

# Solving the Stochastic Steady-State Diffusion Problem Using Multigrid

Tengfei Su

Applied Mathematics and Scientific Computing

Advisor: Howard Elman  
Department of Computer Science

Sept. 29, 2015

# Outline

1 Background

2 Approach

3 Implementation

4 Validation

5 Extension

6 Schedule

7 Deliverables

8 Bibliography

# Background

- Steady-state diffusion equation

$$-\nabla \cdot (c(x)\nabla u(x)) = f(x), \quad x \in D$$

# Background

- Steady-state diffusion equation

$$-\nabla \cdot (c(x)\nabla u(x)) = f(x), x \in D$$

- differential coefficient and source term subject to uncertainty  
(heat conductivity, material porosity)

$$-\nabla \cdot (c(x, \omega)\nabla u(x, \omega)) = f(x, \omega), (x, \omega) \in D \times \Omega$$

# Background

- Steady-state diffusion equation

$$-\nabla \cdot (c(x)\nabla u(x)) = f(x), \quad x \in D$$

- differential coefficient and source term subject to uncertainty  
(heat conductivity, material porosity)

$$-\nabla \cdot (c(x, \omega)\nabla u(x, \omega)) = f(x, \omega), \quad (x, \omega) \in D \times \Omega$$

- Stochastic partial differential equations (SPDEs)

# Background

## Stochastic partial differential equations (SPDEs)

$$-\nabla \cdot (c(x, \omega) \nabla u(x, \omega)) = f(x, \omega), (x, \omega) \in D \times \Omega$$

- Monte Carlo Method (MCM)
  - large numbers of sampling
  - deterministic subproblem

# Background

## Stochastic partial differential equations (SPDEs)

$$-\nabla \cdot (c(x, \omega) \nabla u(x, \omega)) = f(x, \omega), (x, \omega) \in D \times \Omega$$

- Monte Carlo Method (MCM)
  - large numbers of sampling
  - deterministic subproblem
- Stochastic Finite Element Method (SFEM)
  - discretization of sample space
  - solving large linear system

# Background

## Stochastic partial differential equations (SPDEs)

$$-\nabla \cdot (c(x, \omega) \nabla u(x, \omega)) = f(x, \omega), (x, \omega) \in D \times \Omega$$

- Monte Carlo Method (MCM)
  - large numbers of sampling
  - deterministic subproblem
- Stochastic Finite Element Method (SFEM)
  - discretization of sample space
  - solving large linear system

Goal: Solving stochastic PDEs efficiently

- SFEM formulation
- Multigrid

# Boundary value problem

The stochastic steady-state diffusion equation

$$\begin{cases} -\nabla \cdot (c(x, \omega) \nabla u(x, \omega)) = f(x) & \text{in } D \times \Omega \\ u(x, \omega) = 0 & \text{on } \partial D \times \Omega \end{cases}$$

where

- stochastic coefficient  $c(x, \omega) : D \times \Omega \rightarrow \mathbb{R}$
- probability space  $(\Omega, \mathcal{F}, P)$
- random field  $u(x, \omega) : D \times \Omega \rightarrow \mathbb{R}$

# Boundary value problem

The stochastic steady-state diffusion equation

$$\begin{cases} -\nabla \cdot (c(x, \omega) \nabla u(x, \omega)) = f(x) & \text{in } D \times \Omega \\ u(x, \omega) = 0 & \text{on } \partial D \times \Omega \end{cases}$$

where

- stochastic coefficient  $c(x, \omega) : D \times \Omega \rightarrow \mathbb{R}$
- probability space  $(\Omega, \mathcal{F}, P)$
- random field  $u(x, \omega) : D \times \Omega \rightarrow \mathbb{R}$

We seek a weak solution  $u(x, \omega) \in H = H_0^1(D) \otimes L^2(\Omega)$  satisfying

$$\int_{\Omega} \int_D c(x, \omega) \nabla u(x, \omega) \cdot \nabla v(x, \omega) dx dP = \int_{\Omega} \int_D f(x) v(x, \omega) dx dP$$

for  $\forall v \in H$ .

## Karhunen-Loève expansion

If  $c(x, \omega)$  has continuous covariance function  $r(x, y)$ , then

$$c(x, \omega) \approx c_0(x) + \sum_{k=1}^m \sqrt{\lambda_k} c_k(x) \xi_k(\omega).$$

The eigenpair  $(\lambda_k, c_k(x))$  can be computed by

$$\int_D \frac{r(x, y)}{\nu} c_k(x) dx = \lambda_k c_k(y).$$

## Karhunen-Loève expansion

If  $c(x, \omega)$  has continuous covariance function  $r(x, y)$ , then

$$c(x, \omega) \approx c_0(x) + \sum_{k=1}^m \sqrt{\lambda_k} c_k(x) \xi_k(\omega).$$

The eigenpair  $(\lambda_k, c_k(x))$  can be computed by

$$\int_D \frac{r(x, y)}{\nu} c_k(x) dx = \lambda_k c_k(y).$$

Introducing KL expansion,

$$\int_{\Gamma} p(\xi) \int_D c(x, \xi) \nabla u(x, \xi) \cdot \nabla v(x, \xi) dx d\xi = \int_{\Gamma} p(\xi) \int_D f(x) v(x, \xi) dx d\xi$$

where  $p(\xi)$  is the joint density function,  $\Gamma$  is the joint image of  $\{\xi_k\}_{k=1}^m$ .

# SFEM formulation

Need a finite-dimensional subspace:

$$S = \text{span}\{\phi_1(x), \dots, \phi_N(x)\} \subset H_0^1(D)$$

$$T = \text{span}\{\psi_1(\xi), \dots, \psi_M(\xi)\} \subset L^2(\Gamma)$$

$$V^h = S \otimes T = \text{span}\{\phi(x)\psi(\xi), \phi \in S, \psi \in T\}$$

# SFEM formulation

Need a finite-dimensional subspace:

$$S = \text{span}\{\phi_1(x), \dots, \phi_N(x)\} \subset H_0^1(D)$$

$$T = \text{span}\{\psi_1(\xi), \dots, \psi_M(\xi)\} \subset L^2(\Gamma)$$

$$V^h = S \otimes T = \text{span}\{\phi(x)\psi(\xi), \phi \in S, \psi \in T\}$$

- $\phi(x)$  - piecewise linear/bilinear basis function

# SFEM formulation

Need a finite-dimensional subspace:

$$S = \text{span}\{\phi_1(x), \dots, \phi_N(x)\} \subset H_0^1(D)$$

$$T = \text{span}\{\psi_1(\xi), \dots, \psi_M(\xi)\} \subset L^2(\Gamma)$$

$$V^h = S \otimes T = \text{span}\{\phi(x)\psi(\xi), \phi \in S, \psi \in T\}$$

- $\phi(x)$  - piecewise linear/bilinear basis function
- $\psi(\xi)$  -  $m$ -dimensional “polynomial chaos” of order  $p$ 
  - orthogonality relationship

$$\int \psi_i(\xi) \psi_j(\xi) p(\xi) d\xi = \delta_{ij}$$

- dimension of subspace  $T$

$$M = \frac{(m+p)!}{m!p!}$$

# SFEM formulation

Find  $u_{hp} \in V^h$ , satisfying

$$\int_{\Gamma} p(\xi) \int_D c(x, \xi) \nabla u_{hp}(x, \xi) \cdot \nabla v(x, \xi) dx d\xi = \int_{\Gamma} p(\xi) \int_D f(x) v(x, \xi) dx d\xi$$

for  $\forall v \in V^h$ .

$$u_{hp}(x, \xi) = \sum_{j=1}^N \sum_{s=1}^M u_{jl} \phi_j(x) \psi_s(\xi)$$

$$v(x, \xi) = \phi_i(x) \psi_r(\xi), i = 1 : N, r = 1 : M$$

$$c(x, \omega) = c_0(x) + \sum_{k=1}^m \sqrt{\lambda_k} c_k(x) \xi_k(\omega)$$

# Matrix formulation

Find  $\mathbf{u} \in \mathbb{R}^{MN}$ , such that

$$A\mathbf{u} = \mathbf{f},$$

where

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1M} \\ A_{21} & A_{22} & \cdots & A_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{MM} \end{pmatrix}, \mathbf{f} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_M \end{pmatrix},$$

and

$$\mathbf{u} = [u_{11}, \dots, u_{N1}, \dots, u_{1M}, \dots, u_{NM}]^T$$

$$[\mathbf{f}_r]_i = \int_{\Gamma} p(\xi) \int_D f(x) \phi_i(x) \psi_r(\xi) dx d\xi$$

# Matrix formulation

The matrix block

$$A_{rs} = K_0 \int_{\Gamma} \psi_r(\xi) \psi_s(\xi) p(\xi) d\xi + \sum_{k=1}^m K_k \int_{\Gamma} \xi_k \psi_r(\xi) \psi_s(\xi) p(\xi) d\xi,$$

$$K_0(i,j) = \int_D c_0(x) \nabla \phi_i(x) \nabla \phi_j(x) dx,$$

$$K_k(i,j) = \int_D \sqrt{\lambda_k} c_k(x) \nabla \phi_i(x) \nabla \phi_j(x) dx.$$

# Matrix formulation

The matrix block

$$A_{rs} = K_0 \int_{\Gamma} \psi_r(\xi) \psi_s(\xi) p(\xi) d\xi + \sum_{k=1}^m K_k \int_{\Gamma} \xi_k \psi_r(\xi) \psi_s(\xi) p(\xi) d\xi,$$

$$K_0(i,j) = \int_D c_0(x) \nabla \phi_i(x) \nabla \phi_j(x) dx,$$

$$K_k(i,j) = \int_D \sqrt{\lambda_k} c_k(x) \nabla \phi_i(x) \nabla \phi_j(x) dx.$$

In tensor product notation,

$$A = G_0 \otimes K_0 + \sum_{k=1}^m G_k \otimes K_k.$$

# Multigrid

Solving linear system  $A\mathbf{u} = \mathbf{f}$ , where

- $A$  is symmetric and positive definite
- the choice of basis functions ensures that  $A$  is sparse
- $\text{size}(A) = MN \times MN$

$$N \sim \frac{1}{h^2}, M = \frac{(m+p)!}{m!p!}$$

(for  $h = 2^{-7}$ ,  $m = p = 4$ ,  $MN \sim 1,000,000$ )

# Multigrid

Solving linear system  $A\mathbf{u} = \mathbf{f}$ , where

- $A$  is symmetric and positive definite
- the choice of basis functions ensures that  $A$  is sparse
- $\text{size}(A) = MN \times MN$

$$N \sim \frac{1}{h^2}, M = \frac{(m+p)!}{m!p!}$$

(for  $h = 2^{-7}$ ,  $m = p = 4$ ,  $MN \sim 1,000,000$ )

Multigrid method has been successfully used in solving large sparse systems that arise from deterministic problems.

# Two-grid correction scheme

- fine grid space

$$V^h = S^h \otimes T, A\mathbf{u} = \mathbf{f}$$

coarse grid space

$$V^{2h} = S^{2h} \otimes T, \bar{A}\bar{\mathbf{u}} = \bar{\mathbf{f}}$$

fine grid correction space

$$V^h = V^{2h} + B^h$$

# Two-grid correction scheme

- fine grid space

$$V^h = S^h \otimes T, A\mathbf{u} = \mathbf{f}$$

coarse grid space

$$V^{2h} = S^{2h} \otimes T, \bar{A}\bar{\mathbf{u}} = \bar{\mathbf{f}}$$

fine grid correction space

$$V^h = V^{2h} + B^h$$

- prolongation operator

$$I_{2h}^h : V^{2h} \rightarrow V^h$$

restriction operator

$$I_h^{2h} : V^h \rightarrow V^{2h}$$

## Grid transfer operators

- If  $\mathbf{v}^{2h}$  is the coefficient vector of  $v_{2h}$  in  $V^{2h}$ , then the coefficient vector of  $v_{2h}$  in  $V^h$  is  $\mathcal{P}\mathbf{v}^{2h}$ . Prolongation matrix:

$$\mathcal{P} = I \otimes P.$$

- Restriction matrix is defined as

$$\mathcal{R} = I \otimes R = I \otimes P^T.$$

# Grid transfer operators

- If  $\mathbf{v}^{2h}$  is the coefficient vector of  $v_{2h}$  in  $V^{2h}$ , then the coefficient vector of  $v_{2h}$  in  $V^h$  is  $\mathcal{P}\mathbf{v}^{2h}$ . Prolongation matrix:

$$\mathcal{P} = I \otimes P.$$

- Restriction matrix is defined as

$$\mathcal{R} = I \otimes R = I \otimes P^T.$$

- Relations for matrix  $A$  and right-hand side  $\mathbf{f}$

$$\bar{A} = \mathcal{R} A \mathcal{P}, \bar{\mathbf{f}} = \mathcal{R} \mathbf{f}$$

## Two-grid correction scheme

- Smoother - reduce the fine grid component of the error

$$\mathbf{u} - \mathbf{u}^{(0)} = \mathbf{e}^{(0)} = P\mathbf{e}_{V^{2h}}^{(0)} + \mathbf{e}_{B^h}^{(0)}$$

$$\mathbf{e}^{(k)} = (I - Q^{-1}A)^k \mathbf{e}^{(0)} = P\mathbf{e}_{V^{2h}}^{(k)} + \mathbf{e}_{B^h}^{(k)}$$

## Two-grid correction scheme

- Smoother - reduce the fine grid component of the error

$$\mathbf{u} - \mathbf{u}^{(0)} = \mathbf{e}^{(0)} = P\mathbf{e}_{V^{2h}}^{(0)} + \mathbf{e}_{B^h}^{(0)}$$

$$\mathbf{e}^{(k)} = (I - Q^{-1}A)^k \mathbf{e}^{(0)} = P\mathbf{e}_{V^{2h}}^{(k)} + \mathbf{e}_{B^h}^{(k)}$$

- Stationary iteration

$$A = Q - Z, A\mathbf{u} = \mathbf{f} \Rightarrow Q\mathbf{u} = Z\mathbf{u} + \mathbf{f}$$

$$\begin{aligned}\mathbf{u}^{k+1} &= Q^{-1}Z\mathbf{u}^{(k)} + Q^{-1}\mathbf{f} \\ &= Q^{-1}(Q - A)\mathbf{u}^{(k)} + Q^{-1}\mathbf{f} \\ &= (I - Q^{-1}A)\mathbf{u}^{(k)} + Q^{-1}\mathbf{f}\end{aligned}$$

# Two-grid correction scheme

- **Algorithm**

Choose initial guess  $\mathbf{u}^{(0)}$

for  $i = 0$  until convergence

    for  $j = 1 : k$

$$\mathbf{u}^{(i)} = (\mathbf{I} - \mathbf{Q}^{-1}\mathbf{A})\mathbf{u}^{(i)} + \mathbf{Q}^{-1}\mathbf{f} \text{ (smoothing)}$$

    end

$$\bar{\mathbf{r}} = \mathcal{R}(\mathbf{f} - \mathbf{A}\mathbf{u}^{(i)}) \text{ (restrict residual)}$$

$$\text{solve } \bar{\mathbf{A}}\bar{\mathbf{e}} = \bar{\mathbf{r}}$$

$$\mathbf{u}^{(i+1)} = \mathbf{u}^{(i)} + \mathcal{P}\bar{\mathbf{e}} \text{ (prolong and update)}$$

end

- For multigrid, apply the above scheme recursively

# Implementation

- Platform: Macbook Air, 1.6 GHz Intel Core i5, 4 GB 1600 MHz DDR3  
Language: MATLAB R2015a
- IFISS & S-IFISS for producing Galerkin system  
(Incompressible Flow & Iterative Solver Software)
- Multigrid routine
  - grid transfer operators
  - smoother
  - iterative method

# Validation

- Model problem:  $D = (-1, 1)^2$ ,  $f = 1$ . Covariance function

$$r(x, y) = \nu \exp\left(-\frac{1}{b}|x_1 - y_1| - \frac{1}{b}|x_2 - y_2|\right)$$

# Validation

- Model problem:  $D = (-1, 1)^2$ ,  $f = 1$ . Covariance function

$$r(x, y) = \nu \exp\left(-\frac{1}{b}|x_1 - y_1| - \frac{1}{b}|x_2 - y_2|\right)$$

- KL expansion

$$c(x, \omega) = c_0(x) + \sum_{k=1}^m \sqrt{\lambda_k} c_k(x) \xi_k(\omega)$$

- Normal distribution

$$\Omega = \mathbb{R}^m, p(\xi) = \frac{1}{(2\pi\nu)^{\frac{m}{2}}} e^{-\frac{\xi^2}{\nu^2}}, \text{ Hermite polynomials}$$

- Uniform distribution

$$\Omega = (-1, 1)^m, p(\xi) = \frac{1}{2^m}, \text{ Legendre polynomials}$$

# Validation

- Comparison with Monte Carlo
- Multigrid analysis
  - textbook convergence rate, independent of  $h$
  - independent of  $m, p$

# Extension

- Galerkin solution

$$\mathbf{u} = [u_{11}, \dots, u_{N1}, \dots, u_{1M}, \dots, u_{NM}]^T$$

$$U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1M} \\ u_{21} & u_{22} & \cdots & u_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ u_{N1} & u_{N2} & \cdots & u_{NM} \end{pmatrix}$$

# Extension

- Galerkin solution

$$\mathbf{u} = [u_{11}, \dots, u_{N1}, \dots, u_{1M}, \dots, u_{NM}]^T$$

$$U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1M} \\ u_{21} & u_{22} & \cdots & u_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ u_{N1} & u_{N2} & \cdots & u_{NM} \end{pmatrix}$$

- Matrix form

$$A\mathbf{u} = \mathbf{f}, \quad A = G_0 \otimes K_0 + \sum_{k=1}^m G_k \otimes K_k$$

$$\Rightarrow K_0 U G_0 + \sum_{k=1}^m K_k U G_k = F$$

# Extension

- Seek low-rank approximation

$$U \approx U_k = V_k W_k^T, \quad V_k \in \mathbb{R}^{N \times k}, \quad W_k \in \mathbb{R}^{M \times k}, \quad k \ll N, M$$

which significantly reduce the computational cost.

- Seek low-rank approximation

$$U \approx U_k = V_k W_k^T, \quad V_k \in \mathbb{R}^{N \times k}, \quad W_k \in \mathbb{R}^{M \times k}, \quad k \ll N, M$$

which significantly reduce the computational cost.

- Compute  $U_k$  with iterative methods
- Richardson, conjugate gradient(CG), Biconjugate gradient stabilized method(BiCGstab)
- Multigrid

# Schedule

- 10/15 Generate Galerkin system from IFISS/S-IFISS  
Write the multigrid routine
- 11/15 Validation with multigrid analysis and Monte Carlo
- 12/15 Mid-year presentation
- 02/16 Implement multigrid for low-rank approximate solutions
- 03/16 Implement BiCGstab for low-rank approximate solutions (if time permitting)
- 04/16 Collect computational results.
- 05/16 Final presentation

# Deliverables

- Multigrid routine for Stochastic Galerkin system
- Multigrid routine for Low-rank approximation
- Documented code
- Reports and presentations

# References

- ① Ghanem, R. G. & Spanos, P. D. (1991) *Stochastic Finite Elements: A Spectral Approach*. New York: Springer.
- ② Elman, H. & Furnival D. (2007) Solving the stochastic steady-state diffusion problem using multigrid. *IMA Journal of Numerical Analysis* **27**, 675–688.
- ③ Powell, C. & Elman H. (2009) Block-diagonal preconditioning for spectral stochastic finite-element systems. *IMA Journal of Numerical Analysis* **29**, 350–375.
- ④ Kressner D. & Tobler C. (2011) Low-rank tensor Krylov subspace methods for parametrized linear systems. *SIAM Journal of Matrix Analysis and Applications* **32.4**, 1288–1316.
- ⑤ Xiu, D. & Karniadakis G. M. (2003) Modeling uncertainty in flow simulations via generalized polynomial chaos. *Journal of Computational Physics* **187**, 137–167.
- ⑥ Elman, H., Sylvester, D. & Wathen, A. (2014) *Finite Elements and Fast Iterative Solvers: with Applications in Incompressible Fluid Dynamics*. Oxford: Oxford University Press.
- ⑦ Sylvester, D., Elman, H. & Ramage, A. Incompressible Flow and Iterative Solver Software, <http://www.cs.umd.edu/~elman/ifiss/index.html>.

# The End

- Thank you!
- Questions?