Simulating with uncertainty : the rough surface scattering problem

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A problem often encountered in numerical analysis

1. A simulation, $\sigma(\mathbf{x})$, $\mathbf{x} \in \mathbb{D}$ is computationally expensive
2. The input $\mathbf{x}$ or the domain $\mathbb{D}$ displays uncertainty,

   e.g. in simulating the modes of an optical fibre, the refractive index might not be exactly known, or the boundary may be rough

In this light, more useful than $\sigma(\mathbf{x})$ is the expectation $\langle \sigma(\mathbf{x}) \rangle$
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Computing the expectation and standard deviation

Assumptions

Setup: d-dimensional $\mathbf{x} = [x_1, x_2, \ldots, x_d]$

Each x_i is mutually independent, distributed with known pdf ρ_i

Construct a multi-variate pdf, $\rho(\mathbf{x}) = \prod_{i=1}^{n} \rho_i(x_i)$

Quantities of interest

$$\text{Expectation} \quad \langle \sigma(\mathbf{x}) \rangle = \int_{\mathbb{D}} \sigma(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x}$$

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Yes!

$\sigma(\mathbf{x})$ is only known numerically.

Recall: $\sigma(\mathbf{x})$ is the output of an (possibly expensive) simulation

Monte Carlo method

The most commonly used method to estimate expectation.

Instantiate several $\mathbf{x}_i$'s and approximate $\langle\sigma(\mathbf{x})\rangle = \sum_{i=1}^{n} \frac{1}{n}\sigma(\mathbf{x}_i)$

Convergence rate: independent of d, but slow $O(\frac{1}{\sqrt{n}})$

Extra: Create a histogram from $\sigma(\mathbf{x}_i)$ values to estimate pdf of σ.

Objective of this talk: Discuss alternatives to Monte Carlo

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The alternatives to Monte Carlo

Broadly, two families of methods will be discussed:

1. **Galerkin Polynomial Chaos** (gPC)

   Need to code a new solver, works for small range of d values

2. **Stochastic Collocation** (SC)

   Uses an existing solver, works for small–medium range of d values

   Attractive, because compatible with commercial software

What about Monte Carlo?

Use for benchmarking and for large range of d values

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Start with Stochastic Collocation: Polynomial interpolation

For simplicity, consider a 1-D case of the simulation, $\sigma(x)$

Polynomial interpolation and integration

- Choose n-points to evaluate $\sigma(x)$ and construct a $n-1$ degree polynomial (Lagrange interpolation): $\sigma_{n-1}(x) = \sum_{i=1}^{n} \sigma(x_i) L_i(x)$
  Recall, $L_i(x) = \prod_{j=1, j\neq i}^{n} (x - x_j)/(x_i - x_j)$
- Compute expectation as
  $\langle \sigma(x) \rangle \approx \sum_{i=1}^{n} \sigma(x_i) \int L_i(x)\rho(x)dx = \sum_{i=1}^{n} \sigma(x_i)\, \alpha_i$
- α_i can be pre-computed, and $\langle \sigma(x) \rangle$ is accurate to order $n-1$.

Can we do better?

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Stochastic Collocation: Gaussian quadrature

Yes! Gaussian quadrature

- Use the theory of orthogonal polynomials, i.e. find polynomials s.t. $\int p_m(x)p_n(x)\rho(x)dx = \delta_{m,n}$
- Pick the n points, $\{x_i\}$ to be roots of n^{th} degree polynomial, $p_n(x)$
- This also gives $\langle\sigma(x)\rangle \approx \sum_{i=1}^{n} \sigma(x_i)\, \alpha_i$, but now integral is accurate to order $2n-1$

Common orthogonal polynomials

- *Legendre*, $x \in [-1,1]$, $\rho(x) = 1$.
- *Jacobi*, $x \in (-1,1)$, $\rho(x) = (1-x)^{\alpha}(1+x)^{\beta}$, $\alpha, \beta > -1$.
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But our problem is d-dimensional!

Solution: Extend one-dimensional Gaussian quadrature to d dimensions

- With $\mathbf{x} = [x_i, x_2, \ldots, x_d]$, express $\sigma(\mathbf{x}) = \prod_{i=1}^{d} \sigma_i(x_i)$ (implicitly)
- The integral splits up: $\int \sigma(\mathbf{x})\rho(\mathbf{x})d\mathbf{x} = \prod_i \int \sigma_i(x_i)\rho_i(x_i)dx_i$
- Apply n-point Gaussian quadrature (GQ) in each dimension: $\langle\sigma(\mathbf{x})\rangle = \prod_{i=1}^{d} \sum_{j=1}^{n} \sigma_i(x_{i,j})\alpha_j$. Combine the σ_i's to get $\sigma(\mathbf{x}_k)$.
- An example in 2D (x, y) and a 2-point GQ in each dimension: $\langle\sigma(x,y)\rangle = [\sigma_x(x_1)\alpha_1 + \sigma_x(x_2)\alpha_2][\sigma_y(y_1)\alpha_1 + \sigma_y(y_2)\alpha_2] =$ $\sigma(x_1,y_1)\alpha_{1,1} + \sigma(x_1,y_2)\alpha_{1,2} + \sigma(x_2,y_1)\alpha_{2,1} + \sigma(x_2,y_2)\alpha_{2,2}$

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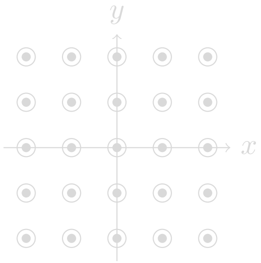
Visualizing the tensor product rule

- E.g. function evaluation points in a 2D 5-point GQ (25 evals) : Denote as $\langle\sigma\rangle_{5,5}$
- Curse of dimensionality is clear: number of function evaluations $= n^d$
- Can we do better?



Theorem: (Mysovskikh 1968, Möller 1976)

To attain a polynomial exactness equal to m, the (optimal) required number of grid-points has lower and upper bounds given by

$$N_{\text{min}} = \binom{d + \lfloor m \rfloor/2}{\lfloor m \rfloor/2} \leq N_{\text{opt}} \leq \binom{d+m}{m} = N_{\text{max}}$$

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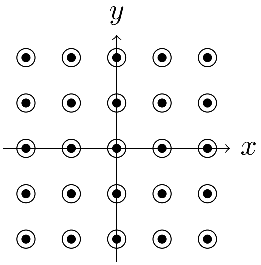

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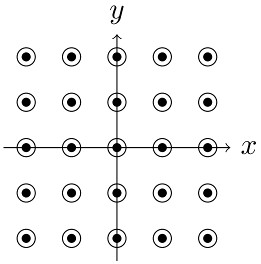

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Sparse Grids: Smolyak (1963)

1. Every $\langle \sigma \rangle_{i,j}$ is an approximation to the actual integral, $\langle \sigma \rangle$
2. Introduce a "level" parameter $k = (i + j)$ and let the max level be denoted by $l = \max\{k\}$

Telescope a series of *different levels* to approximate $\langle \sigma \rangle$

- e.g. (Max) level $l = 4$:
  $\langle \sigma \rangle \approx [\langle \sigma \rangle_{3,1} + \langle \sigma \rangle_{1,3} + \langle \sigma \rangle_{2,2}]_{\text{k=4}} - [\langle \sigma \rangle_{2,1} + \langle \sigma \rangle_{1,2}]_{\text{k=3}}$
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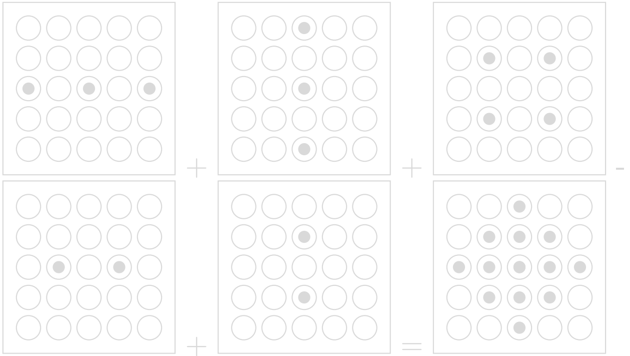
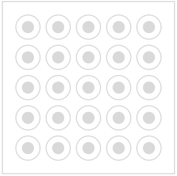


Tensor Grid Points



Substantial savings in higher dims

13 Points (SG) v/s **25** points (TP)!

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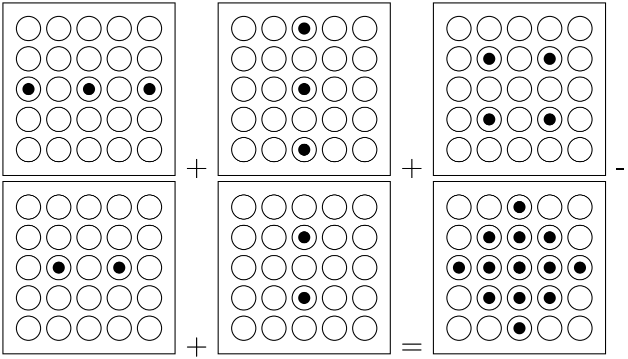

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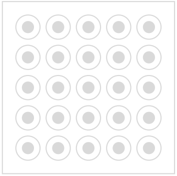

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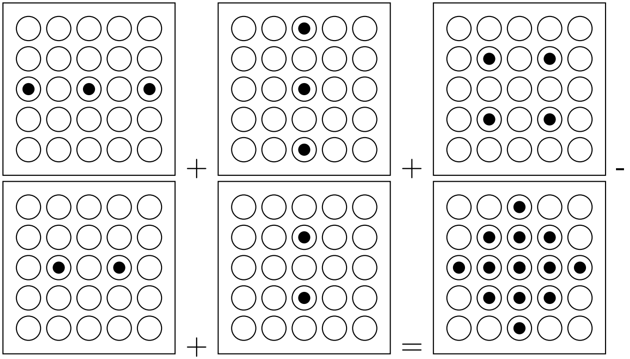

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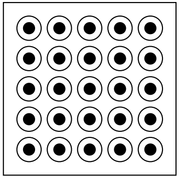

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Sparse Grid rule: finer points

TP rule: $\langle\sigma\rangle = \sum_{i_1=1}^{n_1} \dots \sum_{i_d=1}^{n_d} \sigma(x_{i_1}, \dots, x_{i_d})\alpha_{i_1} \dots \alpha_{i_d}$
$= (Q^{n_1} \times Q^{n_2} \times \dots \times Q^{n_d})[\sigma]$
n_i point quadrature in the i^{th} dim; $\prod n_i \approx n^d$ points

SG rule: With max level l, and $k = k_1 + k_2 + \dots + k_d$:
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- k_i point quadrature in the i^{th} dim; $\approx 2^l d^l / l!$ points
- Nested quadrature rules (e.g. Clenshaw-Curtis, Gauss-Konrad) re-use fn evaluation points between levels.

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- Nested quadrature rules (e.g. Clenshaw-Curtis, Gauss-Konrad) re-use fn evaluation points between levels.

Sparse Grid rule: finer points

TP rule: $\langle\sigma\rangle = \sum_{i_1=1}^{n_1} \ldots \sum_{i_d=1}^{n_d} \sigma(x_{i_1}, \ldots, x_{i_d})\alpha_{i_1} \ldots \alpha_{i_d}$
$= (Q^{n_1} \times Q^{n_2} \times \ldots \times Q^{n_d})[\sigma]$
n_i point quadrature in the i^{th} dim; $\prod n_i \approx n^d$ points

SG rule: With max level l, and $k = k_1 + k_2 + \ldots + k_d$:

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Switching gears: from sampling to projection

The two methods (Monte Carlo, Stochastic Collocation) considered so far were of a "sampling" kind: $\langle\sigma\rangle$ estimated using samples of $\sigma(\mathbf{x})$.

Projection based approach: Overview of Galerkin method

- Governing equation: $\Theta f(\mathbf{x}) = g(\mathbf{x})$, where Θ is an operator, g is a known function, and f is to be determined.
- Project f in a known basis, $\{\phi_j\}$: $f(\mathbf{x}) = \sum_j u_j \phi_j(\mathbf{x})$
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- This is a system of equations; solve for u and get f.

Straightforward when $\mathbf{x}$ is spatio-temporal. But when stochastic?

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generalized Polynomial Chaos (gPC): a very brief history

- Polynomial Chaos (PC): coined by Norbert Wiener studying Gaussian stochastic processes (1938). Used Hermite polynomials as basis.
- Ghanem (1998) used theory of Wiener-Hermite PC to represent random processes in an orthogonal basis of Hermite polynomials.
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The basis functions in gPC

- Start with a RV, call it z as before. Let it have a distribution function, $F_z(\theta) = P(z \leq \theta)$ and a pdf $\rho(\theta)$ s.t. $dF_z(\theta) = \rho(\theta)d\theta$
- The generalized Polynomial Chaos basis functions are orthogonal basis functions, $\psi_i(z)$, satisfying :
  $\langle \psi_i(z)\psi_j(z)\rangle = \int \psi_i(\theta)\psi_j(\theta)\rho(\theta)d\theta = \gamma_i \delta_{ij}$
- Construct linear space of polynomials of degree at most n: $\mathbb{P}_n(z)$
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  - *Legendre*, $\theta \in [-1, 1]$, $\rho(\theta) = 1/2$.
  - *Jacobi*, $\theta \in (-1, 1)$, $\rho(\theta) = (1-\theta)^\alpha(1+\theta)^\beta$, $\alpha, \beta > -1$.
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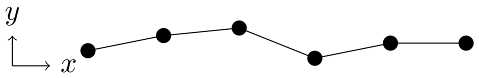
Random inputs? (More than just a collection of RVs!)

Example: A random surface – adjacent points are not independent of each other, there is some correlation:



The Kosambi-Karhunen-Loeve (KL) expansion is widely used to represent random processes: $s(x,\theta) = s_0(x) + \sum_{k=1}^{\infty} \sqrt{\eta_k} f_k(x) z_k(\theta)$

- $s_0(x)$ is the mean of the random process
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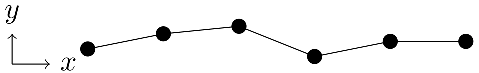

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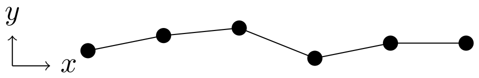

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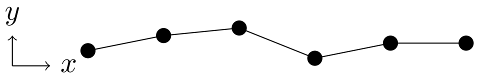

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KL expansion for exponential correlation

$$\boxed{s(x,\theta) = s_0(x) + \sum_{k=1}^{\infty} \sqrt{\eta_k} f_k(x) z_k(\theta)}$$

- KL expansion eigenvalues and functions can be analytically calculated in some cases, e.g. exponential correlation function $C(i,j) = \exp(-|i-j|/l)$, (correlation length l).
- Decay rate of eigenvalues depends inversely on the correlation length $\implies$ *more RVs for smaller l.*

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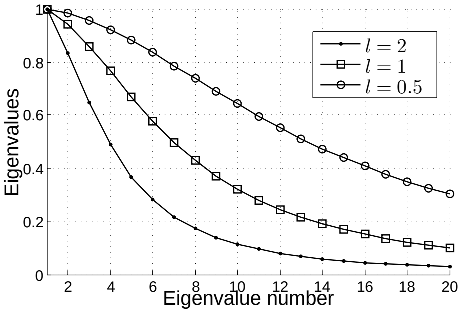
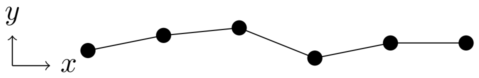


The case of multiple random variables with correlation

Consider again the random rough surface ...



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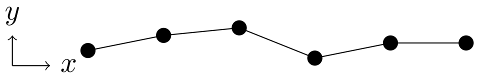

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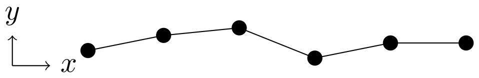

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Changing gears ...

So far ...

This completes an overview of stochastic computation:

1. Monte Carlo (MC)
2. Stochastic Collocation (SC)
3. Stochastic Galerkin (SG) using generalized Polynomial Chaos

Moving on ...

To make matters more concrete, consider the problem of computing the electromagnetic scattering from a random rough surface:
e.g. seen in microwave remote sensing, [MC][a], [SC,SG][b]

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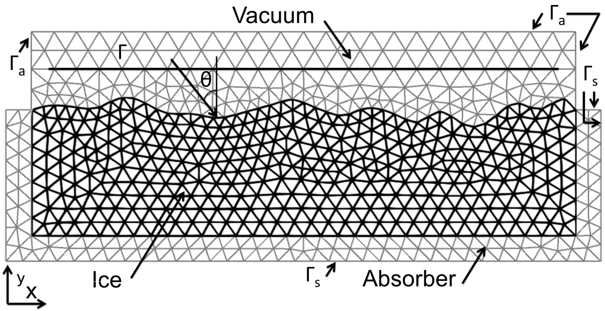
Traditional FEM setup for rough surface scattering



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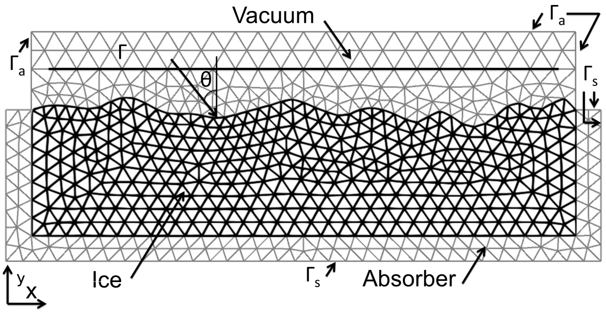

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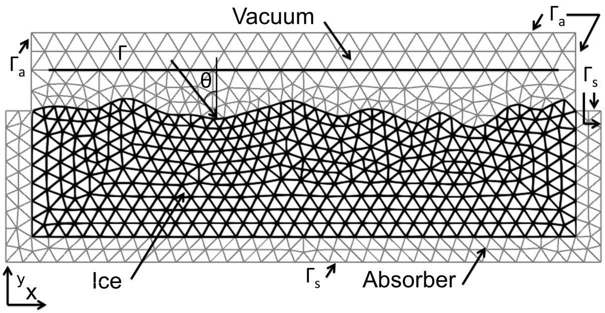

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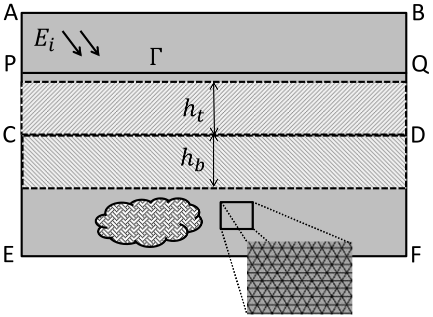

Partition the domain into parts that can move, and those that need not

- Let $s(x)$ define rough surface (e.g. KL expansion)
- Move each node smoothly within 'sandwich' region: $y \to y + \Delta y$

$$\Delta y = \begin{cases} s(x)\left(\frac{h_t - y}{h_t}\right), 0 < y < h_t \\ s(x)\left(\frac{y + h_b}{h_b}\right), -h_b < y < 0 \end{cases}$$

- CD will deform to rough surface
- Zero deformation by the time $y = h_t$ or $y = -h_b$

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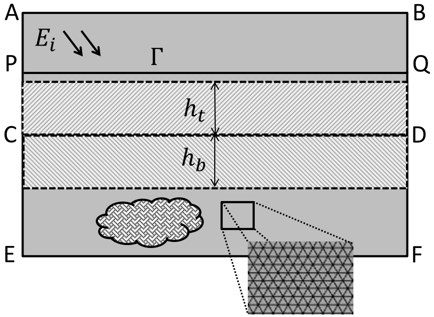

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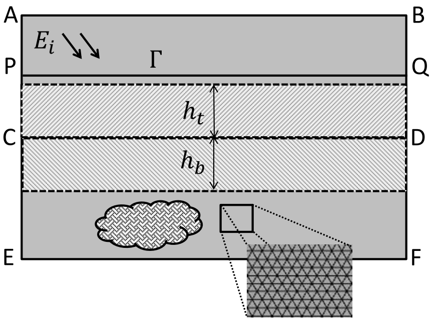

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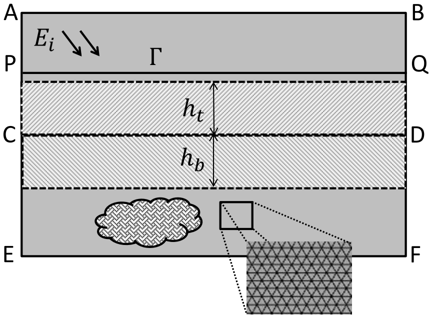

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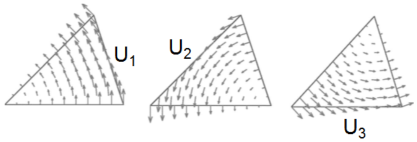

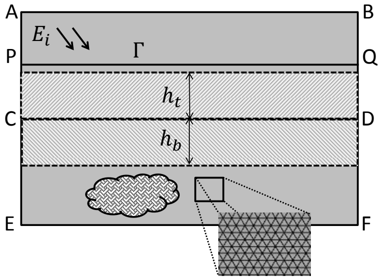

Maxwell's equations in weak form:

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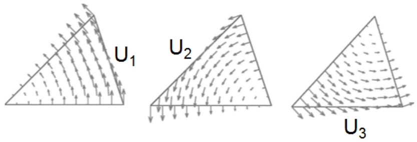

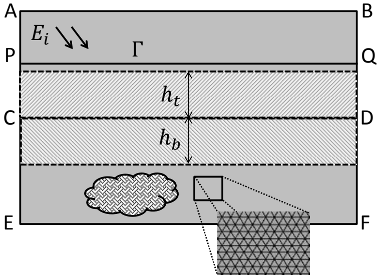

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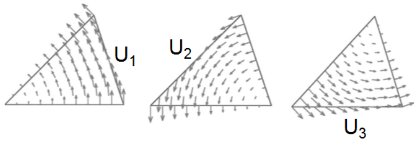

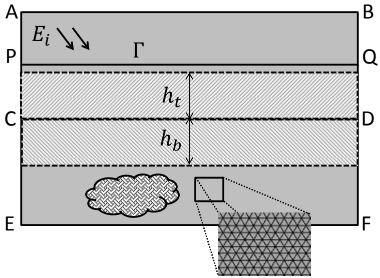

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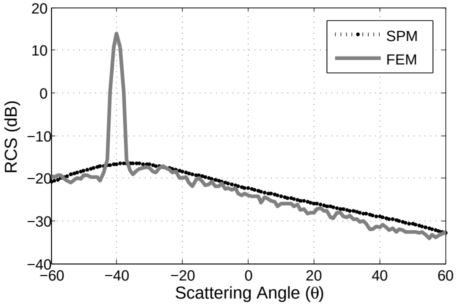

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From Monte Carlo to Stochastic Collocation

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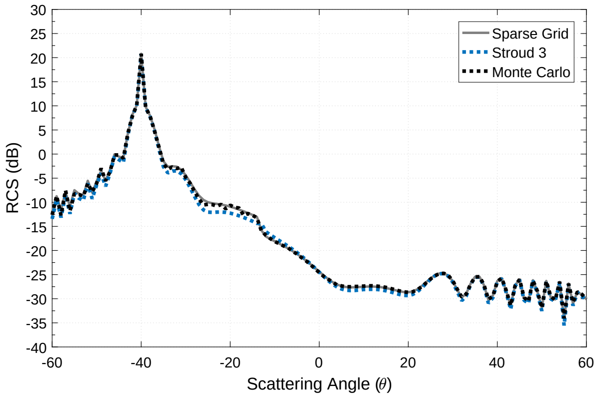

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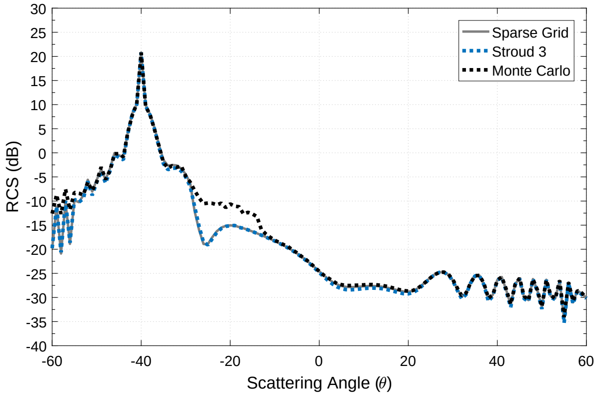

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1. Accomplish the perturbations by Taylor expanding to second order: (1^{st}, 2^{nd} derivatives are computed by finite differences)

$$\tilde{A}_{pq} = \beta_{pq} + \sum_{i=1}^{d} \beta_{pq}^{(i)} z_i + \sum_{i,j=1}^{d} \beta_{pq}^{(i,j)} z_i z_j, \leftarrow \text{matrices } m \times m$$
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Details of Stochastic Galerkin

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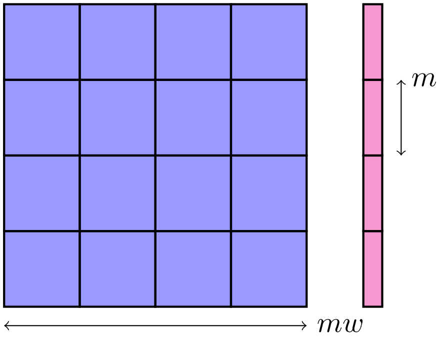

- Each block is sparse, multiplied by stochastic inner products like: $E_{ab} = \langle \Psi_a(\vec{z})\Psi_b(\vec{z})\rangle$, $E_{ab}^{(i)} = \langle \Psi_a(\vec{z}) z_i \Psi_b(\vec{z})\rangle$, $E_{ab}^{(i,j)} = \langle \Psi_a(\vec{z})\, z_i\, z_j\, \Psi_b(\vec{z})\rangle$,
- Needs to be solved only once

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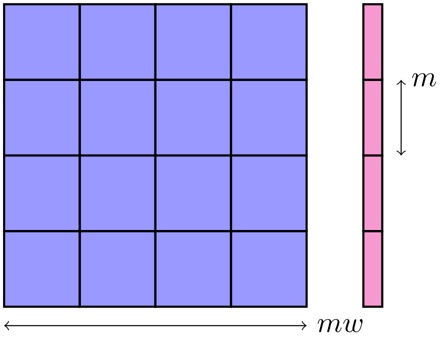
- What is a the structure of: $F\,\mathbf{v} = \mathbf{g}$, $F \in \mathbb{C}^{mw\times mw}$, $\mathbf{v},\mathbf{g} \in \mathbb{C}^{mw}$



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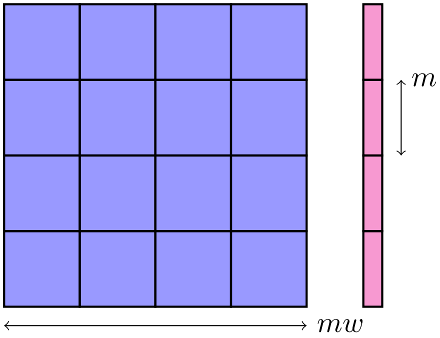

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Computational details of Stochastic Galerkin

In solving $F\,\mathbf{v} = \mathbf{g}$, $F \in \mathbb{C}^{mw \times mw}$, $\mathbf{v}, \mathbf{g} \in \mathbb{C}^{mw}$

- Not a "cheap" computation: ~~direct matrix solvers~~, use an **iterative** method: BiCgStab + block-diagonal, mean-based pre-conditioner
- The matrix F is never stored explicitly, instead we only need to be able to compute the **product** of F with another vector for the iterative method to work
- Compute times and memory demands are still much higher than MC/SC. Scope for lot of research in sparse data structures for F, g

SG-gPC	MC
1200s (10 iters), 10 GB RAM	950s (100 surfaces), 150 MB RAM

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- How do we choose the number of edges in the FEM formulation, m?
  Horizontally: Long enough to capture several correlation lengths
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- How many basis functions to keep, w? Recall:
  $\Psi_{\mathbf{i}}(\vec{z}) = \psi_{i_1}(z_1) \dots \psi_{i_d}(z_d), \quad 0 \le \mathbf{i} = \sum_{j=1}^{d} i_j \le n$ (max degree)
  belong to the space $\mathbb{P}_n^d$ of dimension $w = \binom{n+d}{n}$
  Choose d: no of KL terms till eigenvalue falls by $1/10$
  Choose n: depends on available computer resources

Values of d v/s surface length (a) and correlation length (l)

$\downarrow l \setminus$ a$\rightarrow$	15	30
1	15	29
0.5	29	58

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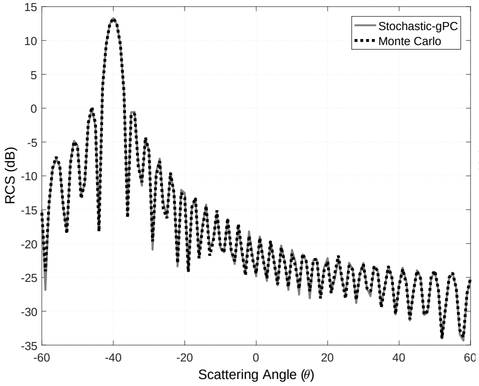
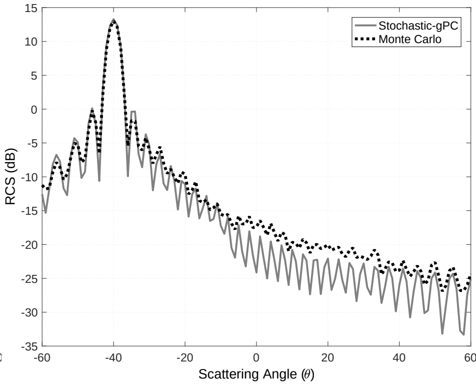
Compare Stochastic Galerkin with Monte Carlo

$h = 0.05/(2\pi)$ $h = 0.20/(2\pi)$





$$\theta_i = 40^\circ, \epsilon_r = 4 - j, a = 20, l = 1, \lambda = 1 \quad d = 15, n = 1$$

Reflections

- SG-gPC is a deal breaker for even small values of d
  $\rightarrow$ Computational innovation required
- For small-moderate values of d, (e.g. $d < 50$) SC methods are a powerful alternative to MC
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Thanks!

Most of this talk was based on:

"Stochastic Solutions to Rough Surface Scattering using the finite element method", Uday K Khankhoje and Shreyas Padhy; *IEEE Transactions on Antennas and Propagation*, 65(08) 2017.

Refer to `http://www.ee.iitm.ac.in/uday` for full-text of relevant papers. Or just Google my name.

E-mail: uday@ee.iitm.ac.in

Aside: Why is Guass quadrature so effective?

- To approximate $\int f(x)w(x)dx$ by an n-point rule, express $f(x)$ in terms of: nth order polynomial $p_n(x)$, a quotient $q(x)$ (degree $< n$), & a remainder $r(x)$ (degree $< n$):
  $$f(x) = q(x) * p_n(x) + r(x) \qquad (1)$$
- Integrate w.r.t. $w(x)$, and use orthogonality property of $p_n(x)$: we get $\int f(x)w(x)dx = \int r(x)w(x)dx$. Next, construct a $n-1$ degree polynomial from n points (Lagrange interpolation) and get:
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- Here's where the choice of points x_i is crucial: If x_i is a root of $p_n(x)$, then from (1) it follows that $f(x_i) = r(x_i)$ and from (2) that:
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