Overview of numerical methods for Uncertainty Quantification

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http://sri-uq.kaust.edu.sa/

Consider

$$A(u; q) = f \quad \Rightarrow \quad u = S(f; q),$$

where S is a solution operator.

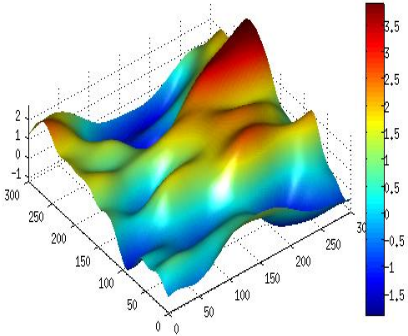
Uncertain Input:

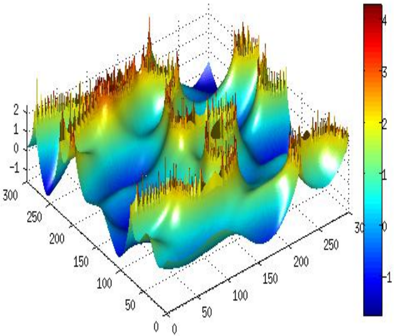
1. Parameter $q := q(\omega)$ (assume moments/cdf/pdf/quantiles of q are given)
2. Boundary and initial conditions, right-hand side
3. Geometry of the domain

Uncertain solution:

1. mean value and variance of u
2. exceedance probabilities $P(u > u^*)$
3. probability density functions (pdf) of u.

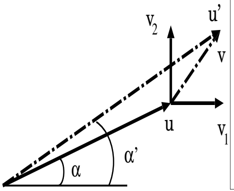
Realisations of random fields

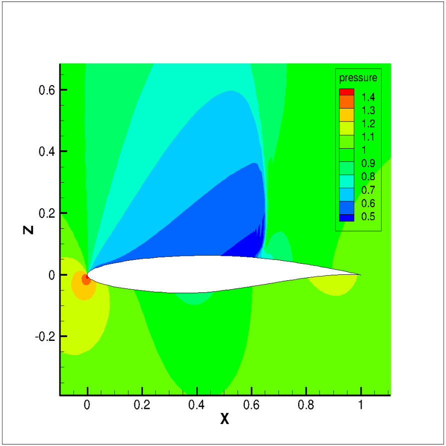




A big example:
UQ in numerical aerodynamics
(described by Navier-Stokes $+$ turbulence modeling)

Example: uncertainties in free stream turbulence





Random vectors $\boldsymbol{v}_1(\theta)$ and $\boldsymbol{v}_2(\theta)$ model free stream turbulence

Example: UQ

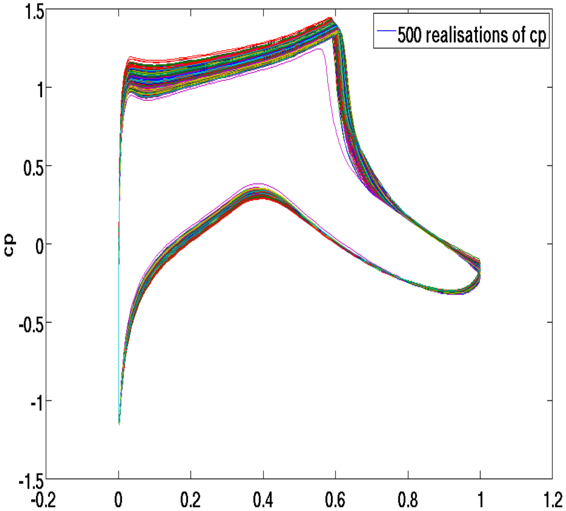
Assume that RVs α and *Ma* are Gaussian with

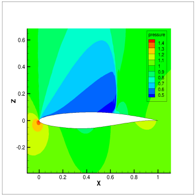
	mean	st. dev. σ	σ/mean
α	2.79	0.1	0.036
Ma	0.734	0.005	0.007

Then uncertainties in the solution lift *CL* and drag *CD* are

CL	0.853	0.0174	0.02
CD	0.0206	0.003	0.146

500 MC realisations of cp in dependence on α_i and Ma_i





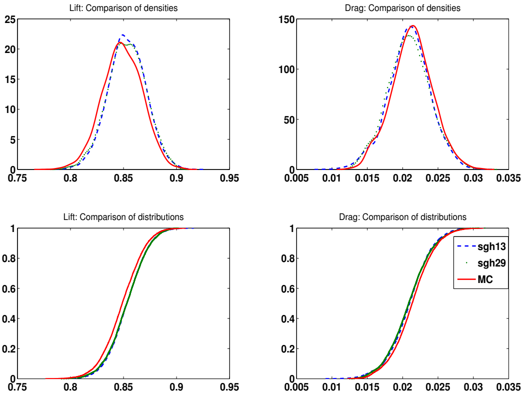


Figure : First row: density functions and the second row: distribution functions of lift and drag correspondingly.

Example: 3sigma intervals

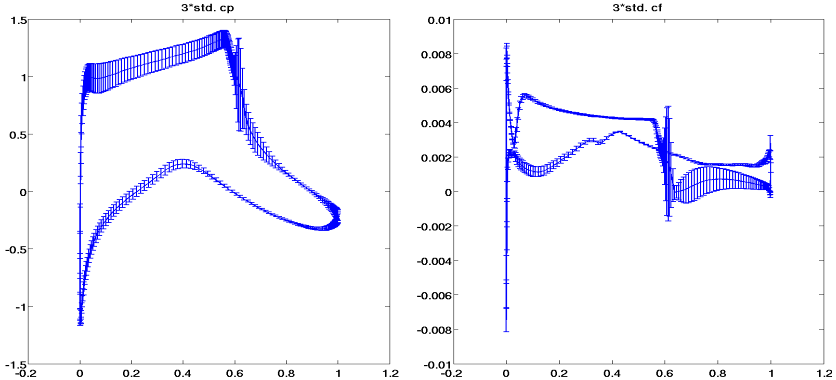
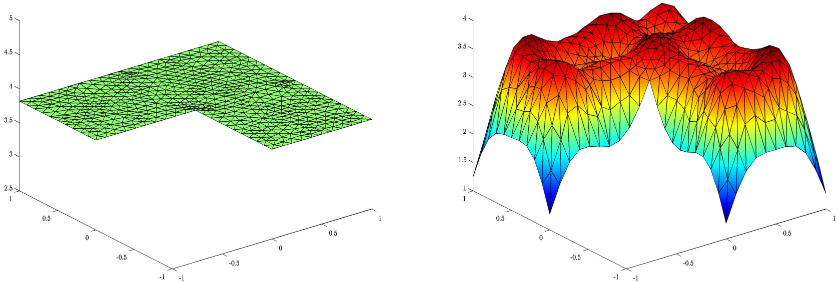


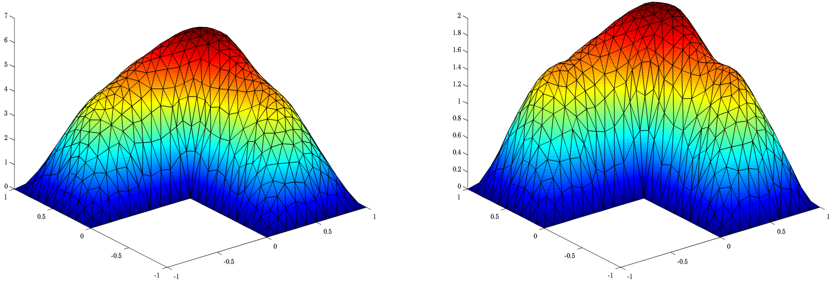
Figure : 3σ interval, σ standard deviation, in each point of RAE2822 airfoil for the pressure (cp) and friction (cf) coefficients.

$$\begin{cases} -\operatorname{div}(\kappa(x,\omega)\nabla u(x,\omega)) = p(x,\omega) & \text{in } \mathcal{G}\times\Omega,\ \mathcal{G}\subset\mathbb{R}^3, \\ u = 0 & \text{on } \partial\mathcal{G}, \end{cases} \tag{1}$$

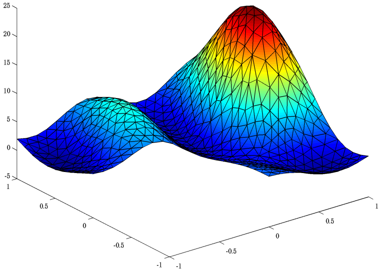
where $\kappa(x,\omega)$ - conductivity coefficient. Since κ positive, usually $\kappa(x,\omega) = e^{\gamma(x,\omega)}$.

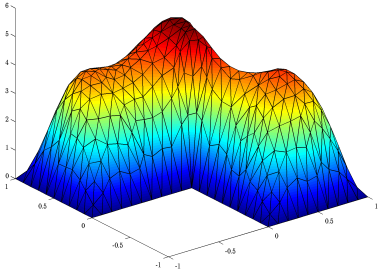


(left) mean and standard deviation (right) of $\kappa(x, \omega)$ (lognormal random field with parameters $\mu = 0.5$ and $\sigma = 1$).



(left) mean and standard deviation (right) of the solution u.





(left) a realization of the permeability and (right) a realisation of the solution).

1. Monte Carlo Simulations (easy to implement, parallelisable, expensive, dim. indepen.).
2. Stoch. collocation methods with global polynomials (easy to implement, parallelisable, cheaper than MC, dim. depen.).
3. Stoch. collocation methods with local polynomials (easy to implement, parallelisable, cheaper than MC, dim. depen.)
4. Stochastic Galerkin (difficult to implement, non-trivial parallelisation, the cheapest from all, dim. depen.)

The Karhunen-Loève expansion is the series

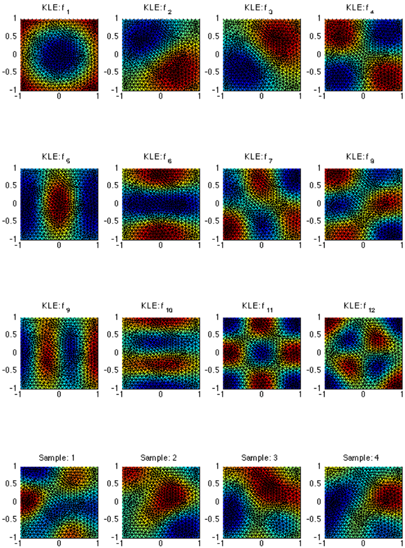
$$\kappa(x,\omega) = \mu_k(x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} k_i(x) \xi_i(\omega), \quad \text{where}$$

$\xi_i(\omega)$ are uncorrelated random variables and k_i are basis functions in $L^2(\mathcal{G})$.
Eigenpairs λ_i, k_i are the solution of

$$Tk_i = \lambda_i k_i, \quad k_i \in L^2(\mathcal{G}), i \in \mathbb{N}, \quad \text{where.}$$

$$T : L^2(\mathcal{G}) \to L^2(\mathcal{G}),$$
$$(Tu)(x) := \int_{\mathcal{G}} \operatorname{cov}_k(x,y) u(y) dy.$$

KLE eigenfunctions in 2D



The random field $\kappa(x,\omega)$ requires to specify its spatial correlation structure

$$\mathrm{cov}_\kappa(x,y) = \mathbb{E}[(\kappa(x,\cdot) - \mu_\kappa(x))(\kappa(y,\cdot) - \mu_\kappa(y))].$$

Let $h = \sqrt{\sum_{i=1}^{3} h_i^2/\ell_i^2}$, where $h_i := x_i - y_i$, $i = 1,2,3$, ℓ_i are cov. lengths.

Examples:
Gaussian $\mathrm{cov}(h) = \exp(-h^2)$,
exponential $\mathrm{cov}(h) = \exp(-h)$.

$$\xi(\omega) \approx \sum_{k=0}^{Z} a_k \Psi_k(\theta_1, \theta_2, ..., \theta_M), \quad \text{where } Z = \frac{(M+p)!}{M!p!}$$

- EXPENSIVE!

$M = 9$, $p = 2$, $Z = 55$
$M = 9$, $p = 4$, $Z = 715$
$M = 100$, $p = 4$, $Z \approx 4 \cdot 10^6$.

How to store and to handle so many coefficients ?

The orthogonality of Ψ_k enables the evaluation

$$a_k = \frac{<\xi\Psi_k>}{<\Psi_k^2>} = \frac{1}{<\Psi_k^2>} \int \xi(\boldsymbol{\theta}(\omega))\Psi_k(\boldsymbol{\theta}(\omega))dP(\omega).$$

(e.g. Ψ_k are Hermite polynomials).

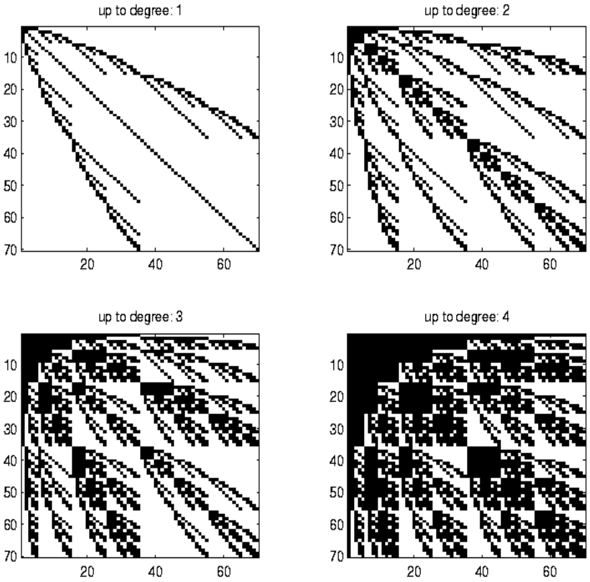
Discrete form

Take weak formulation of the diffusion equation, apply KLE and PCE to the test function $v(x, \omega)$, solution $u(x, \omega)$ and $\kappa(x, \omega)$, obtain

$$\mathbf{Ku} = \left[\sum_{\ell=0}^{m-1} \sum_{\gamma \in J_{M,p}} \boldsymbol{\Delta}^{(\gamma)} \otimes \boldsymbol{K}_\ell \right] \mathbf{u} = \mathbf{p}, \tag{2}$$

where $\boldsymbol{\Delta}^{(\gamma)}$ are some discrete operators which can be computed analytically, $\boldsymbol{K}_\ell \in \mathbb{R}^{n \times n}$ are the stiffness matrices.

Galerkin stiffness matrix **K**



Examples:

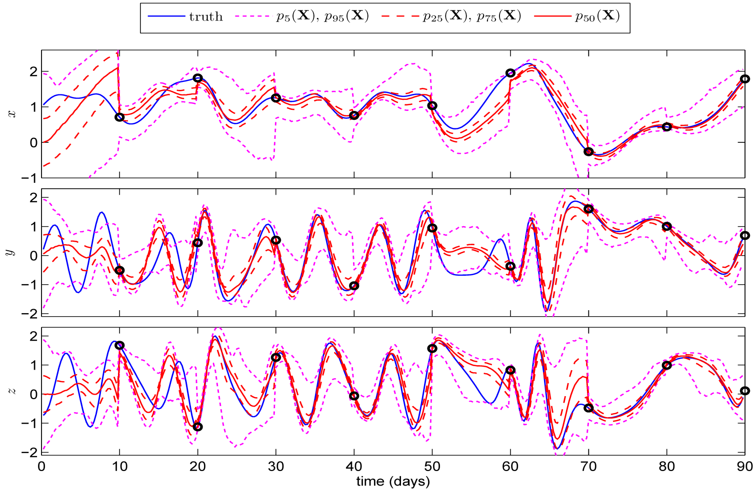
1. Chaotic systems (Lorenz 63)
2. Predator-pray model
3. reaction/combustion/chemical equations

Is a system of ODEs. Has chaotic solutions for certain parameter values and initial conditions.

$$\dot{x} = \sigma(\omega)(y - x)$$
$$\dot{y} = x(\rho(\omega) - z) - y$$
$$\dot{z} = xy - \beta(\omega)z$$

Initial state $q_0(\omega) = (x_0(\omega), y_0(\omega), z_0(\omega))$ are uncertain.

Solving in $t_0, t_1, ..., t_{10}$, Noisy Measur. $\rightarrow$ UPDATE, solving in $t_{11}, t_{12}, ..., t_{20}$, Noisy Measur. $\rightarrow$ UPDATE,...



Trajectories of x,y and z in time. After each update (new information coming) the uncertainty drops. (O. Pajonk)

1. Type in your terminal
   `git clone git://github.com/ezander/sglib.git`
2. To initialize all variables, run `startup.m`

You will find:
generalised PCE, sparse grids, (Q)MC, stochastic Galerkin, linear solvers, KLE, covariance matrices, statistics, quadratures (multivariate Chebyshev, Laguerre, Lagrange, Hermite) etc

There are: many examples, many test, rich demos

Open problems

1. Too many expensive (MC) simulations are required
2. in reality distributions/cov. matrices of random variables are unknown
3. After discretization of random variables the problem becomes high-dimensional.
4. The iterative methods must deal with tensors. The linear algebra becomes multi-linear. The rank truncation issue.

Take to home

1. KLE and PCE are used to discretize the stochastic problem (e.g. for stochastic Galerkin)
2. KLE is optimal, used to separate x from ω
3. PCE is not optimal, used to represent unknown random variable $\xi(\omega)$ by Gaussian random variables $\xi(\omega) = \sum_\alpha \xi^\alpha H_\alpha(\theta)$.
4. KLE contains less terms as PCE, but requires cov. function
5. (Q)MC does not take into account good (e.g. sparse/low-rank) properties of the operator
6. Stochastic Galerkin does
7. sparse grids are often used to compute PCE coeffs