0\) is a positive function)
- \(G_0, G_1, \ldots\) are \textbf{symmetric} and \textbf{sparse}; \textit{eigenvalues known explicitly.}
Example: Groundwater Flow

For the standard **mixed formulation** of elliptic PDE $+\ KL$-type coefficients

$$a(x, y)^{-1}v(x, y) + \nabla u(x, y) = 0$$
$$\nabla \cdot v(x, y) = f(x),$$

we have

$$A = \begin{pmatrix}
G_0 \otimes K_0 + \sum_{i=1}^{m} G_i \otimes K_i & G_0 \otimes B^T \\
G_0 \otimes B & 0
\end{pmatrix}.$$ 

Problem-specific features:

- $A$ is **symmetric** and **indefinite**.
- $K_0, K_1, K_2, \ldots$ are **symmetric** FEM mass matrices
- $K_0$ is **positive definite** (if $a_0$ is a positive function)
- $G_0, G_1, \ldots$ are **symmetric** and **sparse**; eigenvalues known explicitly.
Example: Navier-Stokes Equations

For the **nonlinear** (steady-state) Navier-Stokes equations, with parameter-dependent viscosity $\nu(y) = \nu_0 + \nu_1 y$,

$$-\nu(y) \nabla^2 u(x, y) + u(x, y) \cdot \nabla u(x, y) + \nabla p(x, y) = f(x)$$
$$\nabla \cdot u(x, y) = 0$$

after **linearisation**, we have a **sequence** of linear systems with
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$$\nabla \cdot u(x, y) = 0$$

after linearisation, we have a sequence of linear systems with

$$A_{n+1} = \begin{pmatrix} F_n & 0 & G_0 \otimes B_1^T \\ 0 & F_n & G_0 \otimes B_2^T \\ G_0 \otimes B_1 & G_0 \otimes B_2 & 0 \end{pmatrix}, \quad n = 0, 1, \ldots,$$

where $F_n = (\nu_0 G_0 + \nu_1 G_1) \otimes A + \sum_{\ell=0}^k H_\ell \otimes N_\ell^n$.

Here, $A_{n+1}$ is non-symmetric.
Example: Parabolic PDE

For the **time-dependent** heat equation with KL-type diffusion coefficients

\[
\frac{\partial u}{\partial t} = \nabla \cdot (a(x, y) \nabla u(x, y, t)) + f(x), \quad a(x, y) = a_0(x) + \sum_{i=1}^{m} a_i(x)y_i,
\]

after applying the SGFEM, we have a **system of ODEs**

\[
(G_0 \otimes M) \frac{du(t)}{dt} = \left( G_0 \otimes K_0 + \sum_{i=1}^{m} G_i \otimes K_m \right) u(t) + g_0 \otimes f.
\]

Applying a time-stepping scheme then gives a **sequence** of linear systems

\[ A_n u_n = f_{n-1}, \quad k = 1, 2, \ldots \]
Krylov methods generate approximations \( u_1, u_2, \ldots, u_k \) in a space 

\[
K_k(A, v_0) = \text{span} \{ v_0, Av_0, A^2v_0, \ldots, A^{k-1}v_0 \}.
\]

Widely available in software libraries as \textbf{black-box} tools:

- \texttt{pcg} - preconditioned conjugate gradient method
- \texttt{minres} - minimal residual method
- \texttt{gmres} - generalized residual method
- \texttt{bicgstab} - biconjugate gradient stabilized method
- \texttt{qmr} - quasi minimal residual method
- ...
\[ A = G_0 \otimes K_0 + \sum_{i=1}^{m} G_i \otimes K_i \]

**Golden Rule:** do not try to assemble A! (Forget direct solvers).

Can we solve \( Au = f \) using **standard iterative methods**? Need:

- **multiplications** with \( A \)
- application of \( P^{-1} \) (**preconditioners**) to vectors
- **memory** to store vectors of length \( n \times n_P \)!
\[ \mathbf{A}\mathbf{v} = \text{vec} \left( \sum_{i=0}^{m} K_i (G_i \mathbf{V}^\top)^\top \right), \quad \mathbf{V} = \text{array}(\mathbf{v}) \in \mathbb{R}^{n_X \times n_P} \]

\(\mathbf{A}\mathbf{v}\) can be computed via:

- \(n_X\) decoupled multiplications with the \(n_P \times n_P\) sparse matrices \(G_i\),
- \(n_P\) decoupled multiplications with the \(n_X \times n_X\) sparse matrices \(K_i\).

So, matrix-vector products with \(\mathbf{A}\)

- cost \((m + 1) \times O(n_X n_P)\) work (MC-FEM costs \(N \times O(n_X)\))
- are parallelisable.
SGFEM approximation of PDEs with random inputs leads to linear systems with matrices that are huge and have Kronecker structure.

For stochastically linear problems, choosing orthonormal parametric basis functions \( \{\psi_\alpha(y)\} \) brings sparsity.

Standard Krylov methods cannot be used in a black-box fashion.

What is a feasible preconditioning strategy? [Next Talk]

Memory requirements in particular can be an issue (the underlying continuous problem is high-dimensional). [Next Talk]
MATLAB toolbox for scalar elliptic problem: SIFISS

▷ http://www.manchester.ac.uk/ifiss/sifiss.html

Main contributors:
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▷ Adaptive SGFEM approximation

▷ Solver: Preconditioned conjugate gradient method.
References: UQ, SGFEM & Approximation Theory

Books

▷ R. Smith, Uncertainty Quantification, SIAM, 2014.


Papers


