Efficient Solution Algorithms for Partial Differential Equations with Random Coefficients

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Problem Statement and Assumptions

Diffusion equation $-\nabla \cdot (a(\mathbf{x}, \omega)\nabla u) = f$ on $\mathcal{D} \subset \mathbb{R}^d$,
with suitable boundary conditions

Initial Assumptions

Coercivity: $0 < \alpha_1 \leq a \leq \alpha_2 < \infty \;\Rightarrow$ well posed

Finite expansion: $a(\mathbf{x}, \boldsymbol{\xi}) = a_0 + \sigma \sum_{r=1}^{m} a_r(\mathbf{x})\boldsymbol{\xi}_r$

Independence: $\{\xi_r = \xi_r(\omega)\}$ uncorrelated with density functions $\rho_r(\xi_r)$,
joint density $\rho(\boldsymbol{\xi}) = \rho_1(\xi_1)\rho_2(\xi_2)\cdots\rho_r(\xi_r)$

Stochastic Galerkin: FEM/FD in space,
Polynomial chaos of total degree p in $\boldsymbol{\xi}$

$\longrightarrow$ Requirement: Solve one large algebraic system $A\mathbf{u} = \mathbf{f}$

$$A = G_0 \otimes A_0 + \sum_{r=1}^{m} G_r \otimes A_r$$

Stochastic collocation: "level-p"

$\longrightarrow$ Solve multiple systems of standard structure

Multigrid Methods for the Stochastic Problems

I. Apply multigrid across spatial component (E. & Furnival)

Solving $A\mathbf{u} = \mathbf{f}$, $\quad A = G_0 \otimes A_0^{(h)} + \sum_{r=1}^{m} G_r \otimes A_r^{(h)}$

$$[A_r]_{jk} = \int_{\mathcal{D}} a_r(x) \nabla\phi_k(x) \cdot \nabla\phi_j(x) dx, \quad [G_r]_{lq} = \int_{\Gamma(\Omega)} \xi_r \psi_q(\xi) \psi_l(\xi) \rho(\xi) d\xi$$

Fine grid operators: $A^{(h)}$, $A_r^{(h)}$ spatial discretization parameter h
Course grid operators: $A^{(2h)}$, $A_r^{(2h)}$ spatial discretization parameter $2h$

One multigrid (two-grid) step:

for $j = 1 : k$
$\quad u^{(h)} \leftarrow (I - Q^{-1}A^{(h)})u^{(h)} + Q^{-1}f^{(h)}$ $\quad$ k smoothing steps
end
$r^{(2h)} = \mathcal{R}(f^{(h)} - A^{(h)}u^{(h)})$ $\quad$ Restriction
Solve $A^{(2h)}c^{(2h)} = r^{(2h)}$ $\quad$ Coarse grid correction $\mathcal{R} = I \otimes R$
$u^{(h)} \leftarrow u^{(h)} + \mathcal{P}c^{(2h)}$ $\quad$ Prolongation $\mathcal{P} = I \otimes P$

Sketch of convergence analysis: Use "standard" approach

$$e^{(i+1)} = [(A^{(h)})^{-1} - \mathcal{P}(A^{(2h)})^{-1}\mathcal{R}]\,[A^{(h)}(I - Q^{-1}A^{(h)})^k]\,e^{(i)}$$

Establish for all y

Approximation property $\left\|[(A^{(h)})^{-1} - \mathcal{P}(A^{(2h)})^{-1}\mathcal{R}]y\right\|_{A^{(h)}} \leq \|y\|_2$

Smoothing property $\left\|A^{(h)}(I - Q^{-1}A^{(h)})^k y\right\|_2 \leq \|y\|_{A^{(h)}}$

For approximation property: Introduce *semi-discrete space* $H_0^1(\mathcal{D}) \otimes \mathcal{T}^{(p)}$

$\mathcal{T}^{(p)}$ = discrete stochastic space

Weak formulation: $a(u^{(p)}, v^{(p)}) = (f, v^{(p)})$ for all $v^{(p)} \in H_0^1(\mathcal{D}) \otimes \mathcal{T}^{(p)}$

Then:
$$\begin{aligned}\left\|[(A^{(h)})^{-1} - \mathcal{P}(A^{(2h)})^{-1}\mathcal{R}]y\right\|_{A^{(h)}} &= \|u^{(hp)} - u^{(2h,p)}\|_a \\ &\leq \|u^{(hp)} - u^{(p)}\|_a + \|u^{(p)} - u^{(2h,p)}\|_a \\ &\leq c\|y\|_{A^{(h)}}\end{aligned}$$

Last step: from standard arguments based on approximability, regularity for *every realization* in the semi-discrete space

Mean-Based Multigrid

II. Apply multigrid to mean as preconditioner

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

Preconditioner for use with CG (Kruger, Pellisetti, Ghanem):

Mean $Q = G_0 \otimes A_0$

$A_0 \sim \int_{\mathcal{D}} a_0(x) \nabla \phi_k(x) \cdot \nabla \phi_j(x) dx, \quad G_0 = I$

Further refinement (Le Maitre et al.)

Use multigrid to approximate action of Q^{-1}:

$$Q_{MG}^{-1} \equiv I \otimes A_{0,MG}^{-1}$$

Convergence analysis (E. & Powell):

Coefficient:	$a(\mathbf{x},\boldsymbol{\xi}) = a_0 + \sigma \sum_{r=1}^m a_r(\mathbf{x})\xi_r$
Coefficient matrix:	$A = G_0 \otimes A_0 + \sum_{r=1}^m G_r \otimes A_r$
Mean-based preconditioner:	$Q = G_0 \otimes A_0$
Multigrid preconditioner:	$Q_{MG} = G_0 \otimes A_{0,MG}$

Theorem: For $a_0 = \mu$ constant,

$$1 - \tau \le \frac{(w,Aw)}{(w,Qw)} \le 1 + \tau$$

where $$\tau = (\sigma/\mu)\, c(p) \sum_{r=1}^m \sqrt{\lambda_r}\, \|a_r\|_\infty .$$

If in addition the MG approximation satisfies $\beta_1 \le \frac{(w,Qw)}{(w,Q_{MG}w)} \le \beta_2$, then

$$\frac{(w,Aw)}{(w,Q_{MG}w)} = \frac{(w,Aw)}{(w,Qw)}\ \frac{(w,Qw)}{(w,Q_{MG}w)} \le \left(\frac{1+\tau}{1-\tau}\right)\left(\frac{\beta_2}{\beta_1}\right)$$

Comments

- Establishes textbook convergence of multigrid, rate independent of spatial discretization parameter h
- Minimal dependence on stochastic parameter p.
- Applies to any basis for stochastic space
- Second method: simpler but more dependent on # terms m

Alternative: Collocation Methods

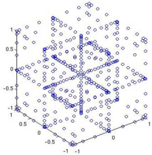
Monte-Carlo (sampling) method: find $u \in H^1_E(\mathcal{D})$ s.t.

$$\int_{\mathcal{D}} a(\mathbf{x}, \boldsymbol{\xi}_k) \nabla u \cdot \nabla v dx \quad \text{for all } v \in H^1_{E_0}(\mathcal{D})$$

for a collection of samples $\{\boldsymbol{\xi}_k\} \in L^2(\Gamma)$

Collocation (Xiu, Hesthaven, Babuška, Nobile, Tempone, Webster)

Choose $\{\boldsymbol{\xi}_k\}$ in a special way (sparse grids), then construct discrete solution $u^{(hp)}(\mathbf{x}, \boldsymbol{\xi}) \in \mathcal{S}^E_h \otimes \mathcal{T}^{(p)}$ to interpolate $\{u_h(\mathbf{x}, \boldsymbol{\xi}_k)\}$



Advantages (vs. stochastic Galerkin):
- decouples algebraic system (like MC)
- applies in a straightforward way to nonlinear random terms

Disadvantage: dimensionality $\sim 2^p \times$ (Galerkin) for comparable accuracy

Experimental Comparison

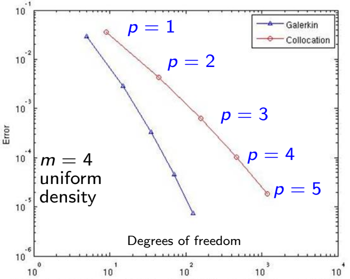
E., Miller, Phipps, Tuminaro

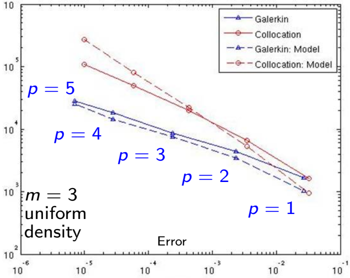
To the right: **Accuracy**

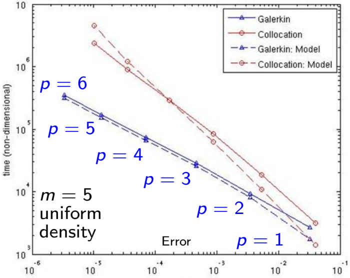
$p =$ polynomial degree for Galerkin
level for collocation
Gaussian abscissas with linear growth

Errors are comparable

Below: **Performance**







Experimental Results: CPU Times

Performed on a serial machine with C code and
CG/AMG code from Trilinos
Truncated Gaussian density

Observation: Galerkin faster, more so as number of stochastic variables (KL terms) grows

	Galerkin			Collocation		
p	$m=5$	$m=10$	$m=12$	$m=5$	$m=10$	$m=12$
1	.058	.147	.263	.069	.163	.218
2	.269	1.20	2.00	.532	2.13	3.17
3	1.20	13.14	24.50	2.41	16.99	29.31
4	3.50	53.79	121.61	8.31	102.60	200.94
5	6.51	117.73		24.56	515.74	

Discussion

Shows Galerkin formulation is tractable

In these circumstances, cheaper than collocation
But: intrusive

Requirements:

- **Linear** dependence on stochastic parameters
- Knowledge of joint density function for parameters

Problem Statement

Diffusion equation $-\nabla \cdot (c(\mathbf{x},\omega)\nabla u) = f$ on $\mathcal{D} \subset \mathbb{R}^d$,
with suitable boundary conditions

Diffusion coefficient $c(\mathbf{x},\omega)$ is a log-normal random field

$$\begin{aligned} k(\mathbf{x},\omega) &= \exp(a(\mathbf{x},\omega)) \\ a(\mathbf{x},\omega) = \log k(\mathbf{x},\omega) &= a_0(\mathbf{x}) + \sigma \textstyle\sum_{m=1}^{\infty} \sqrt{\lambda_m}\, a_m(\mathbf{x})\xi_m(\omega) \\ &\approx \underbrace{a_0(\mathbf{x}) + \sigma \textstyle\sum_{m=1}^{M} \sqrt{\lambda_m}\, a_m(\mathbf{x})\xi_m(\omega)}_{\text{Will use finite-term expression in sequel}^{\dagger}} \end{aligned}$$

Complication: Galerkin much less straightforward when coefficient is nonlinear in $\boldsymbol{\xi}$.

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† For simplicity, we will also take $\{\xi_m\}$ to have *truncated Gaussian distributions*.

New Approach: Convection-Diffusion Formulation

E., Ernst & Ullmann

Diffusion equation $-\nabla \cdot (e^a \nabla u) = f$

Expand using product rule:

$$e^a \left(-\nabla^2 u - \nabla a \cdot \nabla u\right) = f$$

$\longrightarrow$ **Convection-diffusion problem**

$$-\nabla^2 u + \mathbf{w} \cdot \nabla u = e^{-a} f, \quad \mathbf{w} = -\nabla a$$

N.B. This connection is long known, e.g., Varga et al., 1966
Presented in other direction: existence of velocity potential enables recasting of convection-diffusion equation as diffusion equation

Key point:

$$\mathbf{w} = -(\nabla a_0 + \sigma \textstyle\sum_{m=1}^{M} \sqrt{\lambda_m}\, \nabla a_m(\mathbf{x}) \xi_m) \quad \text{is } \textbf{linear} \text{ in } \boldsymbol{\xi}$$

Matrix structure

Extended weak formulation

$$\int_\Gamma \int_{\mathcal{D}} \nabla u \cdot \nabla v - \int_\Gamma \int_{\mathcal{D}} \nabla a_0 \, v - \sigma \sum_{m=1}^{M} \sqrt{\lambda_m} \int_\Gamma \int_{\mathcal{D}} \nabla a_m \, v = \int_\Gamma \int_{\mathcal{D}} e^{-a} f v$$

Generalized polynomial chaos discretization $\longrightarrow$ coefficient matrix:

$$C = I \otimes (L + N_0) + \sum_{m=1}^{M} G_m \otimes N_m$$

L	discrete diffusion operator
N_0	convection term from mean ∇a_0
N_m	convection terms from terms ∇a_m in expansion of ∇a

Advantage: matrix is sparse

Slight disadvantage: matrix is nonsymmetric

For iterative solution: use preconditioned GMRES

Solution Algorithms for Convection-Diffusion Form

Linear system for stochastic Galerkin $Cu = f$

$$C = I \otimes (L + N_0) + \sum_{m=1}^{M} G_m \otimes N_m$$

Right-oriented preconditioning:

Solve $[CP^{-1}]\hat{u} = f$ using GMRES, $u = P^{-1}\hat{u}$

Options for preconditioning

- Diffusion preconditioner: $P = I \otimes L$, n_ξ decoupled diffusion operators
- Mean-based preconditioner: $P = I \otimes (L + N_0)$, n_ξ decoupled *convection-diffusion* operators (provided ∇a_0 is nonzero)
- Refinement: Action of P^{-1}: approximated using multigrid

Representative Analysis

Diffusion preconditioner $P = I \otimes L$:

Consider (generalized) field of values

$$\mathrm{FOV}(C, P) = \left\{ \frac{(\mathbf{v}, C\mathbf{v})}{(\mathbf{v}, P\mathbf{v})} \,:\, \mathbf{v} \in \mathbb{C}^{n_x n_\xi}, \mathbf{v} \neq \mathbf{0} \right\}.$$

Theorem

For the diffusion preconditioner, FOV(C, P) is contained in the circle

$$\{ z \in \mathbb{C} \,:\, |z - 1| \le 2\, c_{\mathcal{D}}\, c_L \}, \quad c_L = \|\nabla a_0\|_\infty + \sigma \nu_{p+1} \sum_{m=1}^{M} \sqrt{\lambda_m} \|\nabla a_m\|_\infty,$$

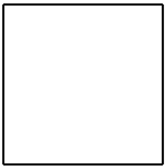
where $\|\nabla a_m\|_\infty = \sup_{\mathbf{x} \in \mathcal{D}} |\nabla a_m(\mathbf{x})|$,

ν_{p+1} = *largest root of orthonormal Rys polynomial of degree* $p + 1$,

$c_{\mathcal{D}} > 0$ *is a constant independent of* h, σ *and* p.

Experimental Results

Benchmark problems



$a = \log k(\mathbf{x}, \boldsymbol{\xi})$ constructed from

$a_0 = 1 + 10x^2$ ($\nabla a_0 \neq 0$)

$\mathrm{Cov}(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp\left(-(\|\mathbf{x} - \mathbf{y}\|_2/\ell)^2\right)$

Problem 1: $\ell = 1$, $M = 5$ term truncated KL exp

Problem 2: $\ell = .5$, $M = 10$-term truncated KL exp

Both: capture 95% of total variance

Iteration Counts

Mean-based $P = I \otimes (L + N_0)$ vs. Diffusion $P = I \otimes L$

Problem 1
$\ell = 1$
$M = 5$

n	σ	p=1	2	3	4	p=1	2	3	4
32	0.1	6	6	6	6	23	25	25	25
64	-	6	6	6	6	23	24	24	24
128	-	5	5	5	5	21	22	22	22
32	1.0	8	9	9	10	26	29	31	32
64	-	7	8	9	9	25	28	30	30
128	-	7	8	8	9	23	26	28	29
32	2.0	10	12	14	15	28	33	36	38
64	-	9	11	13	14	27	31	34	36
128	-	9	11	12	13	25	29	32	34

Problem 2
$\ell = .5$
$M = 10$

n	σ	p=1	2	3	4	p=1	2	3	4
32	0.1	6	6	6	6	24	25	26	25
64	-	6	6	6	6	23	24	25	24
128	-	6	6	5	6	21	23	23	22
32	1.0	10	12	13	14	28	32	34	32
64	-	9	12	13	14	26	30	32	30
128	-	9	11	12	13	25	29	30	29
32	2.0	13	19	24	28	30	37	41	46
64	-	12	18	23	27	29	35	39	44
128	-	12	17	21	26	28	33	37	41

Discussion

- Again: establishes textbook MG convergence wrt spatial mesh
- Overcomes difficulties associated with nonlinearity of lognormal coefficients
- One caveat: for series approximation to ∇a
  Require a to be mean-square continuously differentiable
  (λ_m, a_m): eigenpairs derived from covariance of a, $\mathrm{Cov}(\mathbf{x}, \mathbf{y})$
  OK: $c(\mathbf{x}, \mathbf{y}) = exp\left(-(\|\mathbf{x} - \mathbf{y}\|_2/\ell)^2\right)$
  Not: $c(\mathbf{x}, \mathbf{y}) = exp\left(-\|\mathbf{x} - \mathbf{y}\|_1/\ell\right)$

Restrictions for Ideas Above

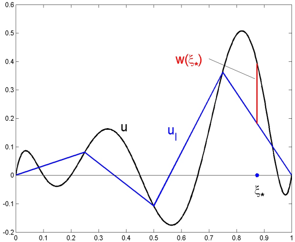
Some restrictions of the approaches just discussed:

- Generally do not have joint pdf for diffusion coefficient
  - Ignored in part I above
  - Worked around in part II (with some limitations)
- Some issues for collocation
  - Simpler than Galerkin (**non-intrusive**), but not cheaper
  - Requires regularity in $\boldsymbol{\xi}$

To address these (E & Miller):

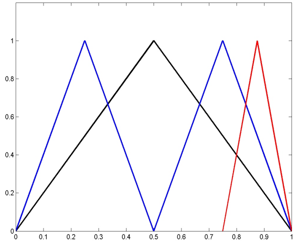
- For pdf: use kernel density estimation methods
- For costs of collocation: use adaptive sparse grid collocation

Adaptive Sparse Grid Collocation



Collocation based on interpolation

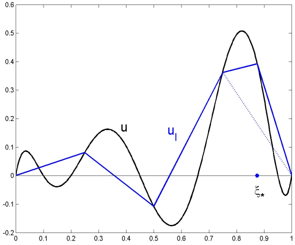
Consider function $u(\xi)$ at left
piecewise linear interpolant $u_I(\xi)$
$\xi_* =$ child, node at next level uniform grid
$w(\xi_*) =$ interpolation error at ξ_*:



Ma & Zabaras: If $u_i(\xi)$ is represented using *hierarchical basis* (left), then
$w(\xi_*) =$ coefficient of basis function in interpolant on refined grid

Strategy: Refine grid using child ξ_* iff $|w(\xi_*)| >$ tolerance

Adaptive Sparse Grid Collocation



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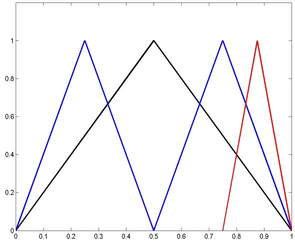


Ma & Zabaras: If $u_i(\xi)$ is represented using *hierarchical basis* (left), then
$w(\xi_*) =$ coefficient of basis function
in interpolant on refined grid

Strategy: Refine grid using child ξ_*
iff $|w(\xi_*)| >$ tolerance

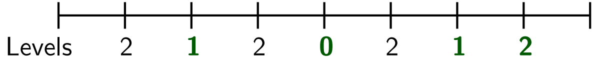
Algorithm: Adaptive interpolation with hierarchical basis functions

Set $\mathcal{A}_0(u)(\xi) = 0$
Set $k = 1$
Set $\Delta\theta^1_{adaptive} = \theta^1$
repeat
  $\Delta\theta^{k+1}_{adaptive} = \emptyset$
  for $\xi_j^{\Delta k} \in \Delta\theta^k_{adaptive}$
    $w_j^k = u(\xi_j^{\Delta k}) - \mathcal{A}_{k-1}(u)(\xi_j^{\Delta k})$
    if $||w_j^k|| > \tau$ **then**
      $\Delta\theta^{k+1}_{adaptive} = \Delta\theta^{k+1}_{adaptive} \cup child(\xi_j^{\Delta k})$
    endif
  endfor
  Set $\mathcal{A}_k(u)(\xi) = \sum_{i=1}^k \sum_j w_j^i \psi_j^i(\xi)$
  $k = k + 1$
until $max(||w_j^{k-1}||) < \tau$

Augment interpolant at refined grid nodes only where interpolation error is too large

Interpolant = sum(levels)
all level-k basis functions

To Use this Idea with Diffusion Equation $-\nabla \cdot (a(\mathbf{x}, \xi) \nabla u) = f$



- Start with $\xi^{(0)}$, compute solution $u(\mathbf{x}, \boldsymbol{\xi}_{(0)})$
  Determines interpolant $[\mathcal{A}^{(0)} u](\mathbf{x}, \xi)$
- Identify children $\{\boldsymbol{\xi}_j^{(1)}\}$ of $\xi^{(0)}$
  Compute solutions $\{u(\mathbf{x}, \boldsymbol{\xi}_j^{(1)})\}$, add $\{\boldsymbol{\xi}_j^{(1)}\}$ to set of collocation points according to adaptive strategy with tolerance test
  $$\|w_j^k\|_\infty \rho(\boldsymbol{\xi}_j^{\Delta k}) > \tau$$
  Determines interpolant $[\mathcal{A}^{(1)} u](\mathbf{x}, \xi)$
- Repeat: identify children of "level-1" points, compute solutions, etc.

Result: Collocation solution $\mathcal{A}^{(k)} u$

Approximate moments, distributions of u using $\mathcal{A}^{(k)} u$

Kernel Density Estimation

Given N samples of ξ, estimate density function by

$$\hat{\rho}(\xi) = \frac{1}{Nh^M} \sum_{k=1}^{N} K\left(\frac{\xi - \xi^{(i)}}{h}\right)$$

For bandwidth h, use *maximum likelihood cross-validation*: maximize

$$CV(h) \equiv \frac{1}{N} \sum_{i=1}^{N} log(\hat{\rho}_{-i}(\xi^{(i)}))$$

where

$$\hat{\rho}_{-i}(\xi) = \frac{1}{Nh^M} \sum_{k=1,k\neq i}^{N} K\left(\frac{\xi - \xi^{(k)}}{h}\right)$$

For $K(\xi)$, use Epanechnikov kernel

$$K(\xi) = \left(\frac{3}{4}\right)^M \prod_{i=1}^{M} (1 - \xi_i^2) \mathbb{1}_{\{-1 \leq \xi_i \leq 1\}}$$

Experimental Results

Test problem:

$$-\frac{d}{dx} a_M(x,\boldsymbol{\xi}) \frac{d}{dx} u(x,\boldsymbol{\xi}) = 1 \quad \forall\ x \in (0,1)$$

$$u(0,\boldsymbol{\xi}) = u(1,\boldsymbol{\xi}) = 0$$

$$a_M = \mu + \sum_{k=0}^{M/2-1} \lambda_k(\xi_{2k} cos(2\pi kx) + \xi_{2k+1} sin(2\pi kx))$$

$$\mu = 3,\ \lambda_k = exp(-k)$$

ξ_k uniformly distributed on $[0,1]$

Experiment: Generate N samples of $\boldsymbol{\xi}$
Use them to generate estimate $\hat{\rho}(\boldsymbol{\xi})$
Use $\hat{\rho}$ to generate adaptive collocation solution $\mathcal{A}u$

Compare with:

Use the same N samples to perform Monte-Carlo simulation

Representative Results: $M = 10$ parameters

N	τ				
	5×10^{-2}	1×10^{-3}	5×10^{-4}	1×10^{-4}	5×10^{-5}
100 9.08×10^{-2}	7.66×10^{-3} **(76)**	8.86×10^{-4} (1026)	4.41×10^{-4} (1655)	4.48×10^{-5} (5026)	8.28×10^{-6} (8111)
500 4.06×10^{-2}	7.13×10^{-3} **(92)**	6.08×10^{-4} (1170)	3.36×10^{-4} (1189)	2.34×10^{-5} (5773)	1.01×10^{-5} (9404)
1000 2.87×10^{-2}	9.19×10^{-3} **(59)**	6.03×10^{-4} (1216)	2.65×10^{-4} (1989)	1.95×10^{-5} (5996)	1.77×10^{-5} (9664)
5000 1.28×10^{-2}	7.16×10^{-3} **(93)**	6.62×10^{-4} **(1120)**	3.03×10^{-4} **(2041)**	2.04×10^{-5} (6095)	1.02×10^{-5} (9787)
20000 6.42×10^{-3}	7.25×10^{-3} **(93)**	6.27×10^{-4} **(1187)**	2.66×10^{-4} **(2127)**	1.96×10^{-5} **(6050)**	5.67×10^{-6} **(9942)**

Monte-Carlo error

Collocation error

$$\left\| \frac{1}{N} \sum_{i=1}^{N} u(x, \boldsymbol{\xi}^{(i)}) - \mathcal{A}(u)(x, \boldsymbol{\xi}^{(i)}) \right\|_{l^2(D)}$$

Parens: Number of DE solves needed for collocation
Green: This number is smaller than N *and* yields smaller error

Concluding Remarks

Various Useful Approaches to Handle Diffusion Problem with Stochastic Coefficient

- Stochastic Galerkin equations with linear dependence on parameters are solvable using multigrid
- Diffusion equation with lognormal coefficent can be handled by transformation to convection-diffusion form
- Adaptive collocation with KDE is general and effective