ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Uncertainty Quantification in Computational Science

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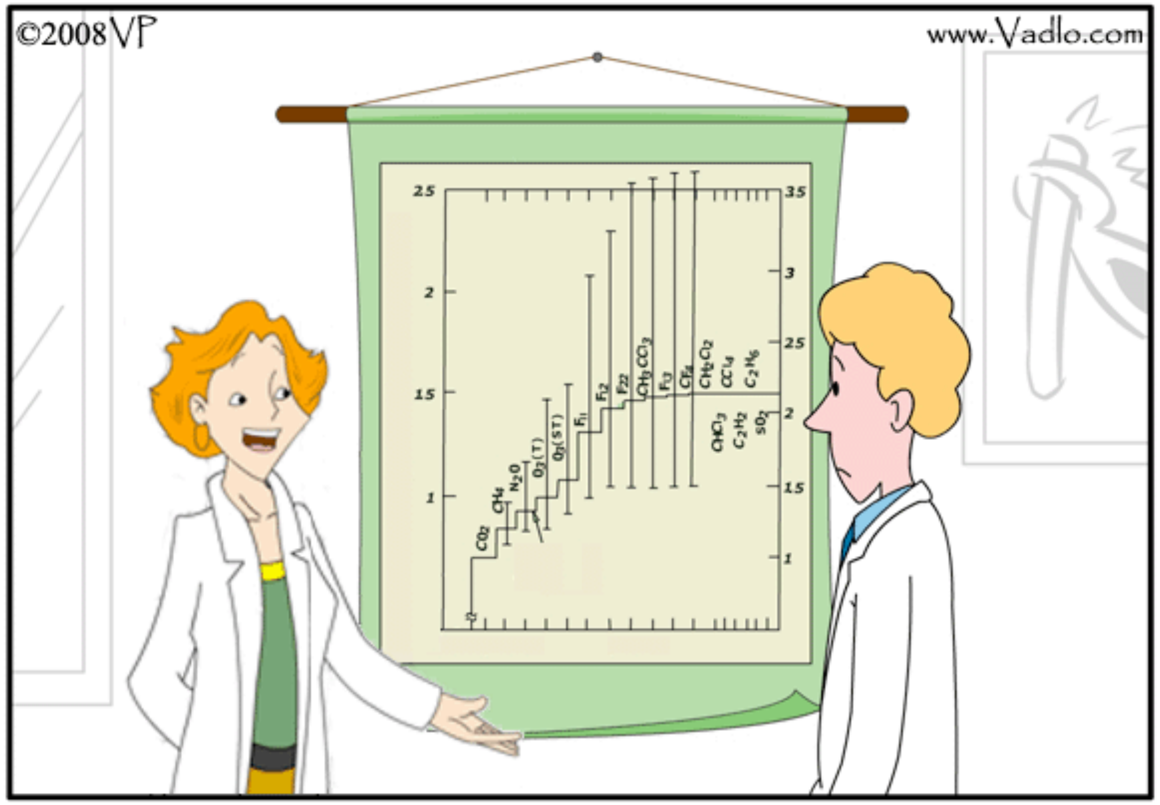


Did you really have to show the error bars?

The global picture

- Lecture I - Introduction to UQ

  Motivation, terminology, background, Wiener chaos expansions.

- Lecture II - Stochastic Galerkin methods

  Formulation, extensions, polynomial chaos, and examples.

- Lecture III - Stochastic Collocation methods

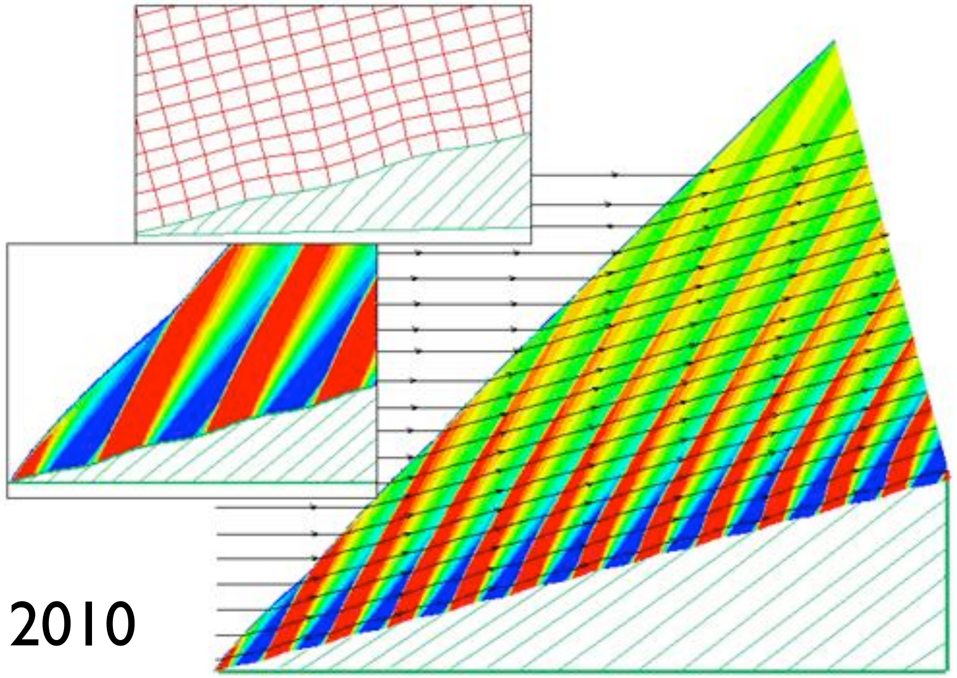
  Motivation, formulation, high-d integration, and examples.

- Lecture IV - Extensions, challenges, open questions

  Geometric uncertainty, ANOVA expansions, reduced order modeling and discussion of some open questions.

The local picture

- A brief overview
- Dealing with geometric uncertainty
- ANOVA expansions and parameter reduction
- Open questions and challenges
- Want to know more ?
- References



Lin et al, 2010

A brief overview

We have the majority of the tools in place

- Wiener Chaos expansion and the generalized Polynomial Chaos (gPC) expansion to represent random variables.
  - Superior performance for 'smooth' random variables

- Developed the Stochastic Galerkin methods to solve SDE/SPDEs with uncertainty.
  - Formal, systematic, general, and rigorous, leading to large systems of equations
  - Requires new solvers to be developed

- Developed the Stochastic Collocation method to improve efficiency and eliminate need to develop new solvers.
  - Reformulates the problem to require the solution of many decoupled problems
  - Connection to approximate high-d integration forms leads to further savings

- Identified the Karhunen-Loeve expansion to represent fields and processes

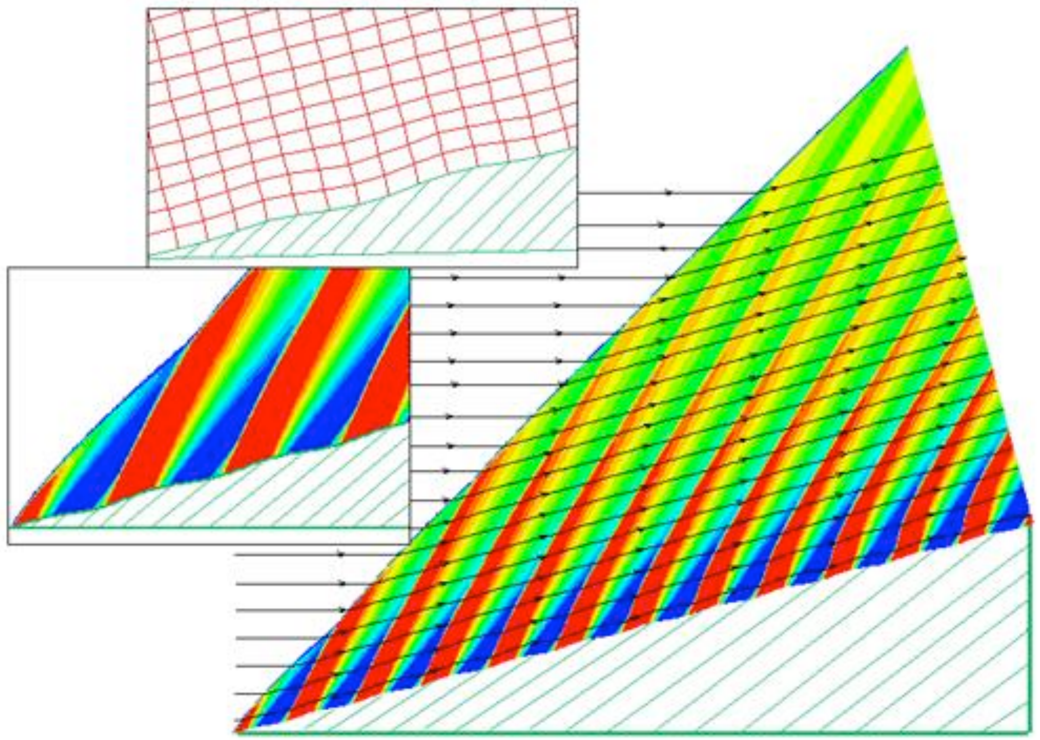
A brief overview

There are a few issues we should still consider

- How to deal with geometric uncertainty
- How to continue to push towards high-d

Shock reflection from rough boundary

From G. Lin et al (2008)



Uncertain geometries

Consider the random domain problem

$$\begin{cases} u_t(x,t) = \mathcal{L}(x;u), & D(Z)\times(0,T], \\ \mathcal{B}(u) = 0, & \partial D(Z)\times[0,T], \\ u = u_0, & D(Z)\times\{t=0\}, \end{cases}$$

Introduce an invertible mapping

$$y = y(x,Z), \qquad x = x(y,Z), \qquad \forall Z\in\mathbb{R}^d,$$

to obtain

$$\begin{cases} v_t(y,t,Z) = L(y,Z;v), & E\times(0,T]\times\mathbb{R}^d, \\ B(v) = 0, & \partial E\times[0,T]\times\mathbb{R}^d, \\ v = v_0, & E\times\{t=0\}\times\mathbb{R}^d, \end{cases}$$

Deterministic problem in random domain is transformed to a stochastic problem in a fixed domain

Uncertain geometries

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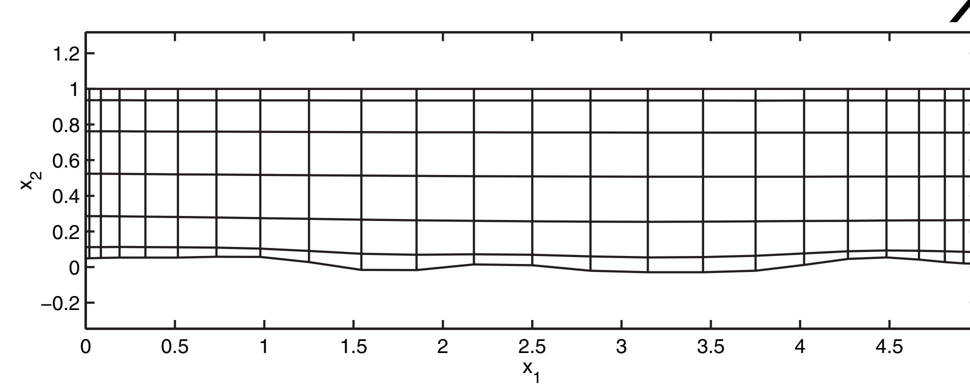
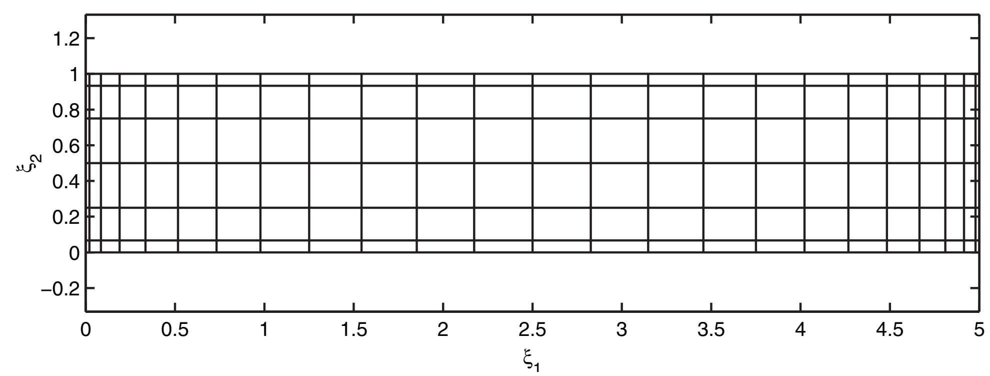
Example: Diffusion in channel - (L,H) with random boundary

Xiu, 2010

$$(x_1, x_2) \in D(\omega) = [0, L] \times [h(x, \omega), H],$$



$$y_1 = x_1, \qquad y_2 = \frac{H}{H - h(x, \omega)}(x_2 - h(x, \omega))$$



Introducing this yields

$$\nabla \cdot [c(x)\nabla u(x, Z)] = a(x) \quad \text{in } D(Z),$$

$$u(x, Z) = 0 \qquad \text{on } \partial D(Z),$$

$$\sum_{i=1}^{\ell} \frac{\partial}{\partial y_i}\left[\kappa(y, Z) \sum_{j=1}^{\ell}\left(\alpha_{ij}(y, Z)\frac{\partial v}{\partial y_j}\right)\right] = J^{-1} f(y, Z)$$

$$J(y, Z) = \frac{\partial(y_1, \ldots, y_\ell)}{\partial(x_1, \ldots, x_\ell)},$$

$$\alpha_{ij}(y, Z) = J^{-1} \nabla y_i \cdot \nabla y_j,$$

Uncertain geometries

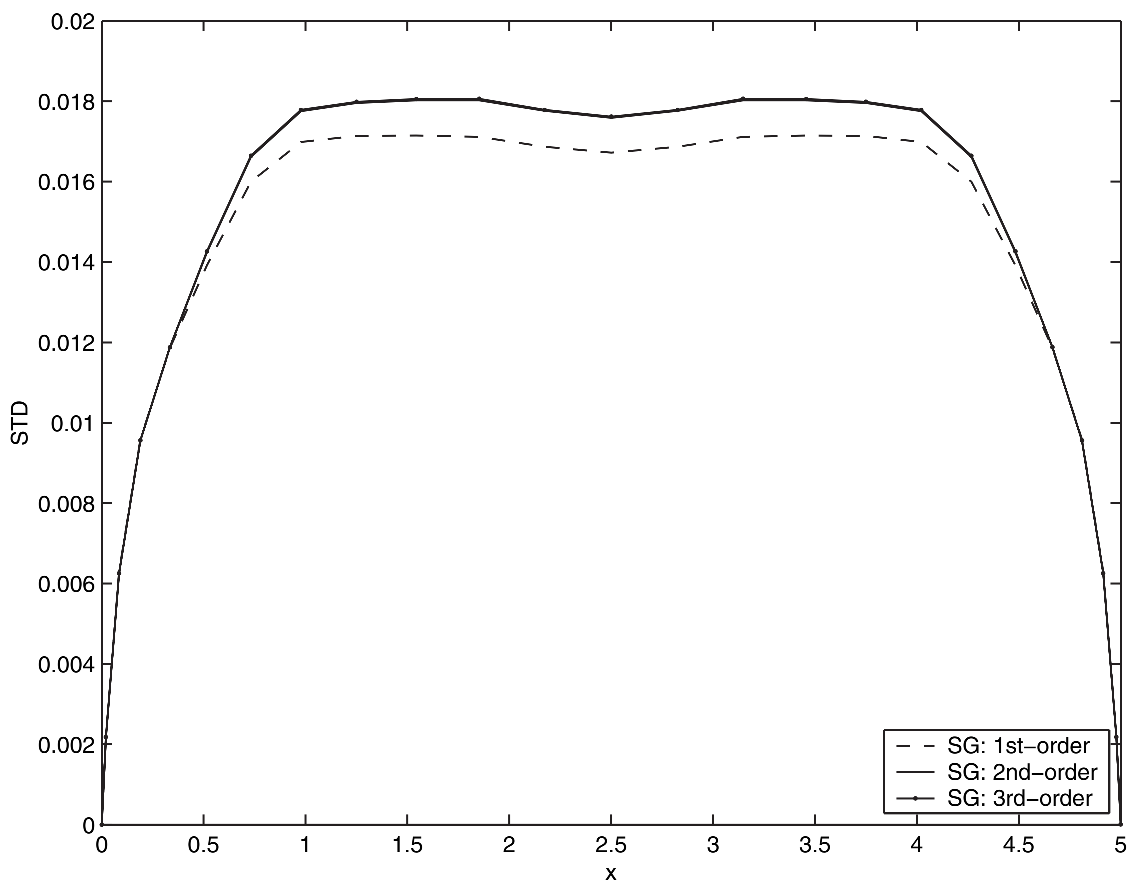
Roughness by covariance

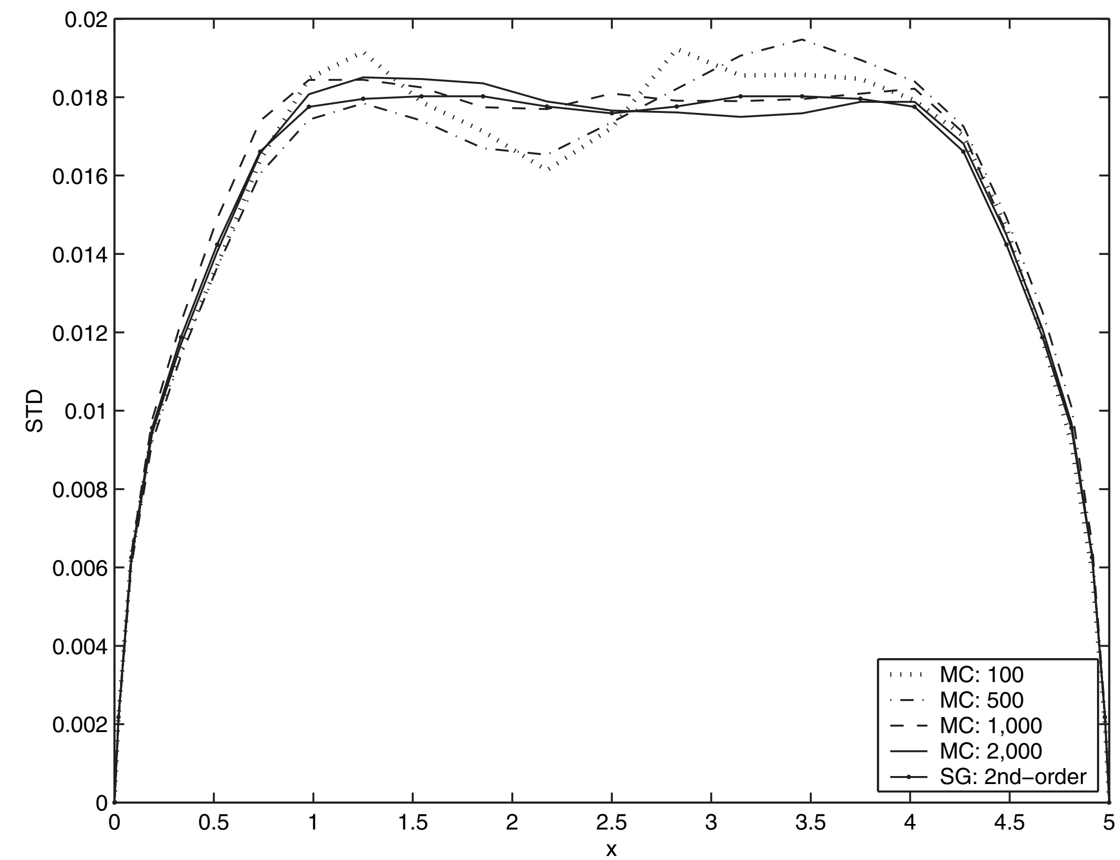
$$C_{hh}(r,s) = \mathbb{E}\left[h(r,\omega)h(s,\omega)\right] = \sigma^2 \exp\left(-\frac{|r-s|}{b}\right)$$

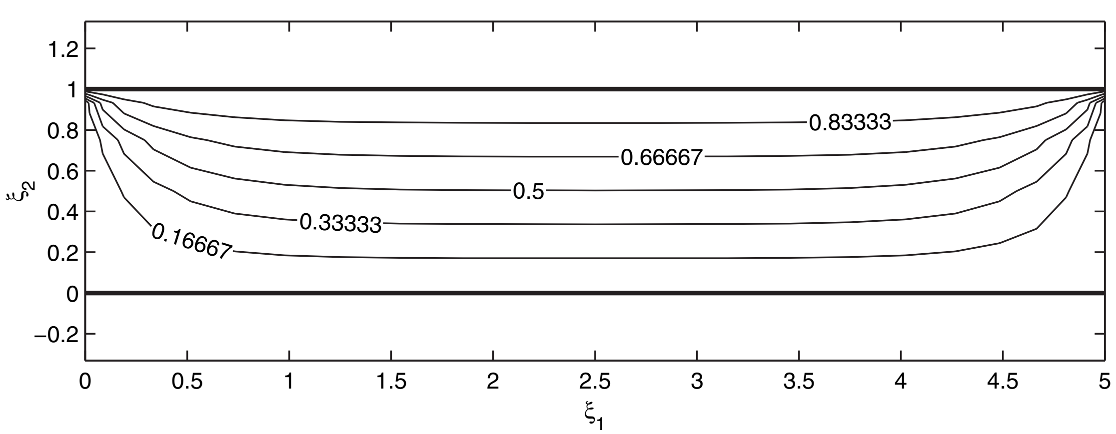
d=10

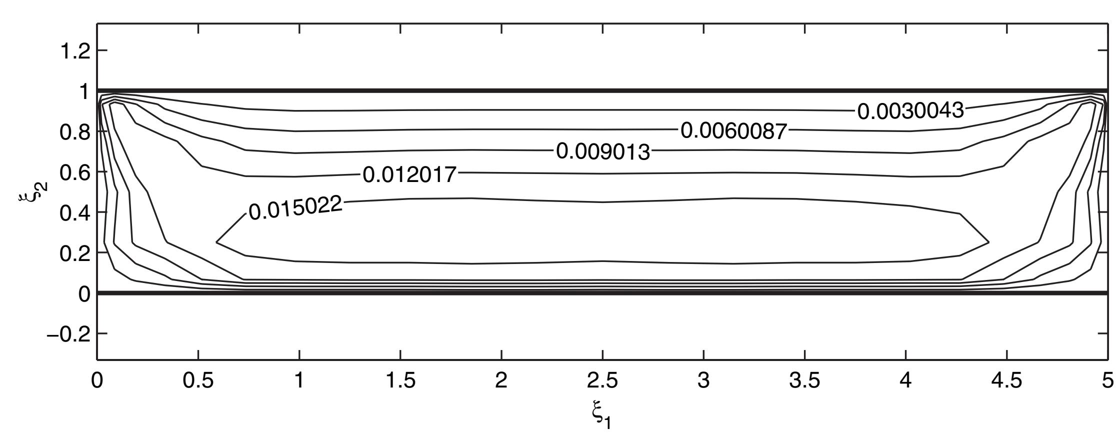
b=L/5

Xiu, 2010



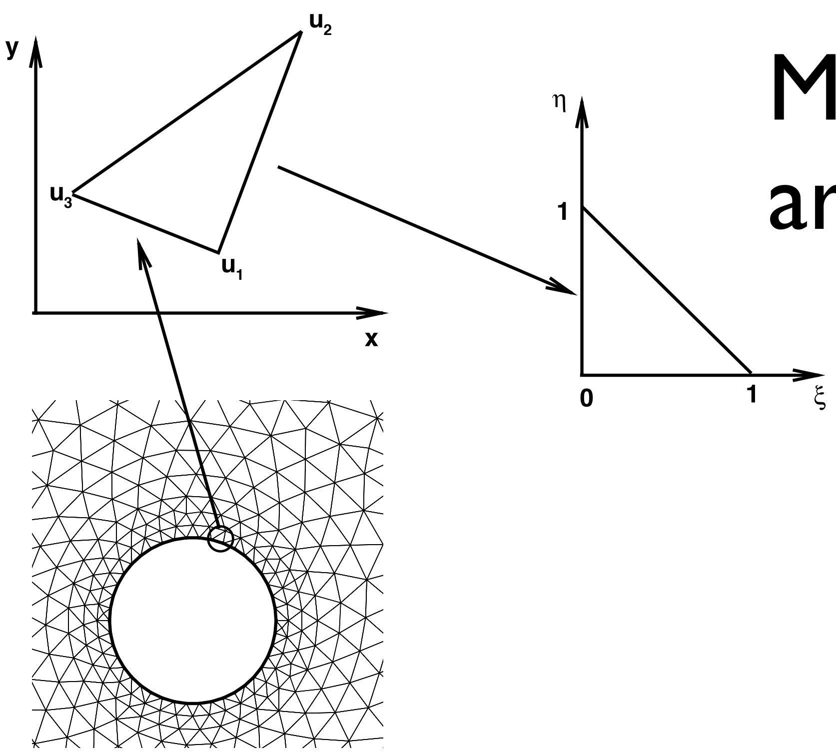




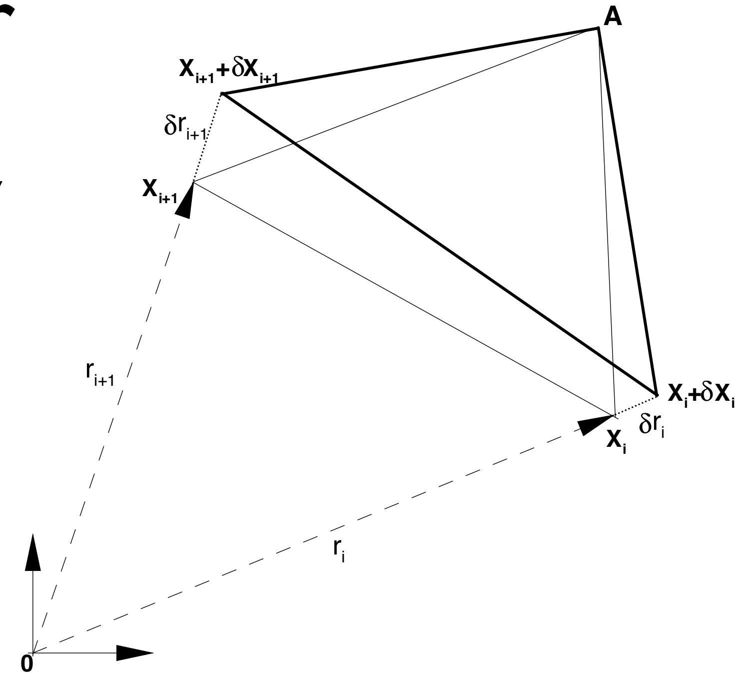


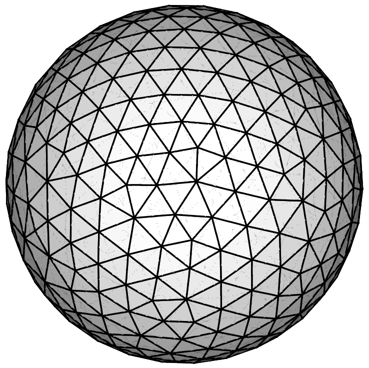
Uncertain geometries

For an element based scheme, it is similar

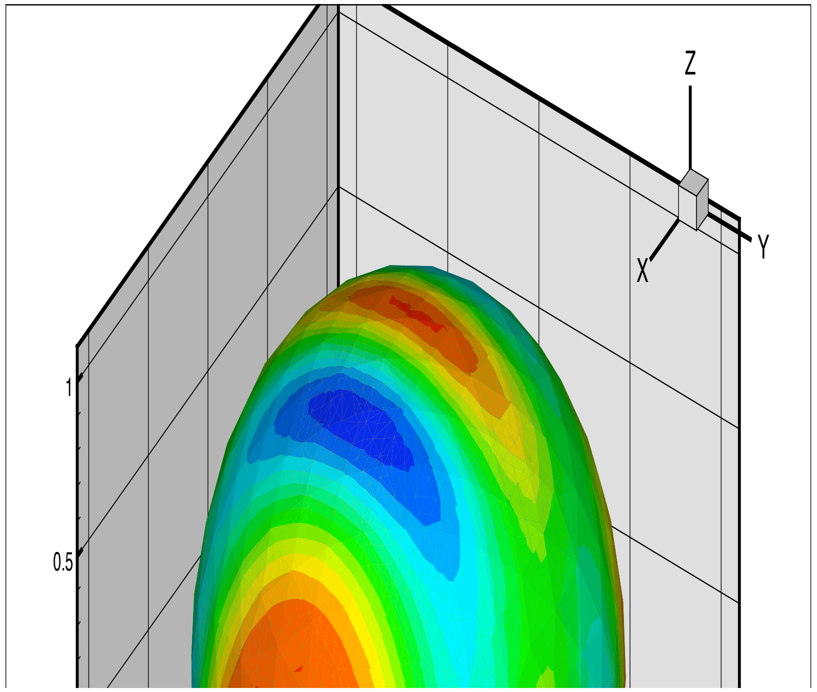


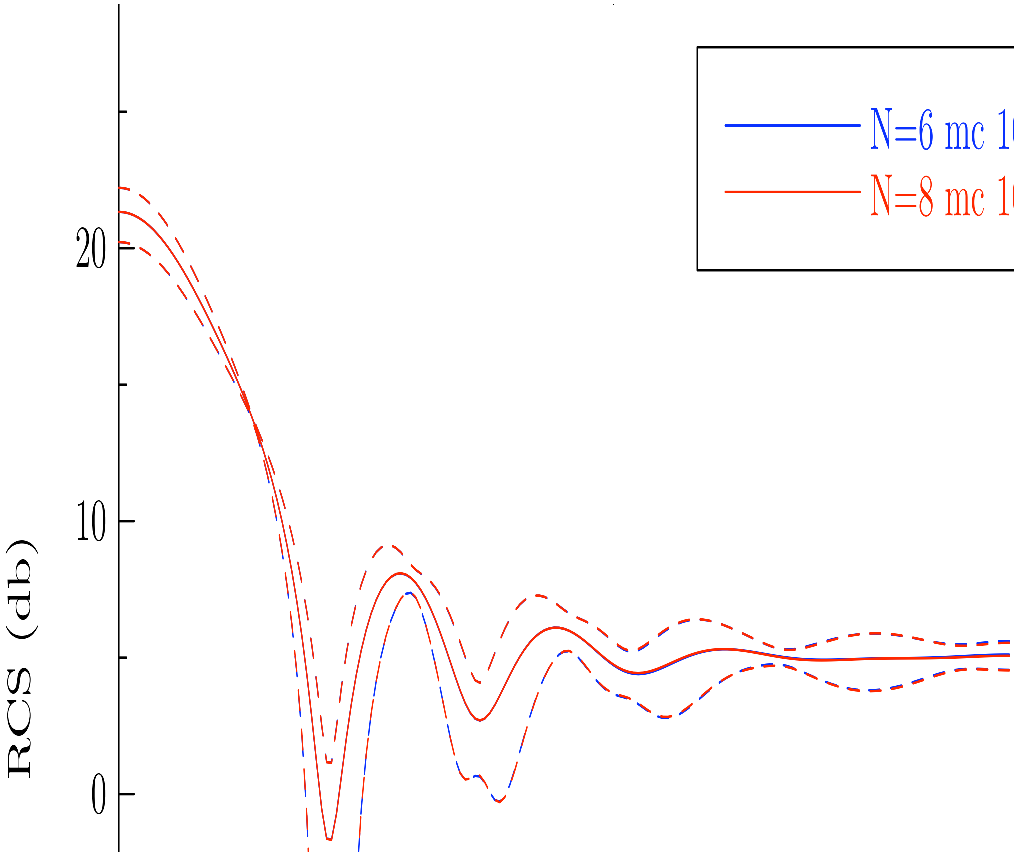
Mapping is essentially around a mean grid



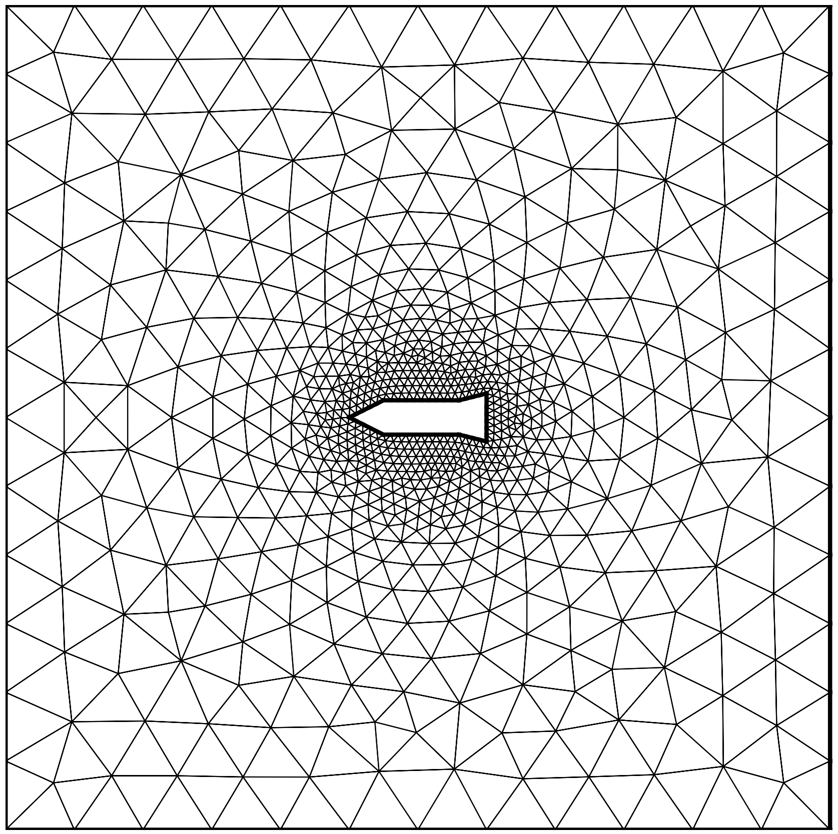


10% uncertain radius

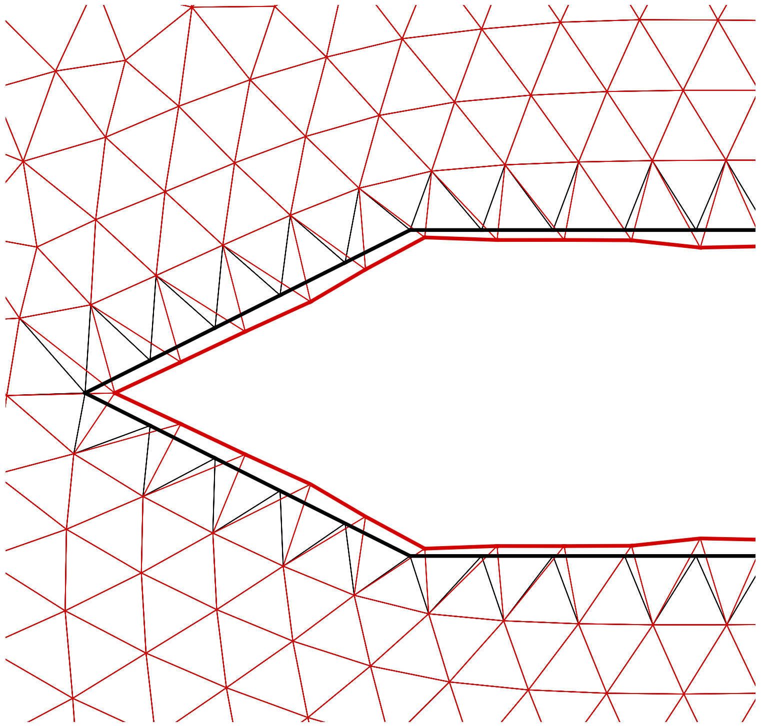


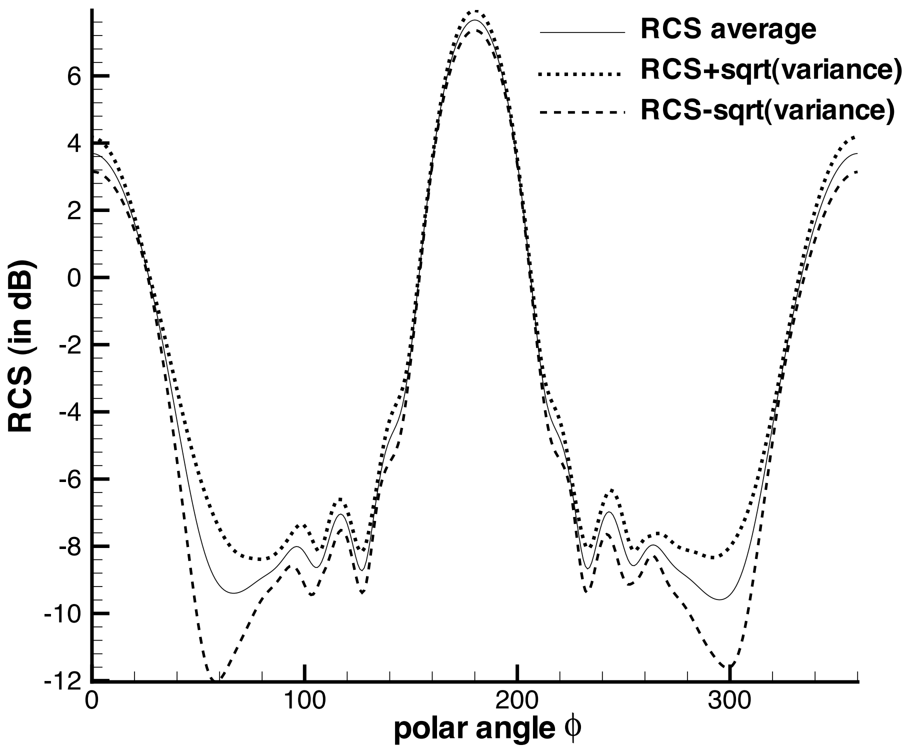


Uncertain geometries



Correlation length is about 1/5 of total length





d=22

Stroud-3 is used

Summary

The use of random mappings in combination with the Stochastic collocation approach is flexible and robust.

We can now address and have demonstrated the ability to deal with uncertainty of a variety of types

- Geometrics
- Initial and boundary conditions
- Materials
- Sources
- Both steady and unsteady problems
- etc

Computational cost is becoming problematic for d>>1

ANOVA Expansions

In many cases we are left with wanting to evaluate

$$f(\mathbf{X}(x)) \qquad \int f(\mathbf{X}(x))\,dx \qquad \mathbf{X} = (X_1, \ldots, X_d), \quad d \gg 1$$

which quickly becomes an expensive exercise.

Q: Can we reduce the cost without loosing accuracy ?

DEF: The ANOVA expansion

$$f(\mathbf{X}) = f_0 + \sum_{t \subseteq \mathcal{D}} f_t(\mathbf{X}^t)$$

$$f_t(\mathbf{X}^t) = \int_{A^{d-|t|}} f(\mathbf{X}) d\mathbf{X}_{\mathcal{D}/t} - \sum_{w \subset t} f_w(\mathbf{X}^w) - f_0$$

$$f_0 = \int_{A^d} f(\mathbf{X})\,d\mathbf{X}, \quad \int_{A^0} f(\mathbf{X})\,d\mathbf{X}^0 = f(\mathbf{X})$$

$$\mathcal{D} = \{1, \ldots, d\}$$

$$\Omega = [0, 1]^d$$

$$A^{|t|}$$

|t| dimensional hypercube

$$\mathbf{X}^t$$

t indexed sub-vector

ANOVA Expansions

A few characteristics -

- The ANOVA expansion is unique and exact
- It is a finite expansion with 2^d terms
- All terms are mutually orthogonal

Example:

$$f(\alpha_1, \alpha_2, \alpha_3) = f_0 + \sum_{i=1}^{3} \hat{f}_i(\alpha_i) + \sum_{1=i<j<d} \hat{f}_{ij}(\alpha_i, \alpha_j)$$

We have not achieved much yet.

Now define the truncated expansion

$$f(\mathbf{X}, s) = f_0 + \sum_{t \subseteq \mathcal{D}; |t| \leq s} f_t(\mathbf{X}^t)$$

S = truncation dimension

ANOVA Expansions

Let us first introduce

$$V_t(f) = \int_{A^d} (f_t(\mathbf{X}^t))^2 \, d\mathbf{X}, \quad V(f) = \sum_{|t|>0} V_t(f)$$

... subset specific variances

Define the effective dimension through

$$\sum_{0<|t|\leq p_s} V_t(f) \geq qV(f) \qquad\qquad q \leq 1$$

Then one can prove $\quad \mathrm{Err}(\mathbf{X}, p_s) \leq 1 - q$

$$\mathrm{Err}(\mathbf{X}, p_s) = \frac{1}{V(f)} \int_{A^d} [f\mathbf{X} - f(\mathbf{X}, p_s)]^2 \, d\mathbf{X}$$

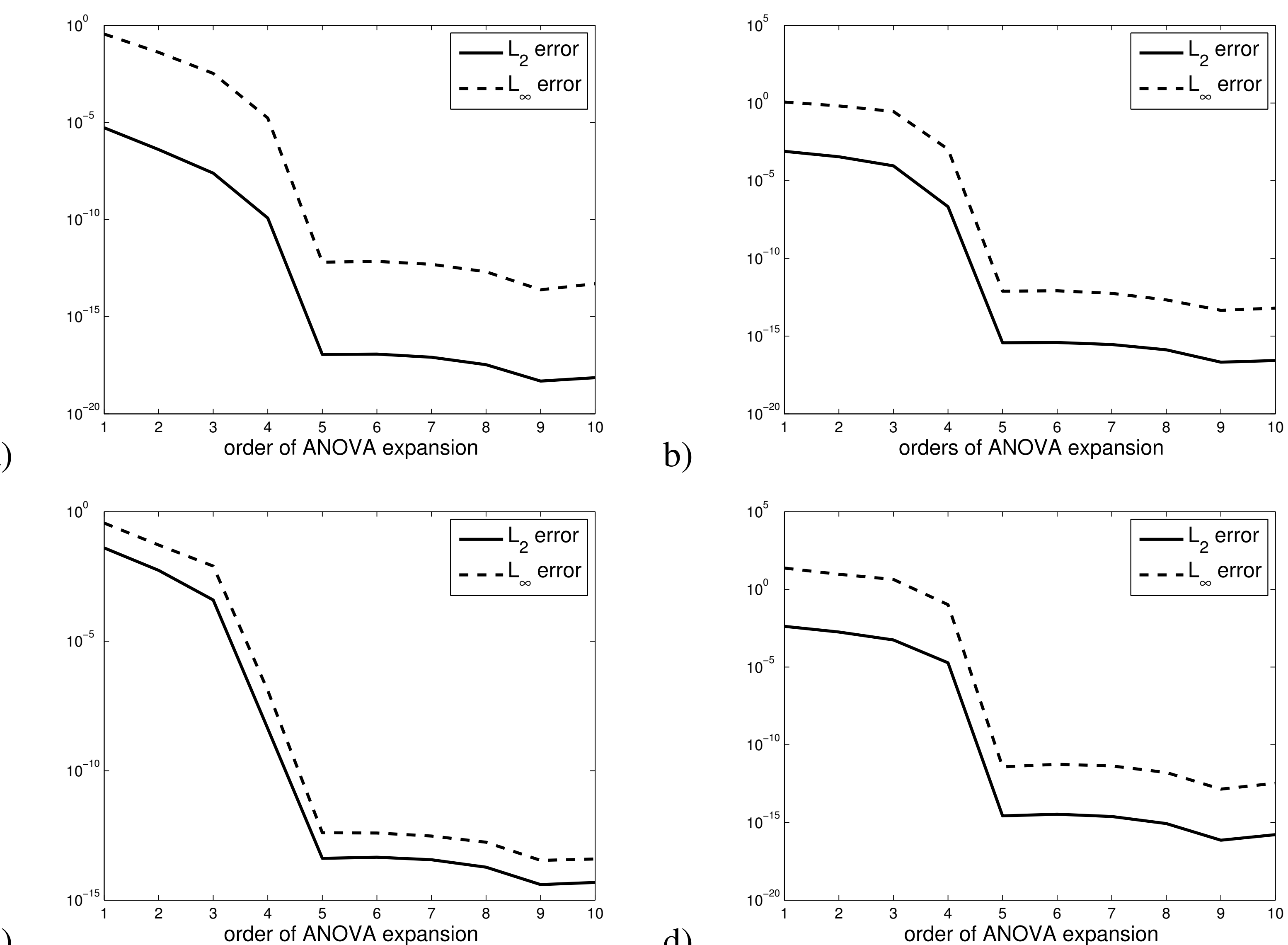
NOTE: If p<<d there is hope!

ANOVA Expansions

Is that relevant ?

d=10

- Product Peak function: $u_1(x) = \prod_{i=1}^{p} (c_i^{-2} + (x_i - \omega_i)^2)^{-1}$,
- Corner Peak function: $u_2(x) = (1 + \sum_{i=1}^{p} c_i x_i)^{-(p+1)}$,
- Gaussian function: $u_3(x) = \exp(-\sum_{i=1}^{p} c_i^2 (x_i - \omega_i)^2)$,
- Continuous function: $u_4(x) = \exp(-\sum_{i=1}^{p} c_i |x_i - \omega_i|)|$,



Observation:
The majority of high-dimensional functions have a low effective dimension.

The ANOVA expansion exposes this and makes it accessible

ANOVA Expansions

Lets take it one step further and define

Sensitivity index: $S(t) = \frac{V_t}{V},$

Then sensitivity of variable "i" is measured through

$$\sum_{i \in t} S(t) + \sum_{i \notin t} S(t) \quad = \quad 1, \qquad\qquad i = \{1, \ldots, d\}, \mathbf{X}^i$$

We can now measure impact of variable on output of interest

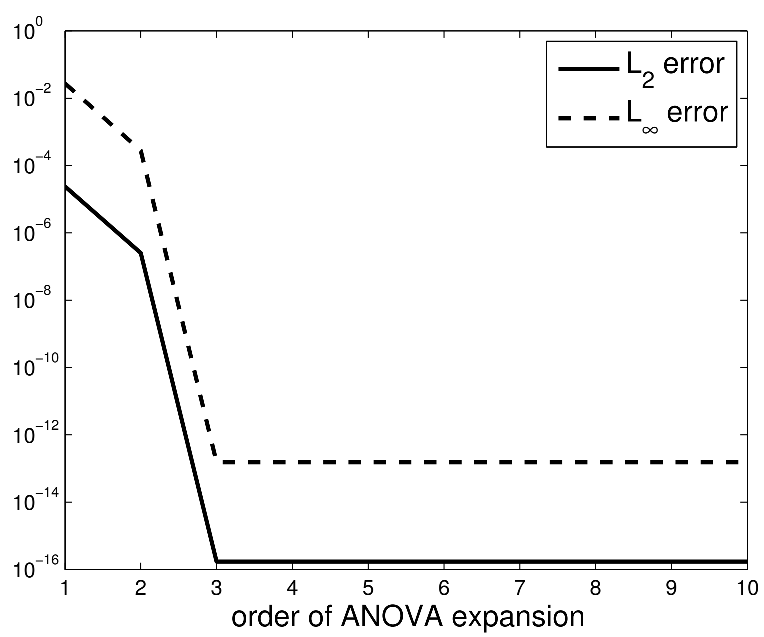
- Compute ANOVA expansion using Stroud-2/3 rule
- Evaluate which parameters are of importance
- Compress parameter set to these and maintain the remaining at expectation value.
- Compute ANOVA expansion of compressed set
- Evaluate statistics of compressed problem

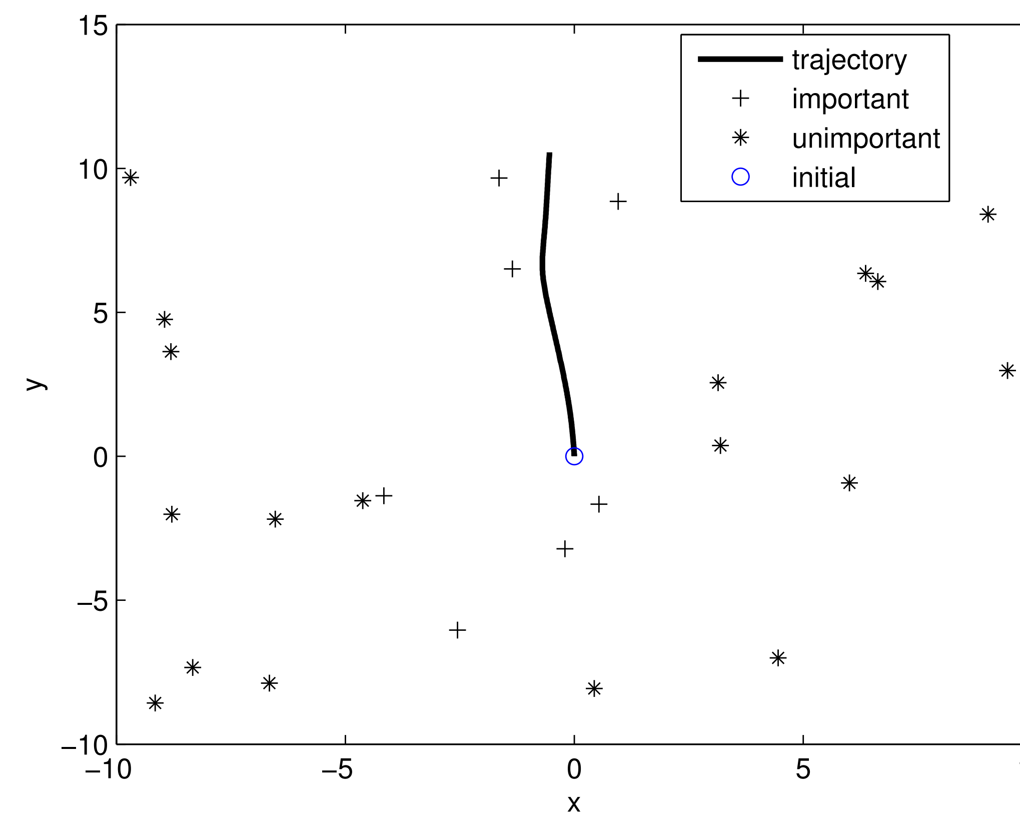
ANOVA Expansions

Example: 25 planets of uncertain mass pull in a unit mass space-ship

$$\ddot{\mathbf{x}}(t) = \sum_{i=1}^{p} m_i \hat{\mathbf{r}}_i / r_i^2, \qquad \mathbf{x}(\mathbf{t_0}) = \mathbf{x_0}. \qquad m_i = \frac{1}{p+1}[1 + 0.1 * U(-1,1)]$$

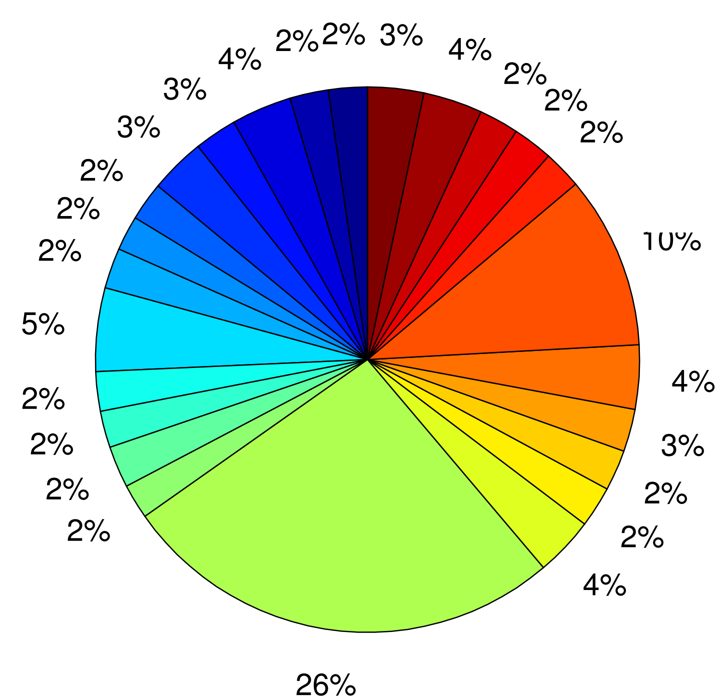
Full ANOVA based on Stroud-3





Active and passive "planets"

Sensitivity index



Active # of parameters is 7 >3%

ANOVA Expansions

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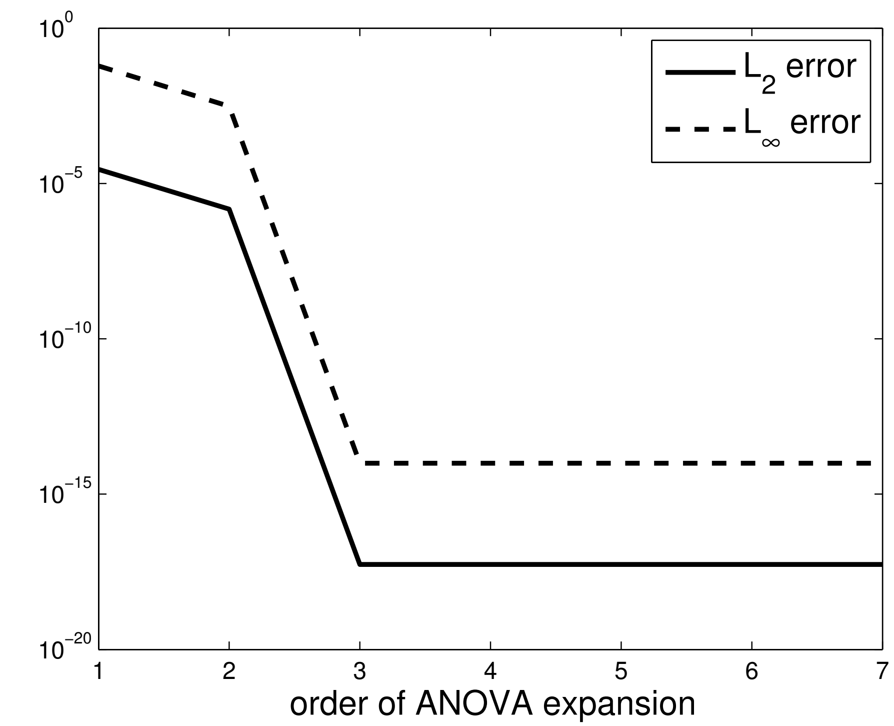
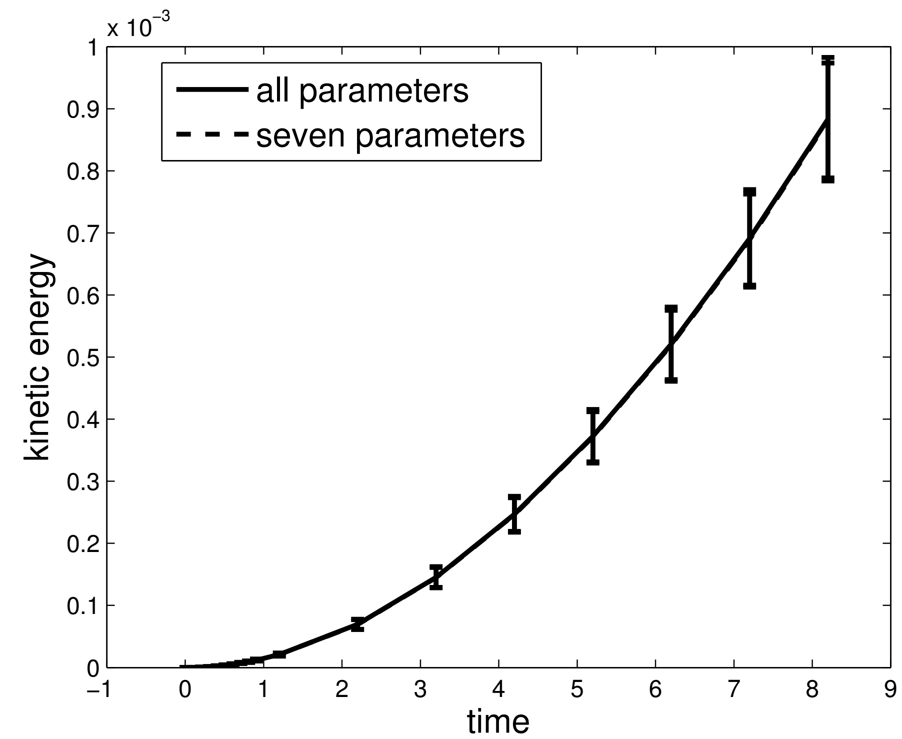
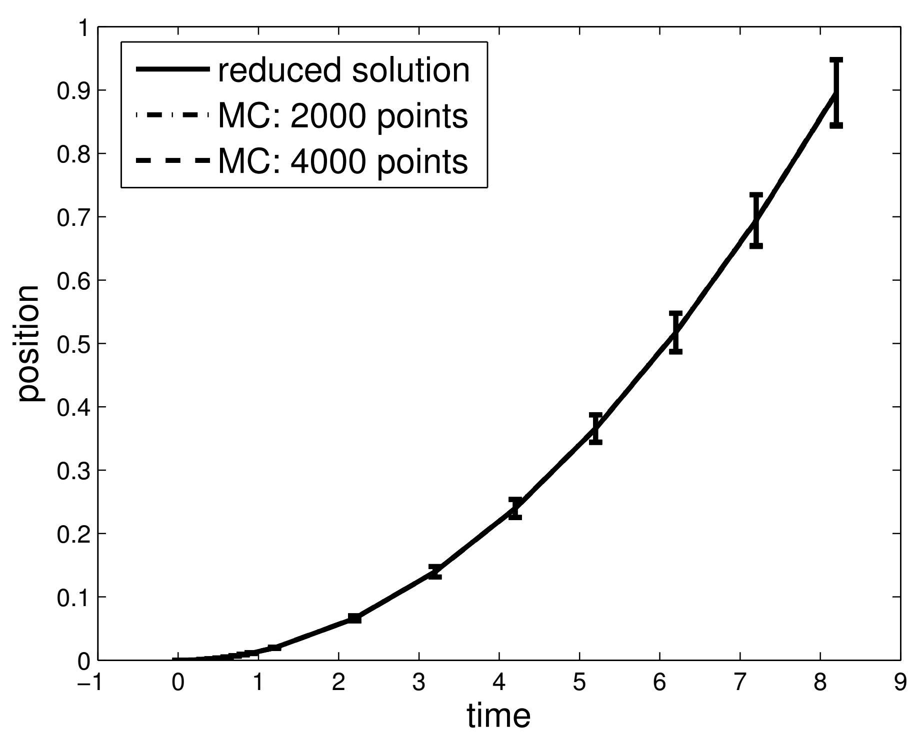
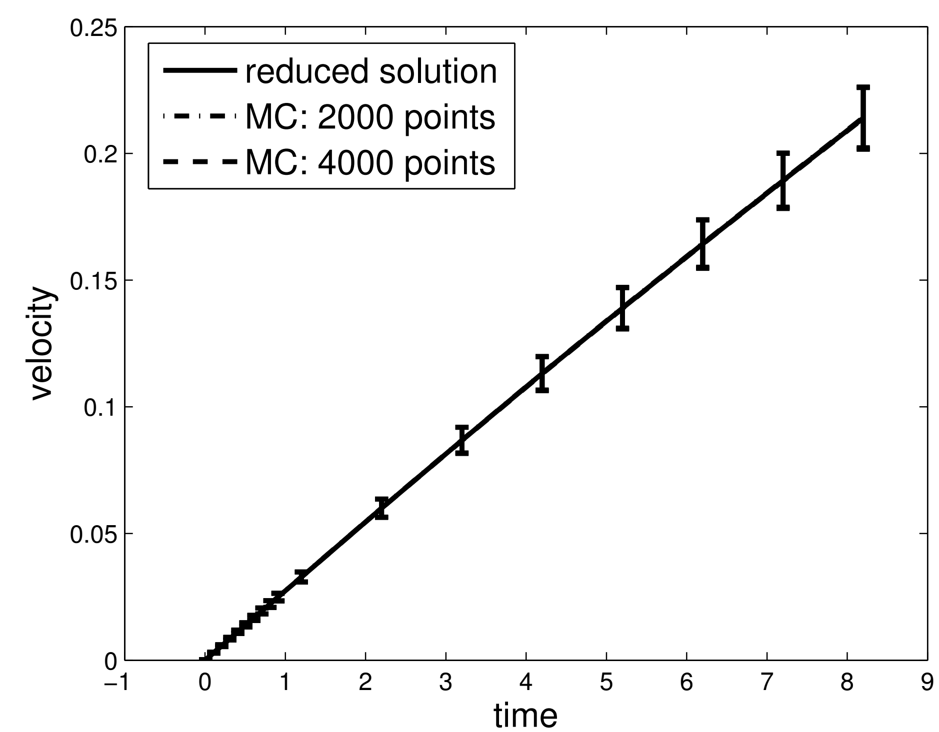
Does it work ?





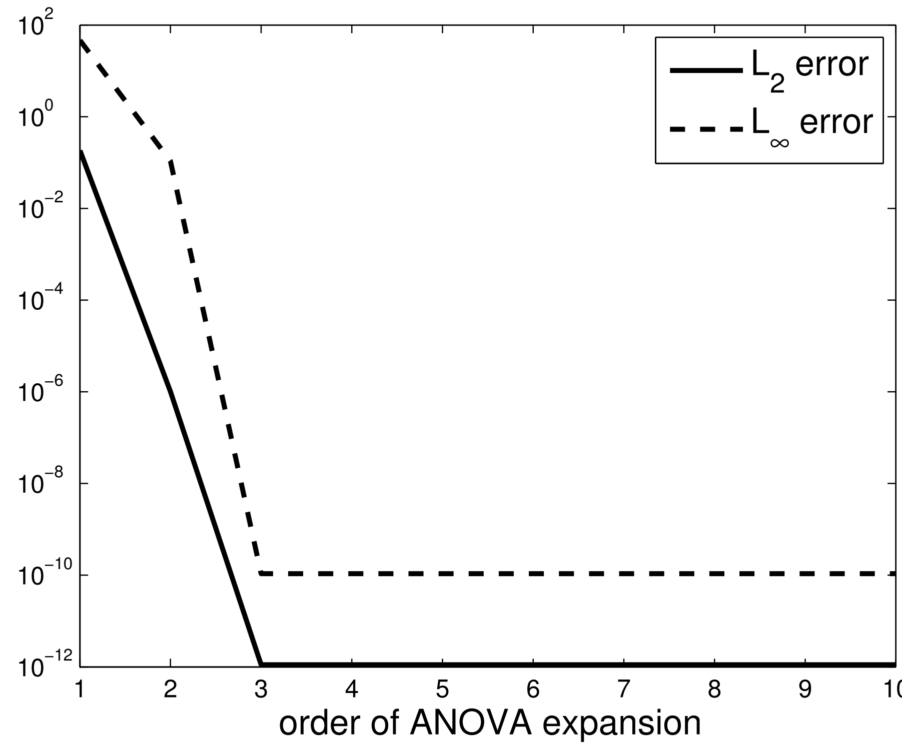


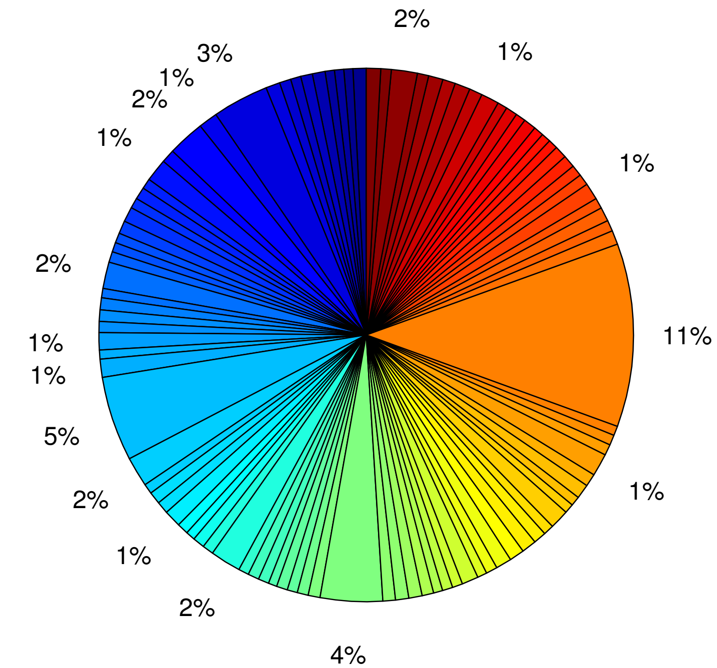


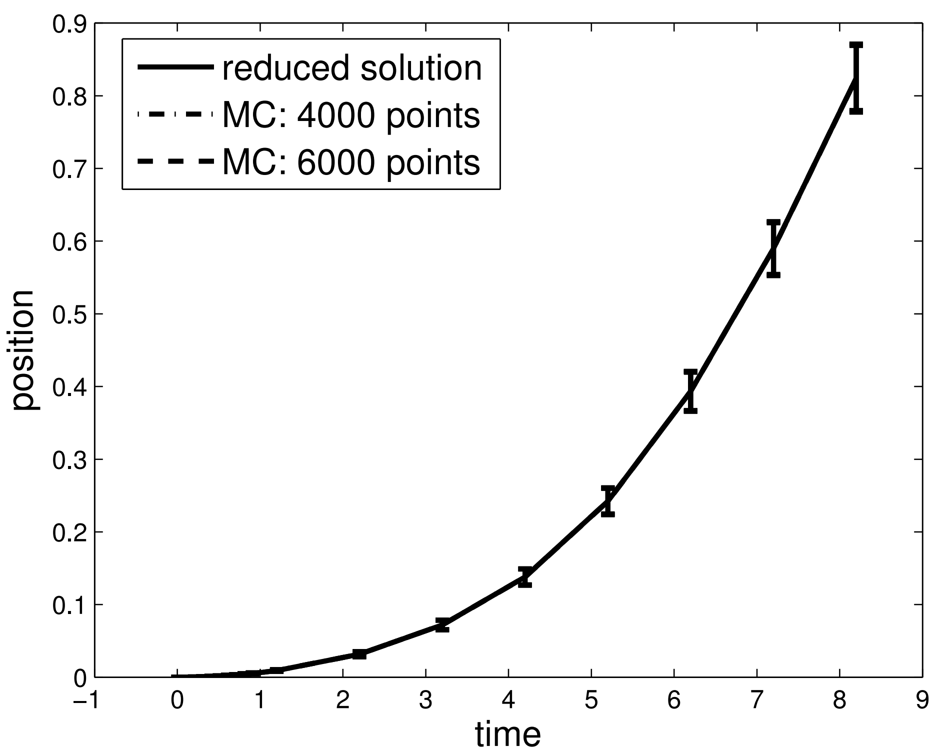
ANOVA Expansions

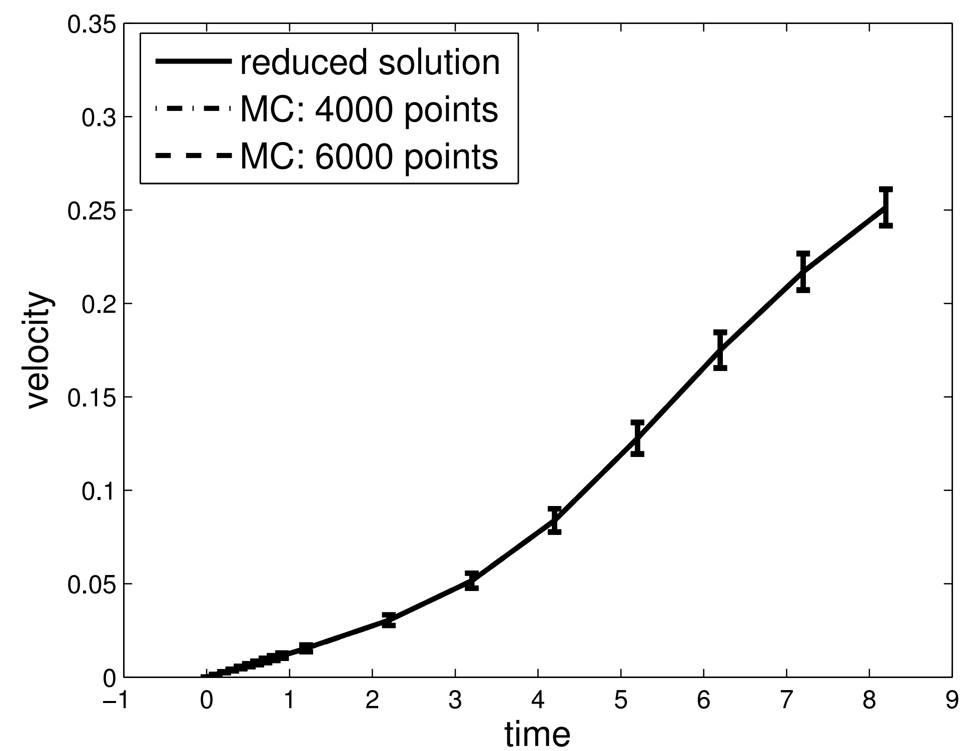
p=100 instead

Active # of parameters is 10









ANOVA Expansions

Consider again the toggle-problem

$$\frac{du}{dt} = \frac{\alpha_1}{1+v^{\beta}} - u,$$

$$\frac{dv}{dt} = \frac{\alpha_2}{1+\omega^{\gamma}} - v,$$

$$\omega = \frac{u}{(1+[IPTG]/\mathscr{K})^{\eta}}$$

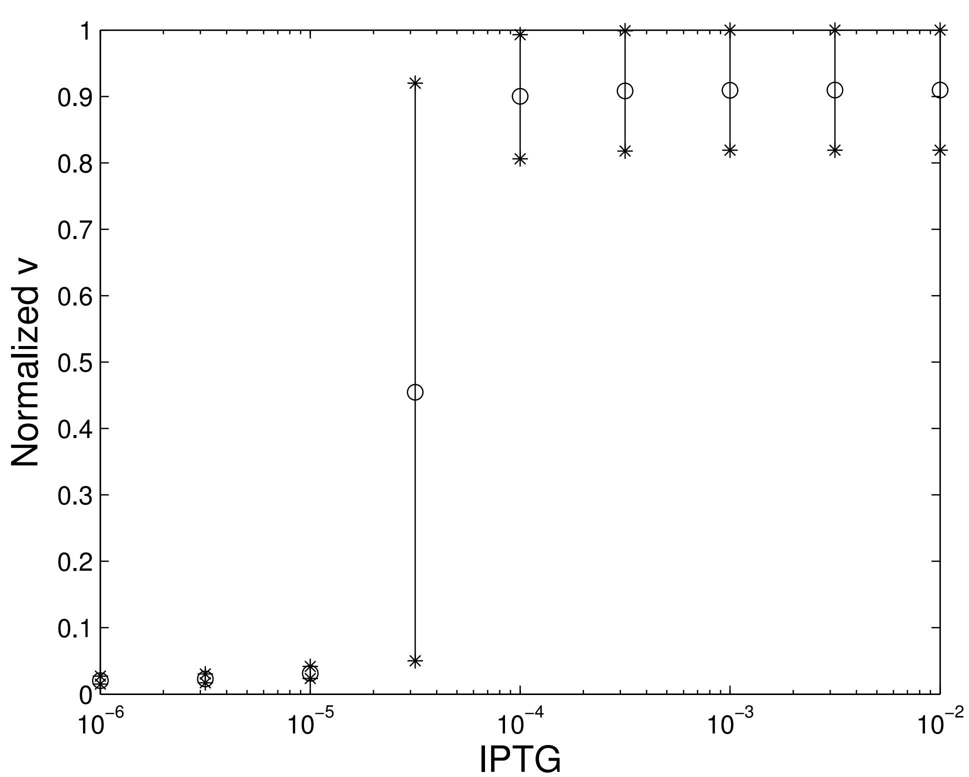
$$\alpha = (\alpha_1, \cdots, \alpha_6) = (\alpha_1, \alpha_2, \beta, \gamma, \eta, \mathscr{K})$$

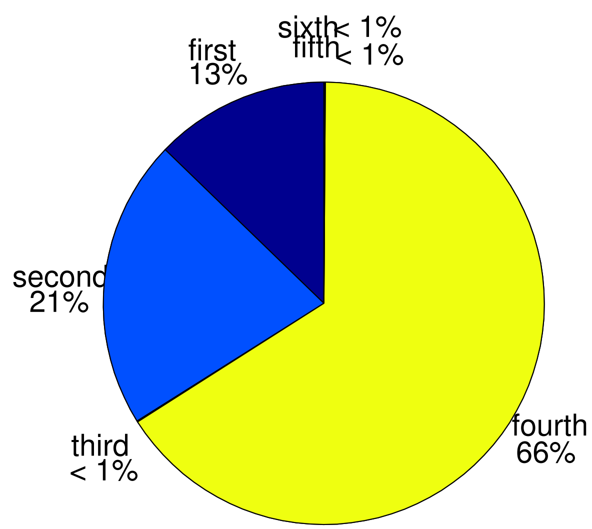
IPTG is a control parameter

$$\alpha(\mathbf{X}) = <\alpha> (1 + \sigma \mathbf{X})$$

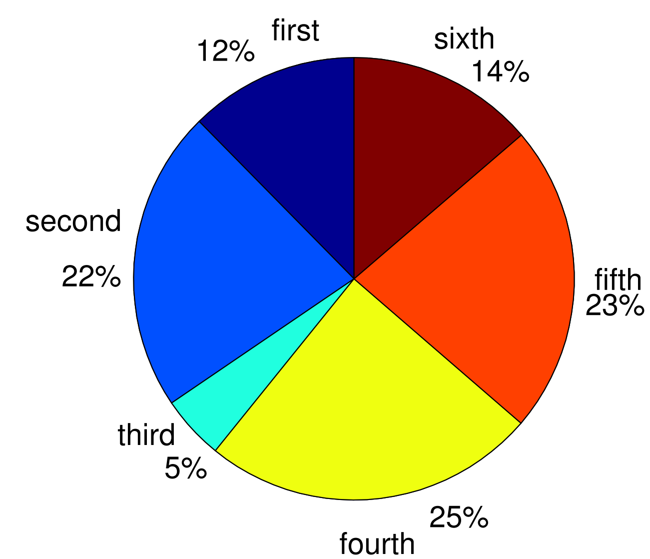
$$f_{X_i} = U(-1,1)$$

$$\sigma = 0.1$$





IPTG = 1E-6



IPTG = 1E-4.5

Parametric importance is nicely reflected in sensitivity index

ANOVA Expansions

Consider a problem of pollution chemistry

$$\mathbf{f}(\mathbf{u}) = \begin{cases} -\sum_{j\in\{1,10,14,23,24\}} r_j + \sum_{j\in\{2,3,9,11,12,22,25\}} r_j \\ -r_2 - r_3 - r_9 - r_{12} + r_1 + r_{21} \\ -r_{15} + r_1 + r_{17} + r_{19} + r_{22} \\ -r_2 - r_{16} - r_{17} - r_{23} + r_{15} \\ -r_3 + 2 * r_4 + r_6 + r_7 + r_{13} + r_{20} \\ -r_6 - r_8 - r_{14} - r_{20} + r_3 + 2 * r_{18} \\ -r_4 - r_5 - r_6 + r_{13} \\ r_4 + r_5 + r_6 + r_7 \\ -r_7 - r_8 \\ -r_{12} + r_7 + r_9 \\ -r_9 - r_{10} + r_8 + r_{11} \\ r_9 \\ -r_{11} + r_{10} \\ -r_{13} + r_{12} \\ r_{14} \\ -r_{18} - r_{19} + r_{16} \\ -r_{20} \\ r_{20} \\ -r_{21} - r_{22} - r_{24} + r_{23} + r_{25} \\ -r_{25} + r_{24} \end{cases}$$

$r_1 = k_1 \cdot u_1$	$r_{10} = k_{10} \cdot u_1 \cdot u_{11}$	$r_{19} = k_{19} \cdot u_{16}$
$r_2 = k_2 \cdot u_2 \cdot u_3$	$r_{11} = k_{11} \cdot u_{13}$	$r_{20} = k_{20} \cdot u_6 \cdot u_{17}$
$r_3 = k_3 \cdot u_2 \cdot u_5$	$r_{12} = k_{12} \cdot u_2 \cdot u_{10}$	$r_{21} = k_{21} \cdot u_{19}$
$r_4 = k_4 \cdot u_7$	$r_{13} = k_{13} \cdot u_{14}$	$r_{22} = k_{22} \cdot u_{19}$
$r_5 = k_5 \cdot u_7$	$r_{14} = k_{14} \cdot u_1 \cdot u_6$	$r_{23} = k_{23} \cdot u_1 \cdot u_4$
$r_6 = k_6 \cdot u_6 \cdot u_7$	$r_{15} = k_{15} \cdot u_3$	$r_{24} = k_{24} \cdot u_1 \cdot u_{19}$
$r_7 = k_7 \cdot u_9$	$r_{16} = k_{16} \cdot u_4$	$r_{25} = k_{25} \cdot u_{20}$
$r_8 = k_8 \cdot u_6 \cdot u_9$	$r_{17} = k_{17} \cdot u_4$	
$r_9 = k_9 \cdot u_2 \cdot u_{11}$	$r_{18} = k_{18} \cdot u_{16}$	

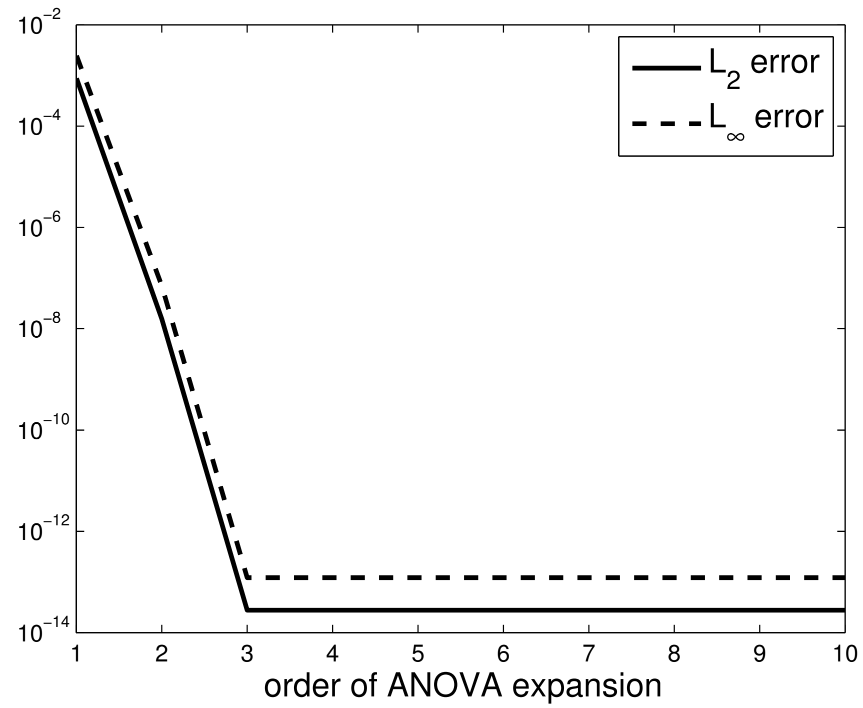
$k_1 = 0.350$	$k_{10} = 0.900 \cdot 10^4$	$k_{19} = 0.444 \cdot 10^{12}$
$k_2 = 0.266 \cdot 10^2$	$k_{11} = 0.220 \cdot 10^{-1}$	$k_{20} = 0.124 \cdot 10^4$
$k_3 = 0.123 \cdot 10^5$	$k_{12} = 0.120 \cdot 10^5$	$k_{21} = 0.210 \cdot 10$
$k_4 = 0.860 \cdot 10^{-3}$	$k_{13} = 0.188 \cdot 10$	$k_{22} = 0.578 \cdot 10$
$k_5 = 0.820 \cdot 10^{-3}$	$k_{14} = 0.163 \cdot 10^5$	$k_{23} = 0.474 \cdot 10^{-1}$
$k_6 = 0.150 \cdot 10^5$	$k_{15} = 0.480 \cdot 10^7$	$k_{24} = 0.178 \cdot 10^4$
$k_7 = 0.130 \cdot 10^{-5}$	$k_{16} = 0.350 \cdot 10^{-3}$	$k_{25} = 0.312 \cdot 10$
$k_8 = 0.240 \cdot 10^5$	$k_{17} = 0.175 \cdot 10^{-1}$	
$k_9 = 0.165 \cdot 10^5$	$k_{18} = 0.100 \cdot 10^9$	

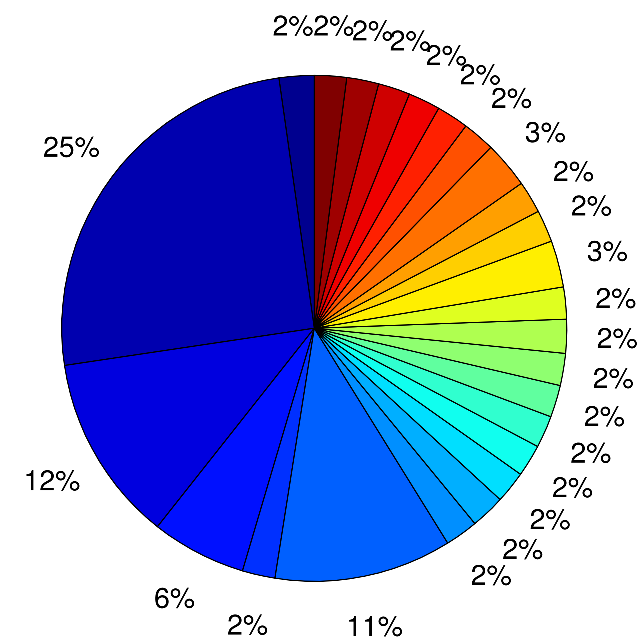
20 equations

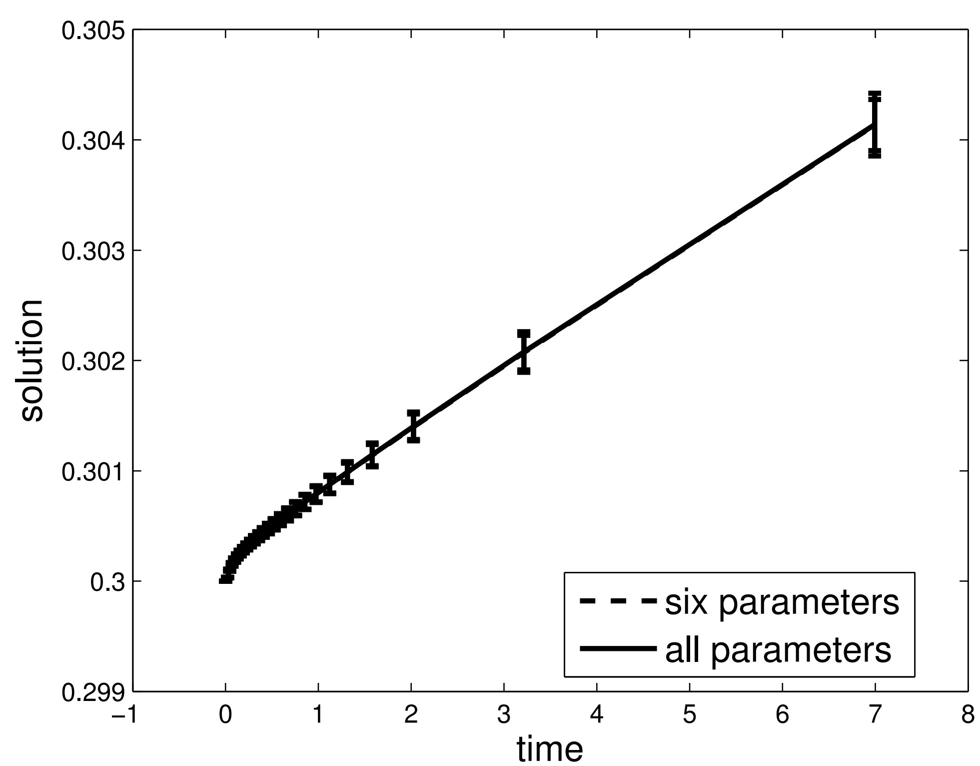
25 RV (Uniformly distributed with 10%)

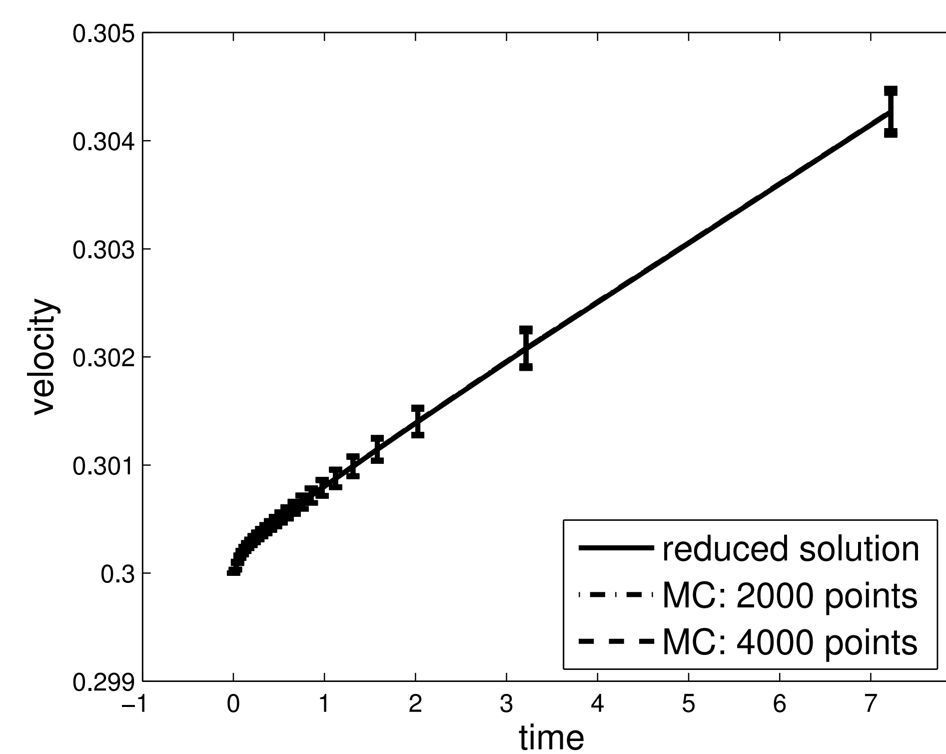
ANOVA Expansions

Active # of parameters is 6





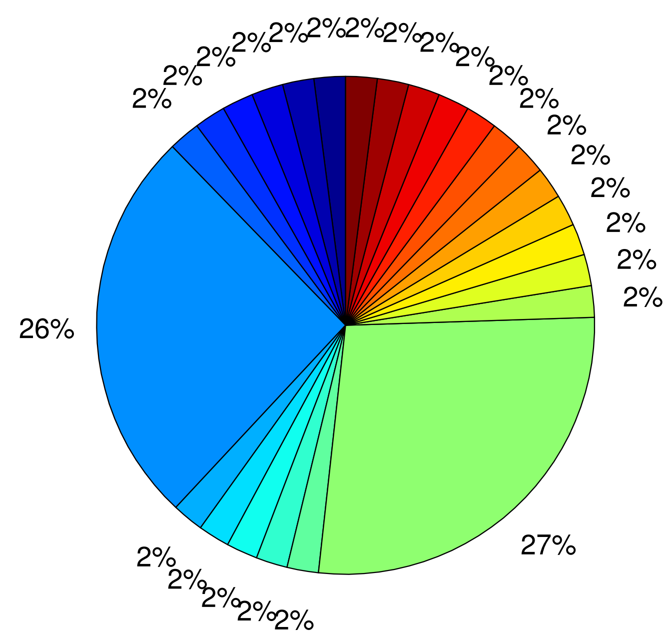


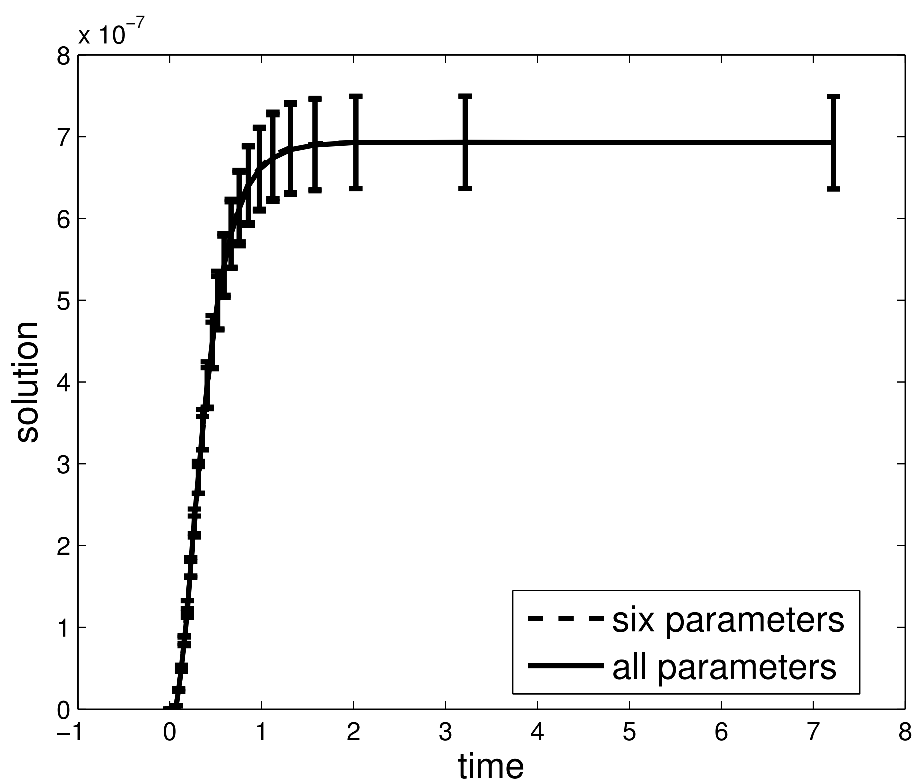


ANOVA Expansions

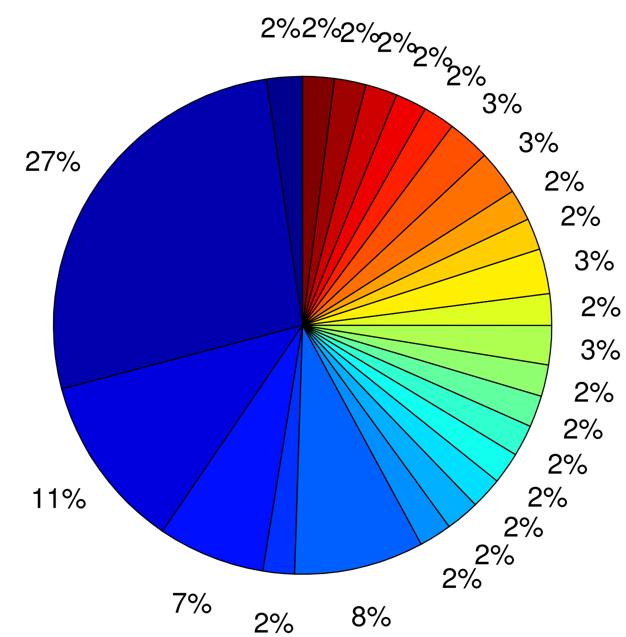
Active parameters depends on output of interest

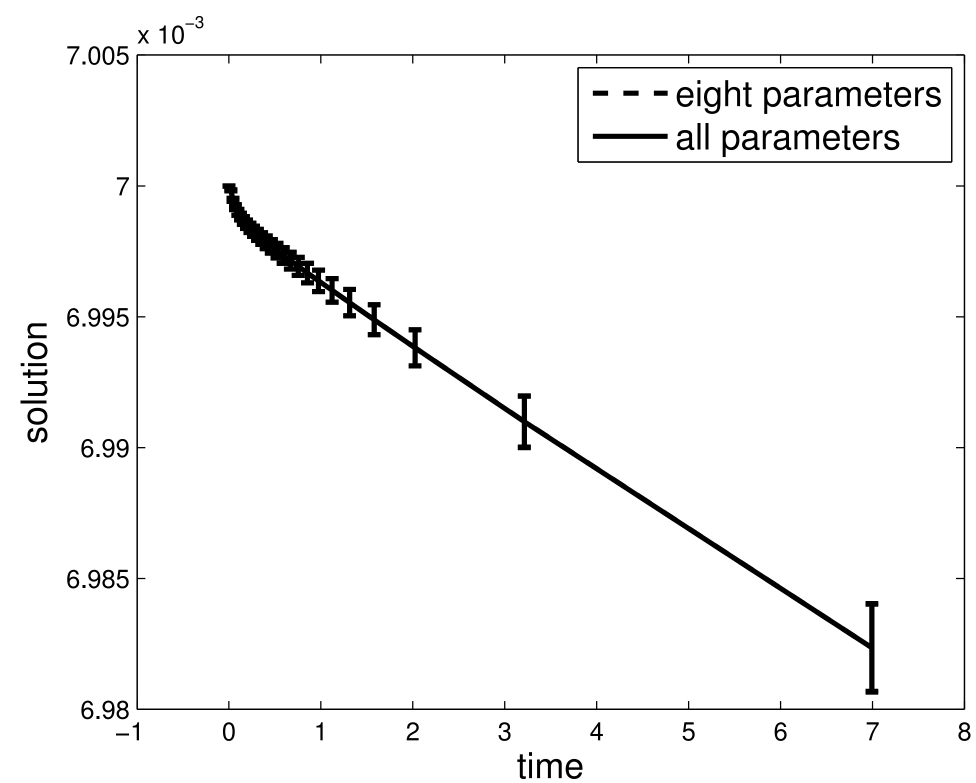
u14 - Active # of parameters is 8





u17 - Active # of parameters is 8





ANOVA Expansions

It is valuable tool to analyze and compress functions of many parameters:

- It is exact and finite
- It nicely exposes low-dimensional effective dimensions
- It provides a practical tool for parametric compression

Only one bottleneck left

$$f_0 = \int_{A^d} f(\mathbf{X})\, d\mathbf{X}, \quad \int_{A^0} f(\mathbf{X})\, d\mathbf{X}^0 = f(\mathbf{X})$$

This is a full high-d integration -

if done accurately, it is very expensive

ANOVA Expansions

The ANOVA expansion can be expressed with an arbitrary measure -

$$\int_{A^d} f(\mathbf{X})\, d\mathbf{X} = \int_{A^d} f(\mathbf{X})\, d\mu(\mathbf{X})$$

Let us choose the measure $\mu(\mathbf{X}) = \delta(\mathbf{X} - \beta)$

With the anchor point $\beta = (\beta_1, \ldots, \beta_d)$

In that case we get the expansion

$$f_t(\mathbf{X}^t) = f(\beta_1, \ldots, \beta_d, \mathbf{X}^t) - \sum_{w \subset t} f_w(\mathbf{X}^w) - f_0$$

$$f_0 = f(\beta_1, \ldots, \beta_d)$$

No integrals - just function evaluations

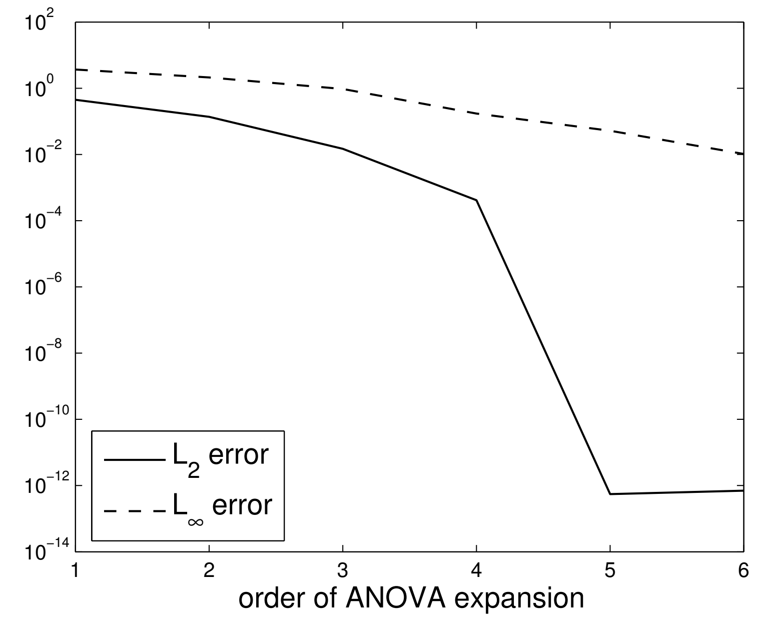
ANOVA Expansions

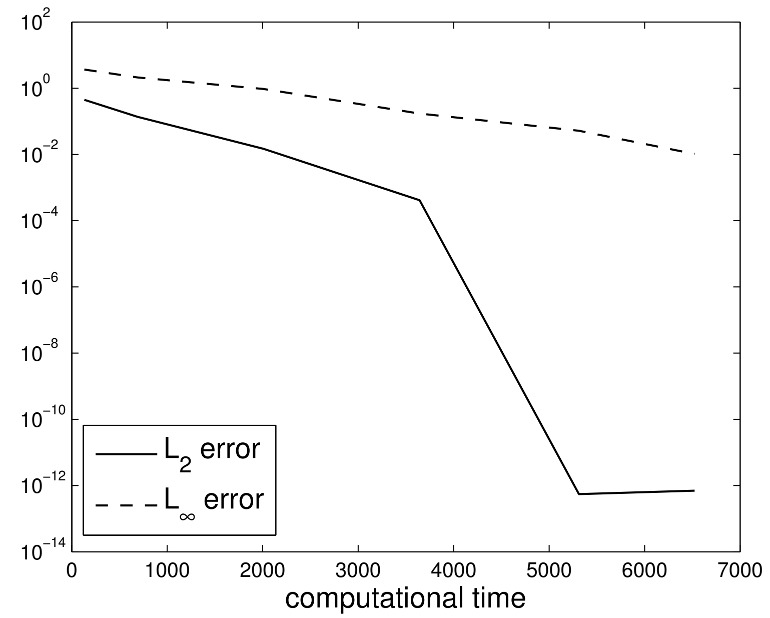
Does this really work ?

$$u_1(\alpha) = \cos(2\pi\omega_1 + \sum_{i=1}^{p} c_i\alpha_i).$$

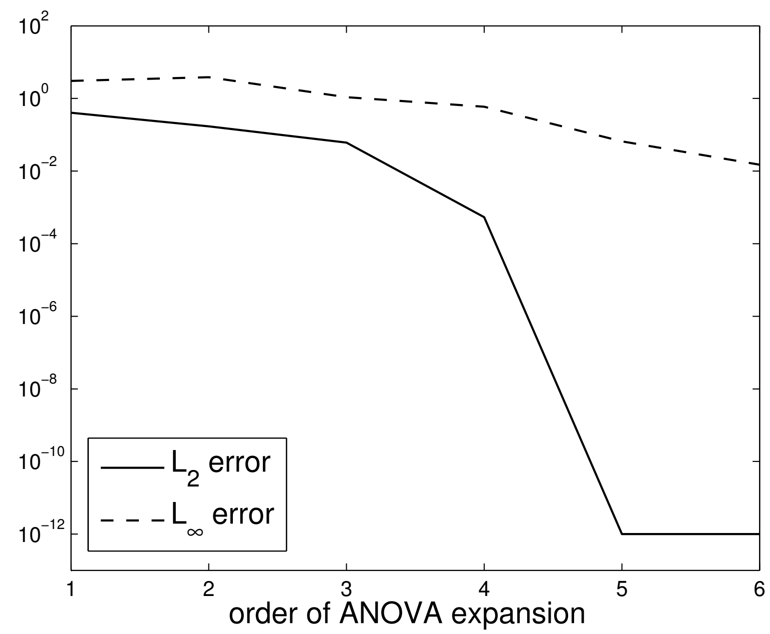
p=10

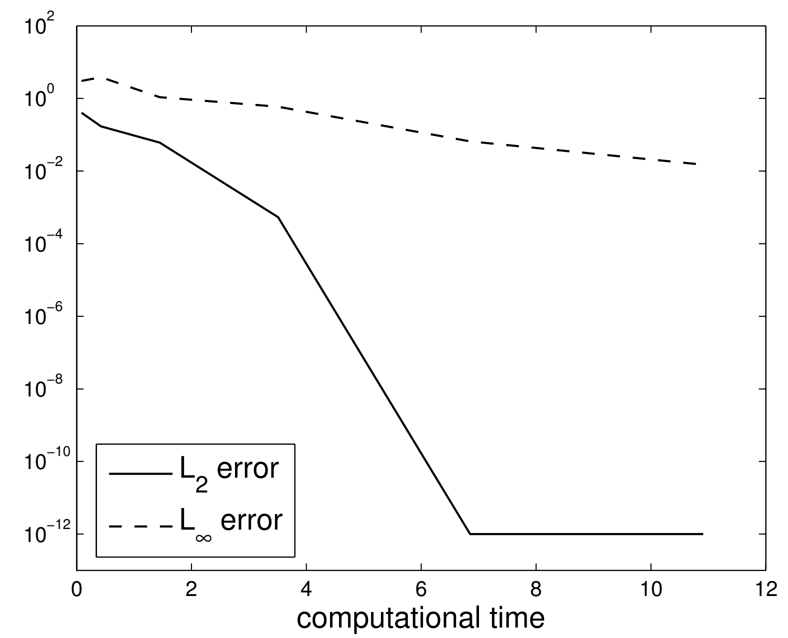
Lebesgue ANOVA





Dirac ANOVA



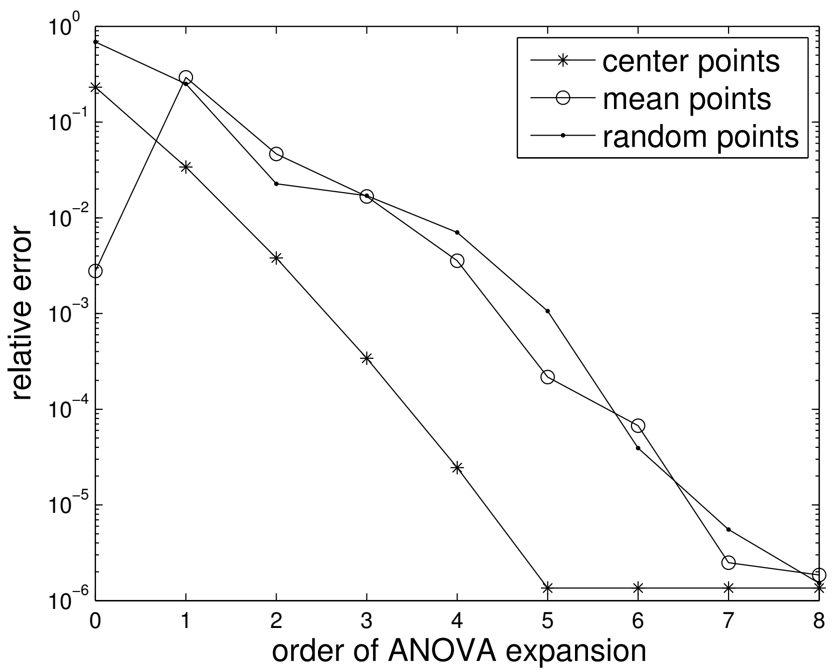


ANOVA Expansions

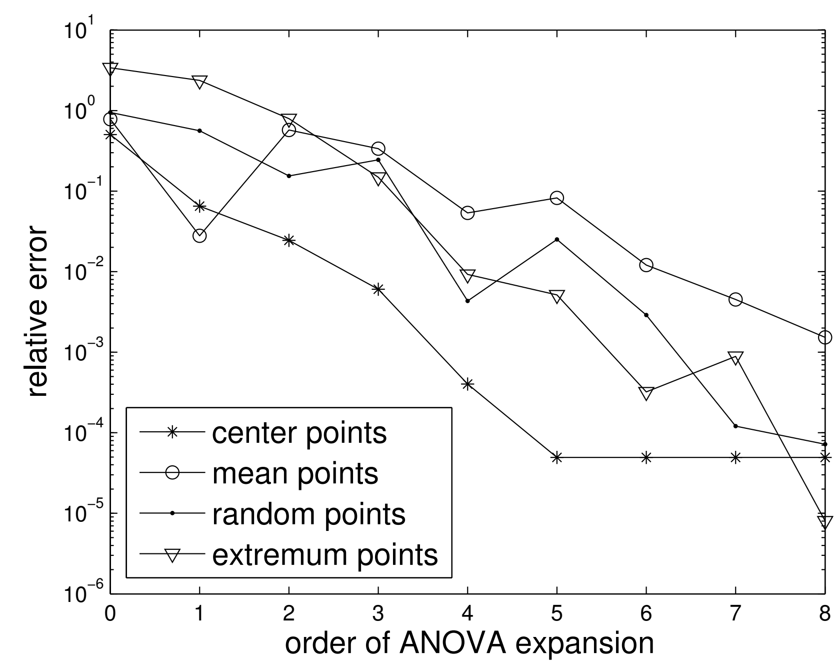
The key out-standing issue is now the choice of anchor

- Randomly chose the point
- Always choose the center point
- Choose a MC based mean point
- Centroid of associated sparse grid

$$u_3(\alpha) = (1 + \sum_{i=1}^{p} c_i \alpha_i)^{-(p+1)},$$



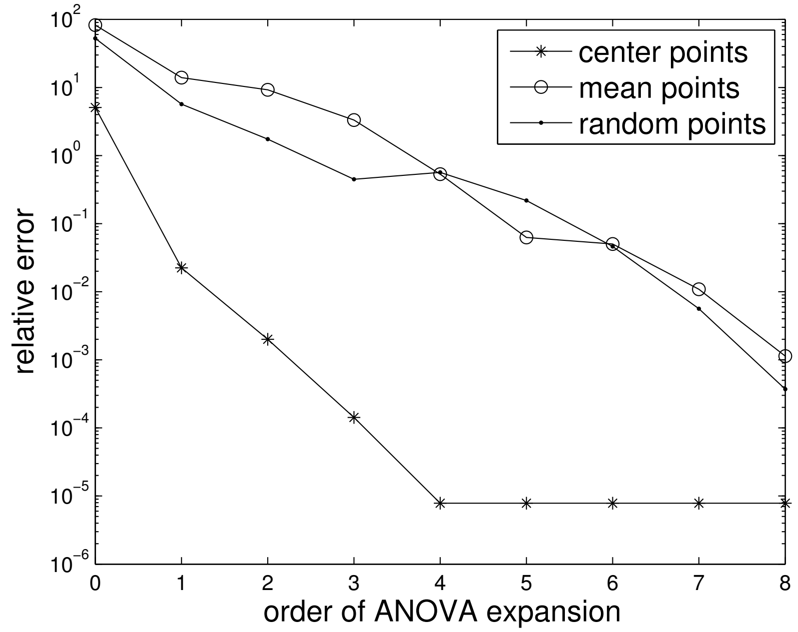
$$u_5(\alpha) = \exp(-\sum_{i=1}^{p} c_i |\alpha_i - \xi_i)|,$$

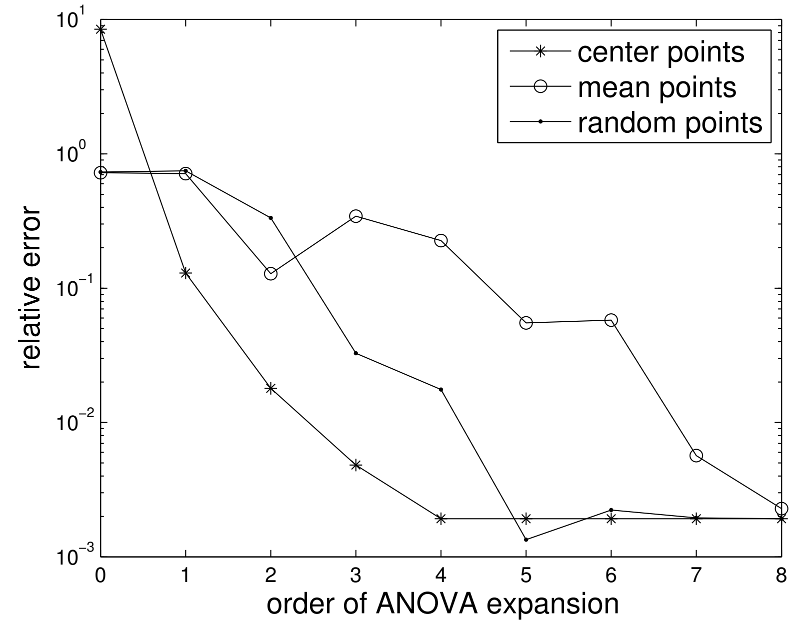


The choice matters a great deal

ANOVA Expansions

For non-uniformly distributed variables it is worse

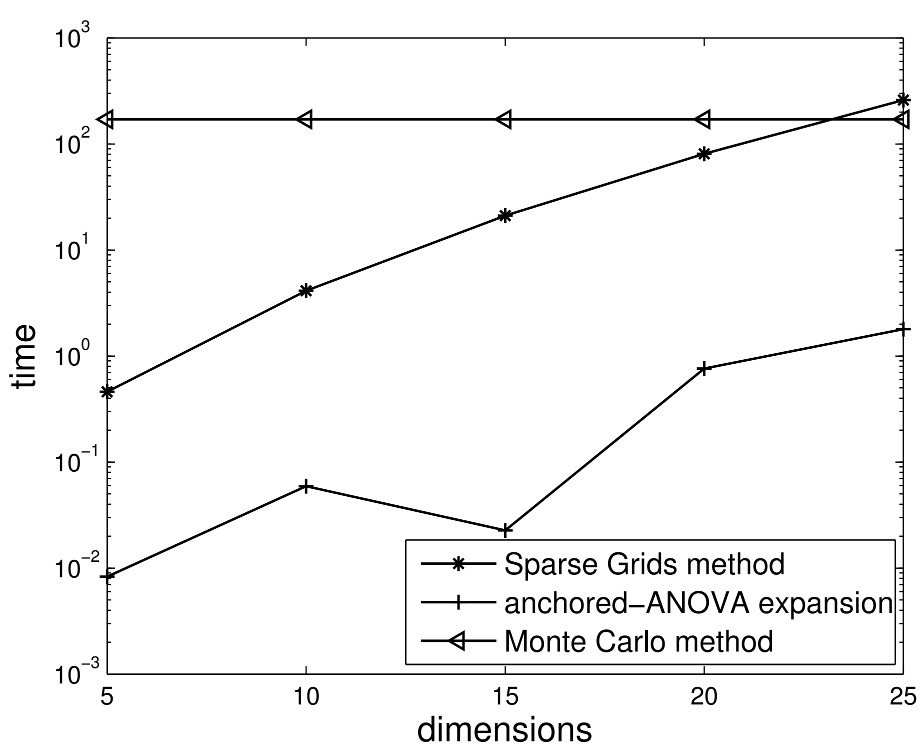


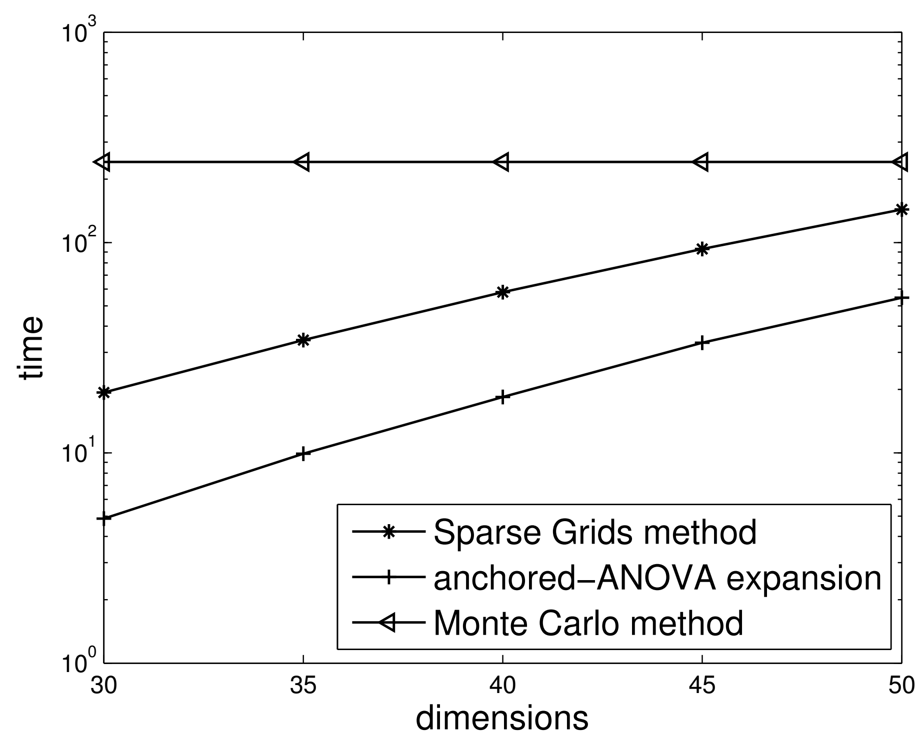


$$X_i \sim (1+x)^{1/2}(1-x)^{1/3}$$

Small order => low cost

Directly comparing cost of integration





Cost for comparable accuracy

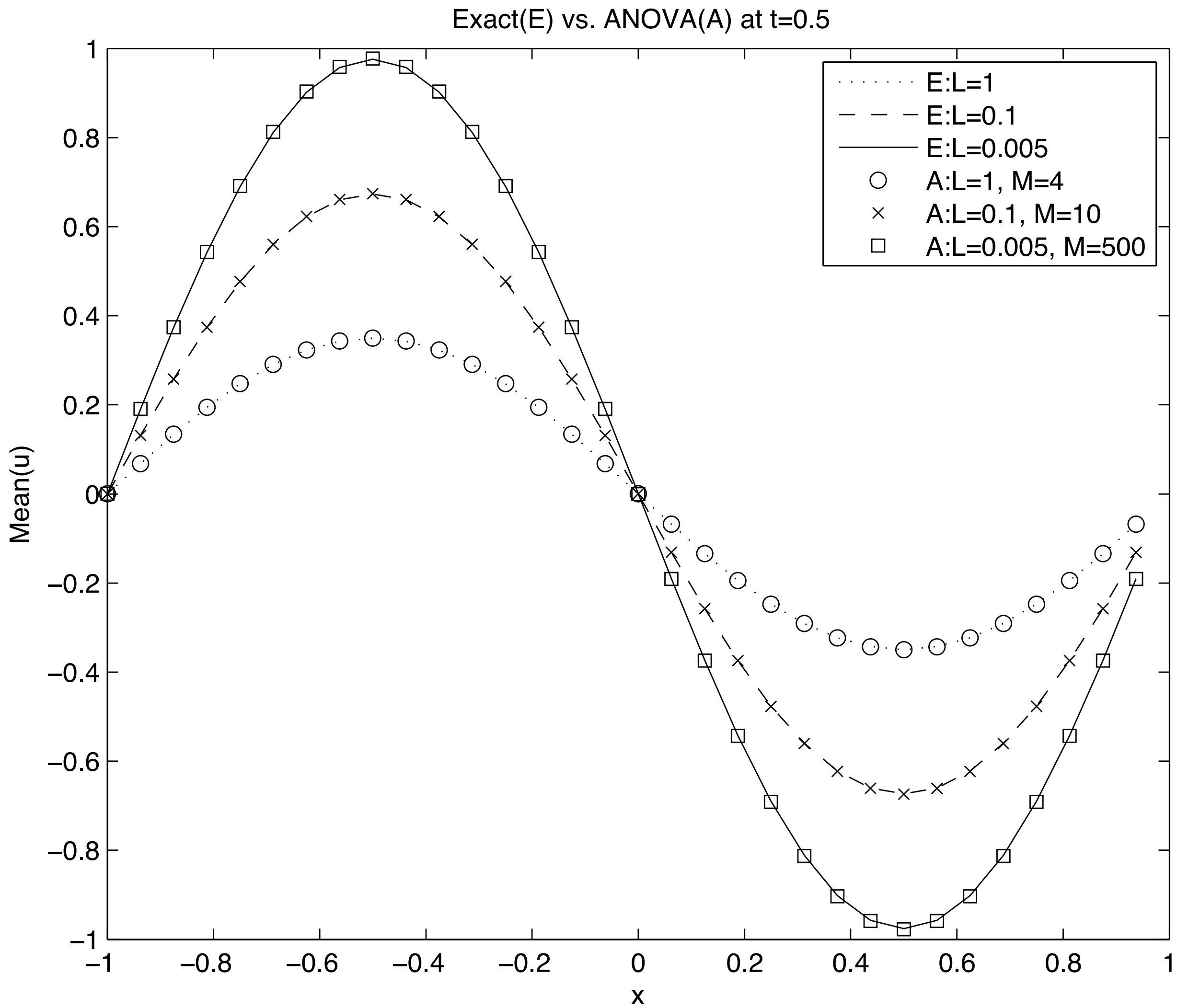
ANOVA Expansions

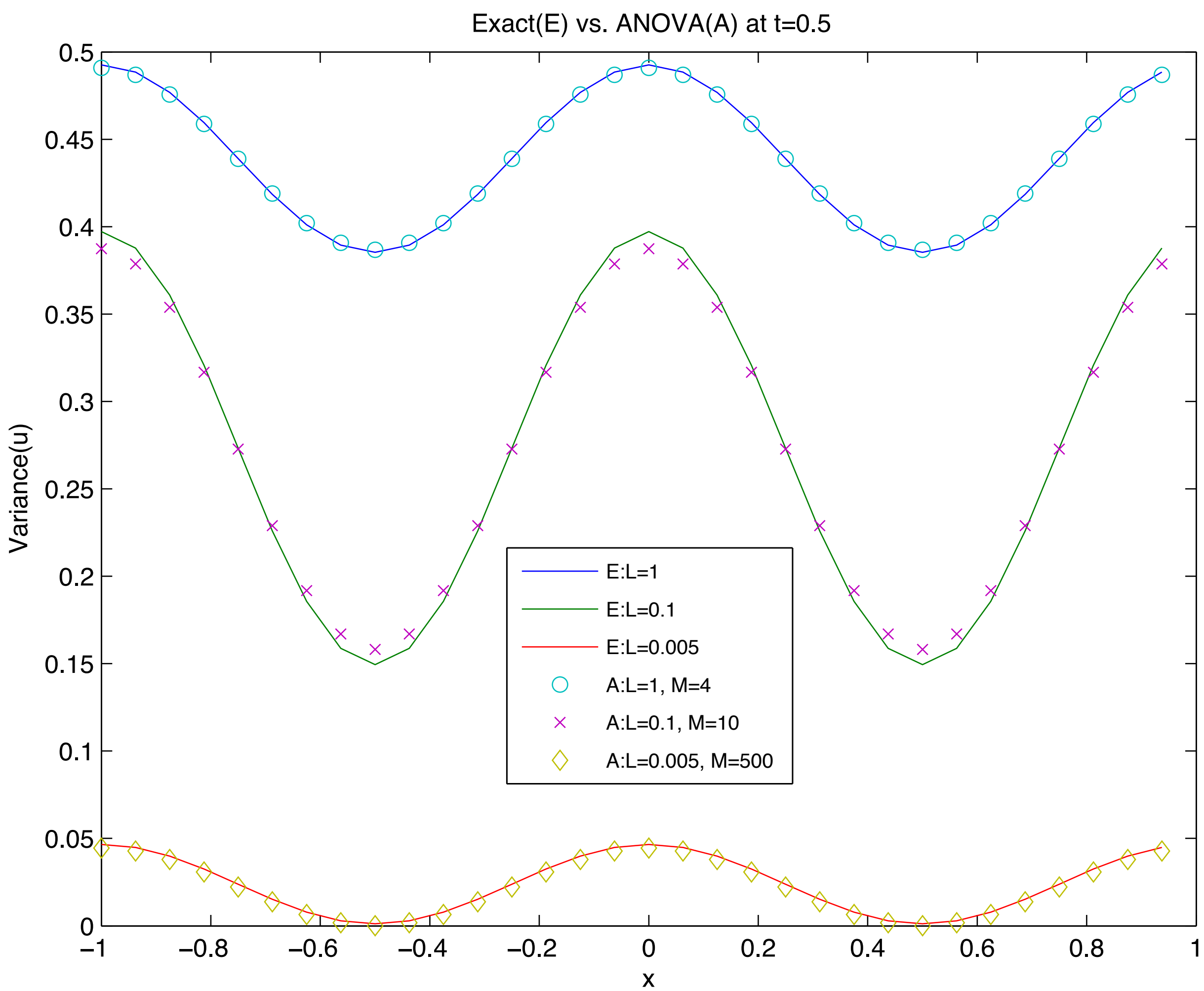
Final example

$$\frac{\partial u}{\partial t} + V(t;\xi)\frac{\partial u}{\partial x} = 0 \qquad x \in [-1,1]$$

$$V(t,\xi) = \sum_{k=0}^{M} \sqrt{\lambda_k}\psi_k(t)\xi_k \qquad \xi \sim U(-1,1) \qquad \mathrm{cov}(V(t_1),V(t_2)) = \exp(-|t_1 - t_2|/L)$$

$$(L,M) = (1,4); (0.1,10); (0.005,500) \qquad p_s = (2,2,1)$$





Z. Zhang et al, 2009

UQ using reduced order models

What we need is an accurate way to evaluate the solution at new parameter values at reduced complexity.

input: parameter value $\boldsymbol{\mu} \in \mathcal{D}$

PDE solver

$$\mathcal{L}_h(u_h(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0$$

output: $s_h(\boldsymbol{\mu}) = l(u_h(\boldsymbol{\mu}); \boldsymbol{\mu})$

.. but WHY ?

Assume we are interested in

$$-\nabla^2 u(\mathbf{x},\mu) = \mathbf{f}(\mathbf{x},\mu) \qquad \mathbf{x} \in \boldsymbol{\Omega}$$

and wish to solve it accurately for many values of 'some' parameter μ

We can use our favorite numerical method

$$\mathrm{A}_h \mathbf{u}_h(\mathbf{x},\mu) = \mathbf{f}_\mathbf{h}(\mathbf{x},\mu) \qquad \dim(\mathbf{u}_h) = \mathcal{N} \gg 1$$

For many parameter values, this is expensive - and slow !

.. but WHY (con't)

Assume we (somehow) know

$$\mathbf{u_h}(\mathbf{x},\mu) \simeq \mathbf{u_{RB}}(\mathbf{x},\mu) = \mathrm{V}\mathbf{a}(\mu) \qquad \mathrm{V}^T\mathrm{V} = \mathrm{I}$$

$$\dim(\mathbf{a}) = N \qquad \dim(V) = \mathcal{N} \times N$$

Then we can recover a solution for a new parameter as little cost

$$(\mathrm{V}^T\mathrm{A}_h\mathrm{V})\mathrm{V}^T\mathbf{u}_h(\mu) = \mathrm{V}^T\mathbf{f}_h(\mu)$$

$N \times N$ $\qquad N$ $\qquad N$

.. if this behaves !

.. but WHY (con't)

So IF

- .. we know the orthonormal basis - V
- .. and it allows an accurate representation - $u_{RB}(\mu)$
- .. and we can evaluate RHS 'fast'-

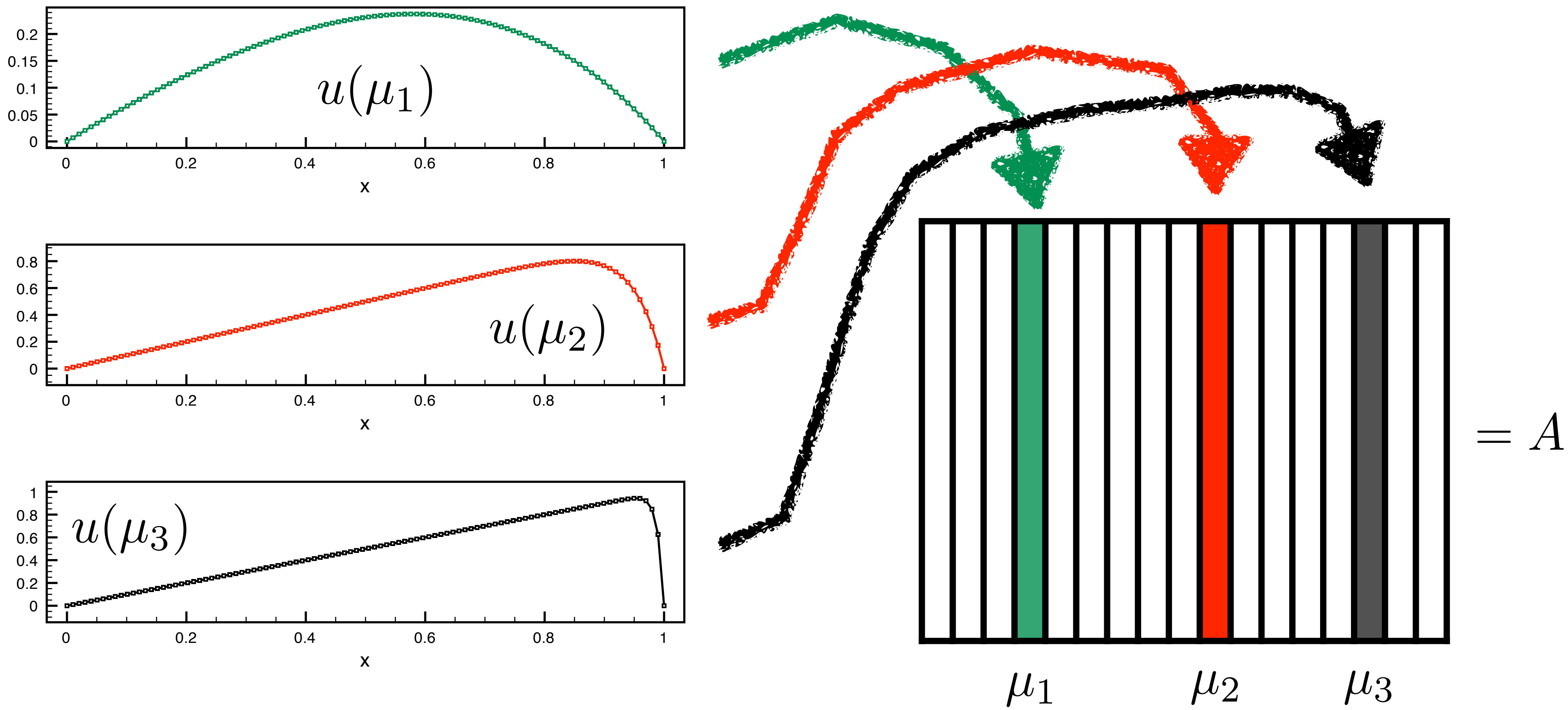
we can evaluate new solutions at cost -

So WHY ? - promise to do sampling at low cost

Does this even work ?

We can get a good sense by a feasibility study

- Define a point-set $\mathbb{P}_h = \{\mu_1, \ldots, \mu_M\} \subset \mathbb{P}$.
- Compute for each μ_i the truth solution $u(\mu_i)$ using a simplified model.
- Store the degrees of freedom row-wise in a matrix A.

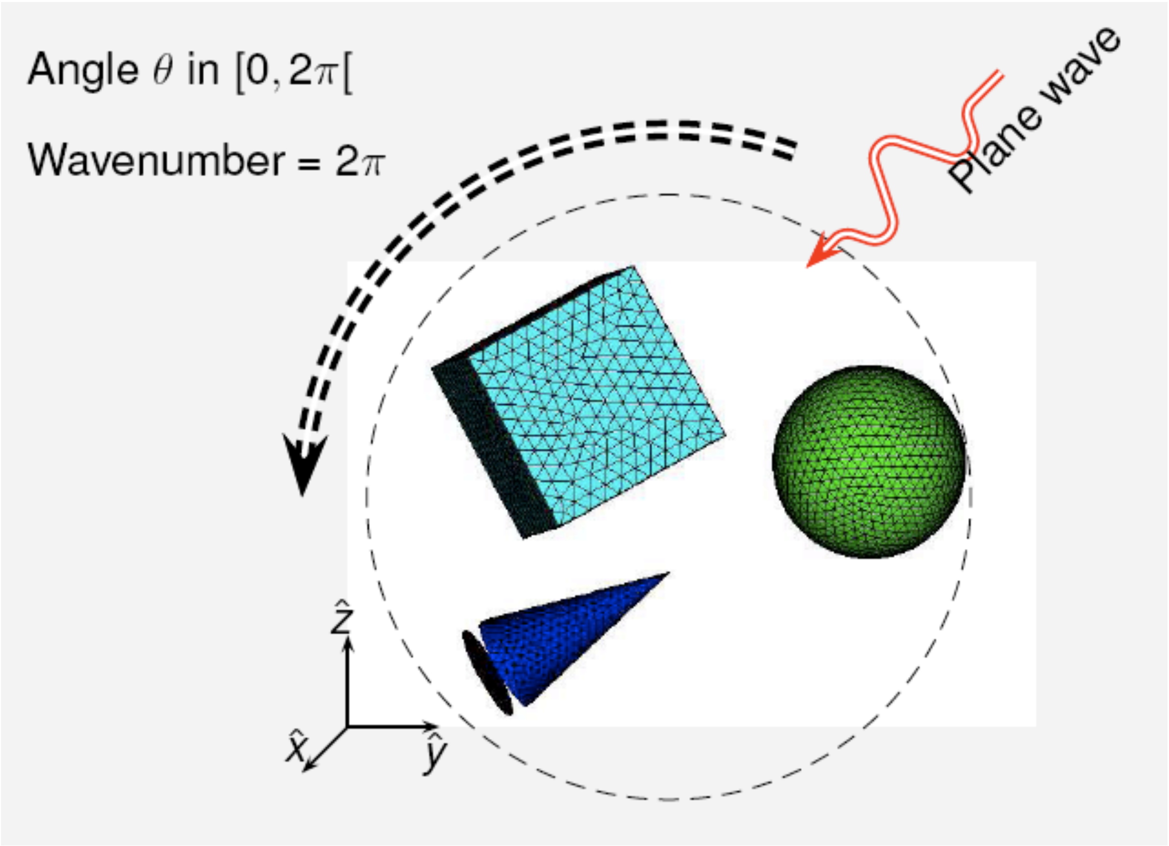


This samples the solution manifold

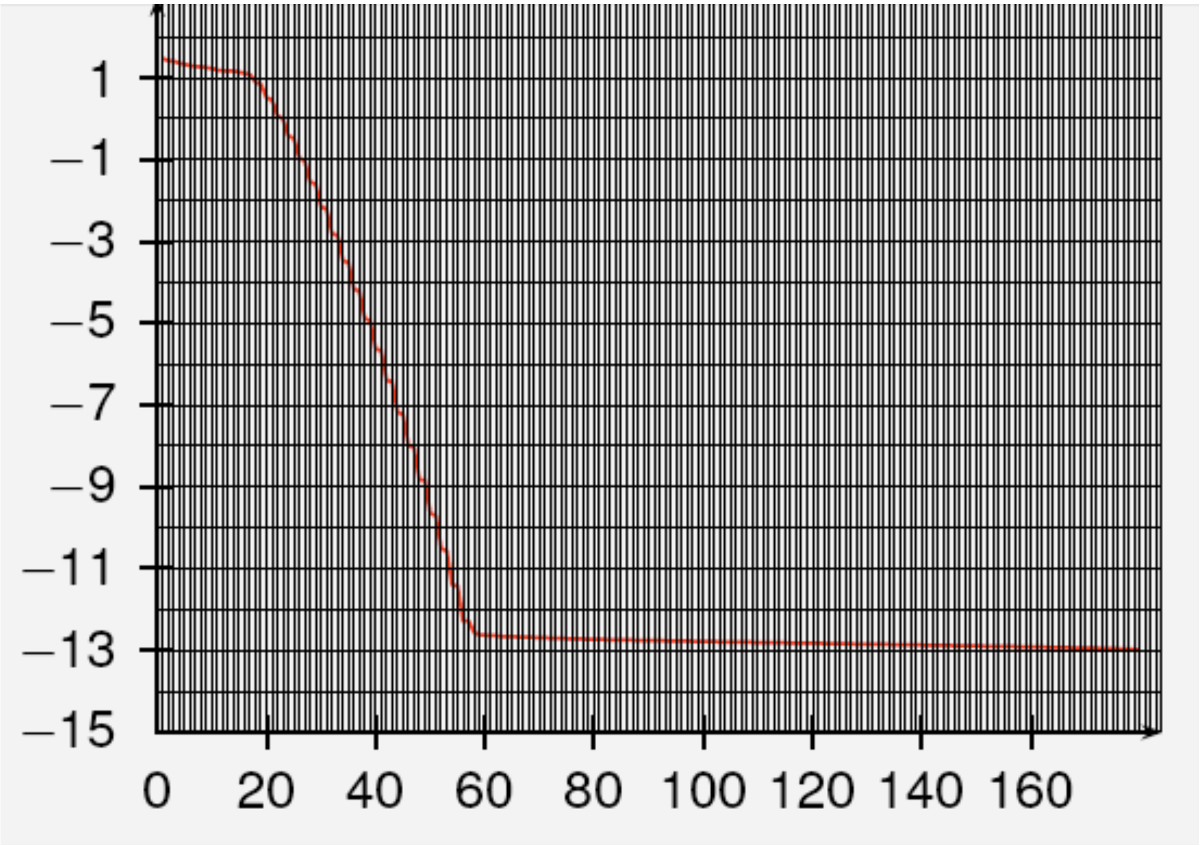
Solution manifold

3D EM scattering with the angle varying 0-360 deg. RCS is computed every 2 deg.

Computing the SVD of the 180 solutions shows that less than 60 samples would suffice -- and likely much less for applications



Computation by CERFACS



Basic setting

We consider physical systems of the form

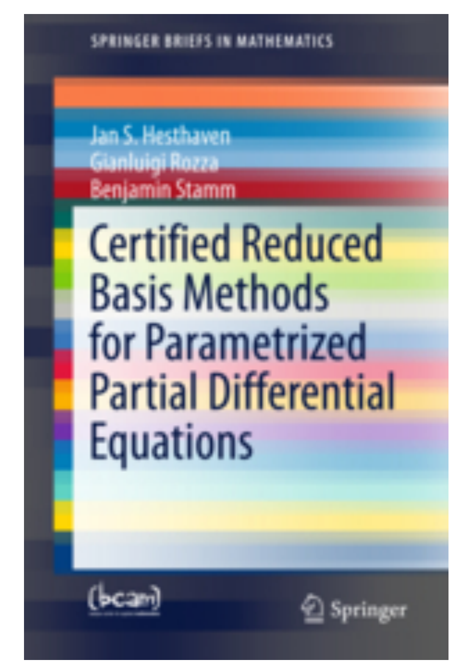
$$\mathcal{L}(\mathbf{x},\mu)u(\mathbf{x},\mu) = f(\mathbf{x},\mu) \qquad \mathbf{x} \in \Omega$$

$$u(\mathbf{x},\mu) = g(\mathbf{x},\mu) \qquad \mathbf{x} \in \partial\Omega$$

where the solutions are implicitly parameterized by

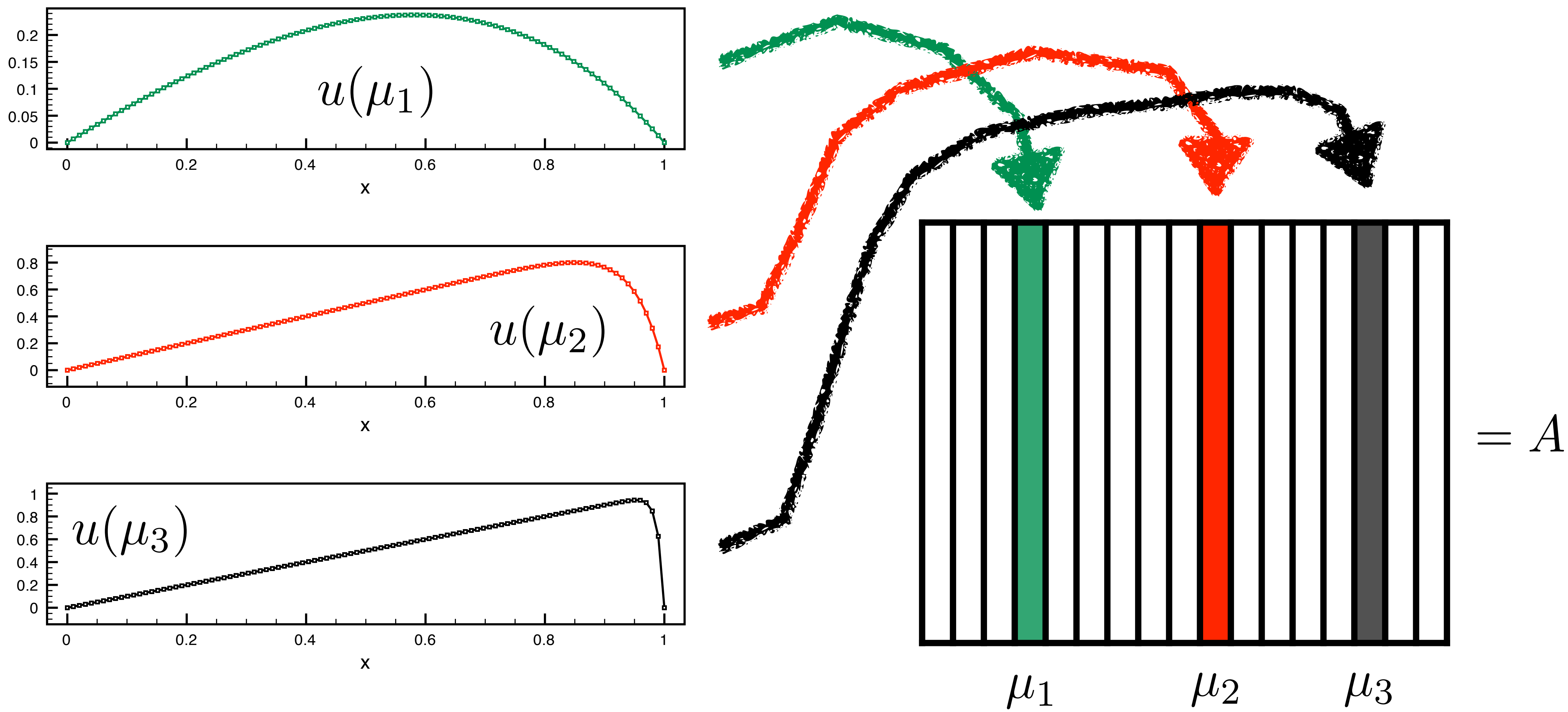
$$\mu \in \mathcal{D} \in \mathcal{R}^N$$

- How do we find the basis.
- How do we ensure accuracy under parameter variation ?
- What about speed ?



Free: https://infoscience.epfl.ch/record/213266?ln=en

Basis by POD approach



$$C = A^* M_\delta A$$

Find eigen-decomposition of C

Basis by POD approach

The reduced model is now obtained as

$$A_h u_\delta = f_h \qquad \Rightarrow$$

$$(V^T A_h V) V^T u_\delta = V^T f_h \qquad V^T V = I$$

or

$$A_{rb} u_{rb} = f_{rb}$$

and the output of interest is

$$s(u) \simeq s(u_\delta) \simeq s(\mathrm{V} u_{rb})$$

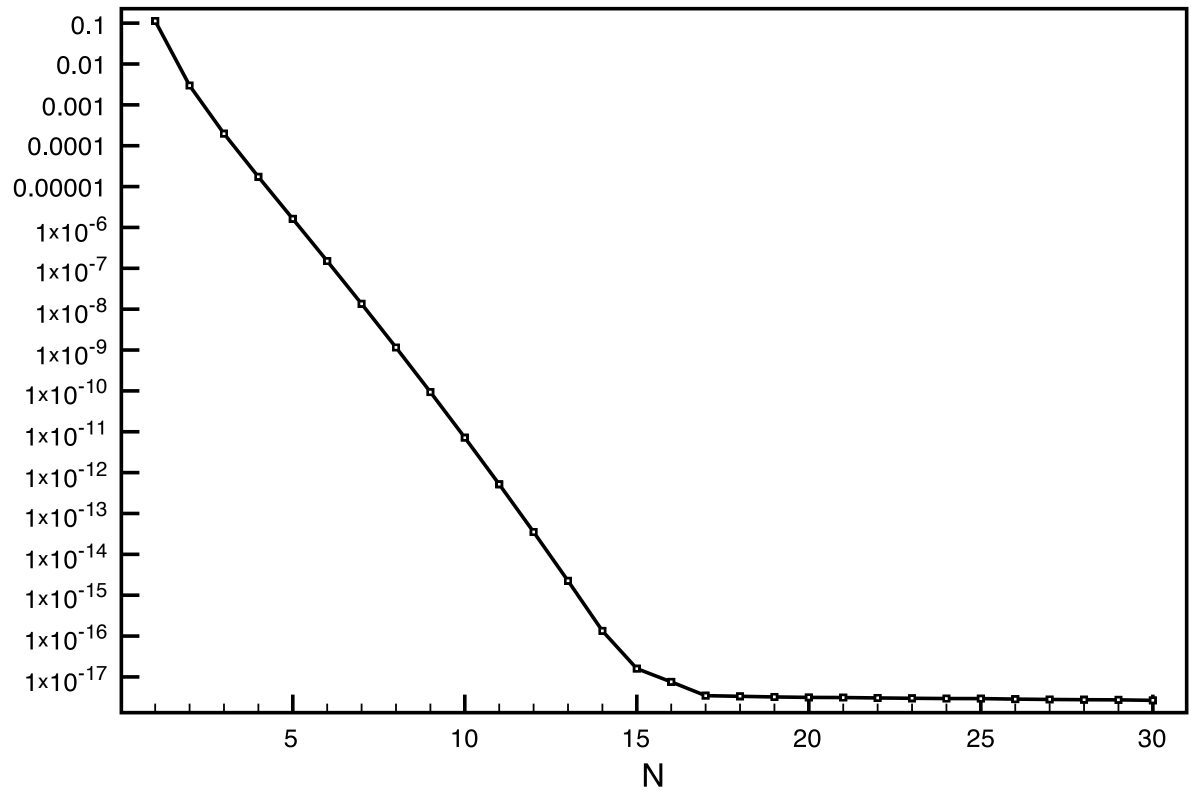
Since $N \ll \mathcal{N}$ we have the potential for speed

POD example - Ex 1

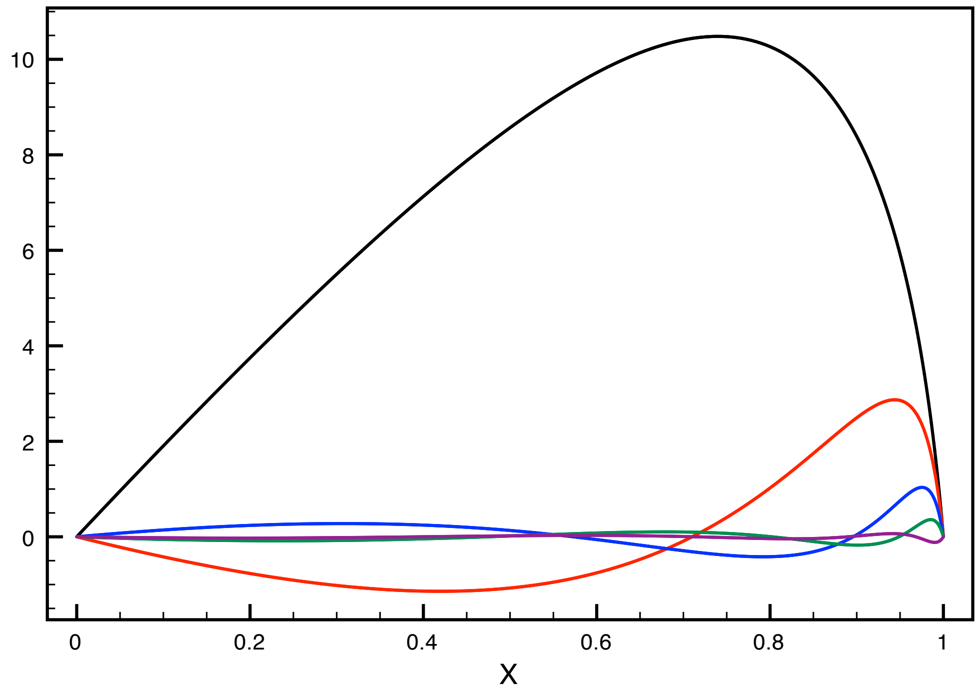
- Nodal values of exact solutions used instead of FE-approximations.
- $\mathbb{P}_h$: 491 equidistant points in $\mathbb{P} = [0.01, 0.5]$.

$$\varepsilon u'' + u' = 1, \qquad \text{in } (0,1),$$
$$u(0) = u(1) = 0.$$

Eigenvalues:

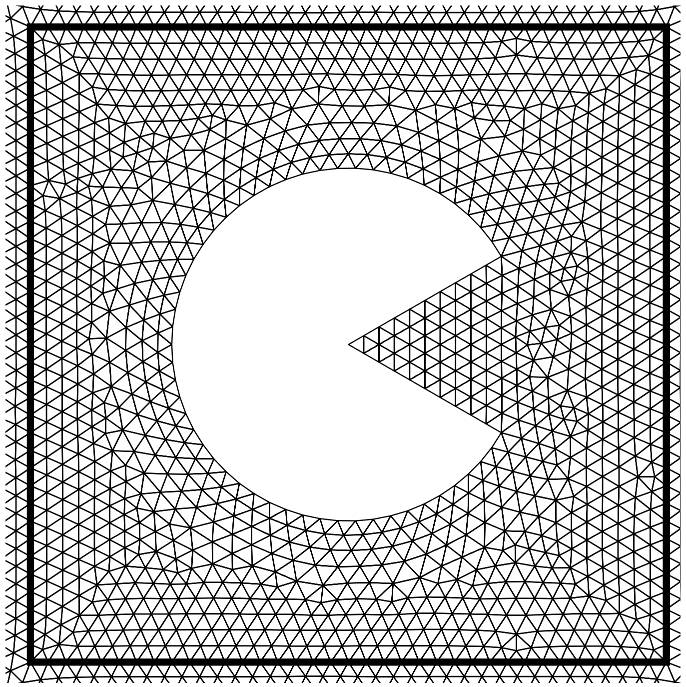


5 first basis functions:



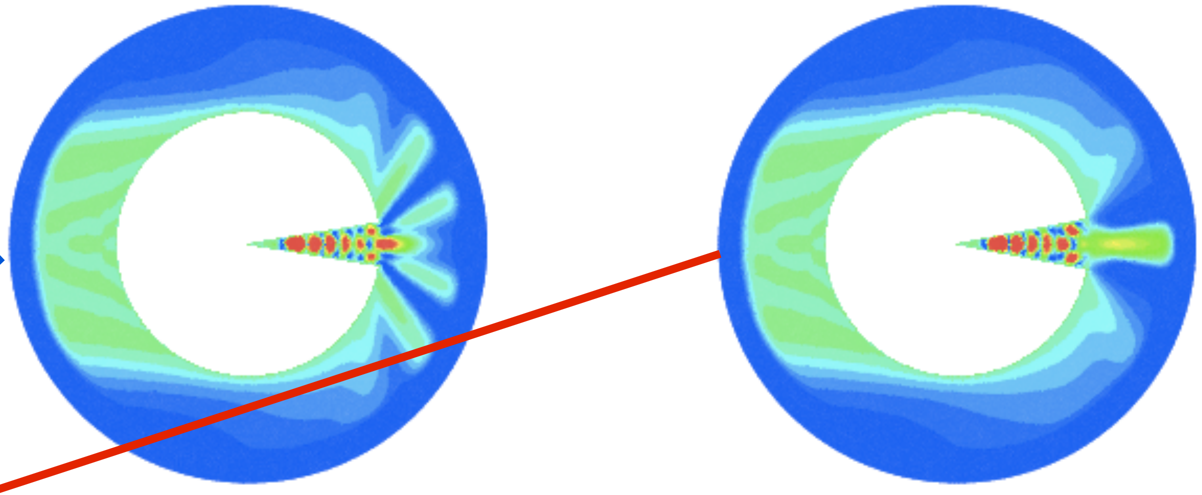
$\Rightarrow$ Precision of $\sim 10^{-6}$ with 5 basis functions.

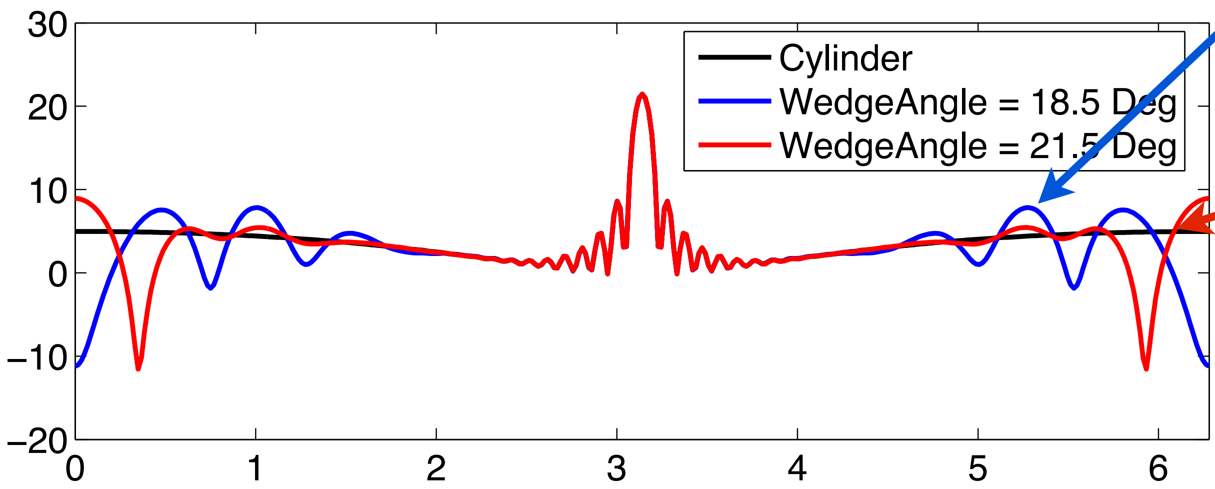
2D Pacman problem



Scattering by 2D PEC Pacman

Backscatter depends very sensitively on cutout angle and frequency.



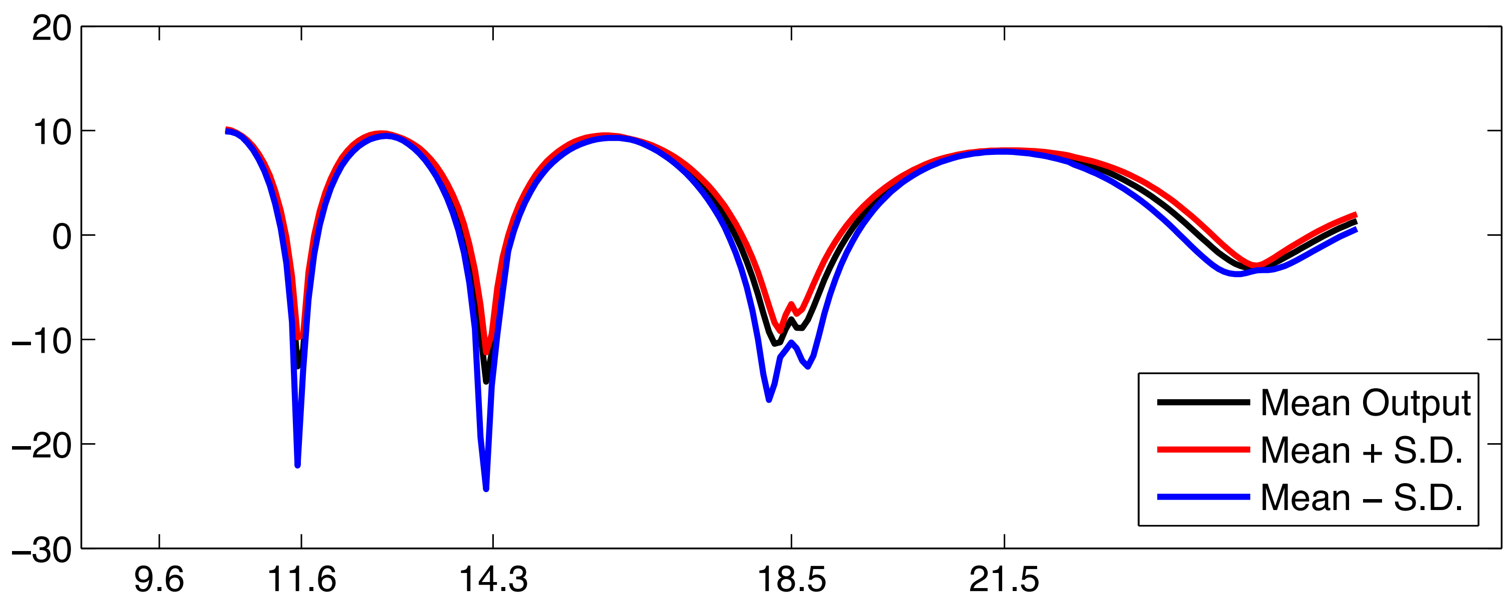


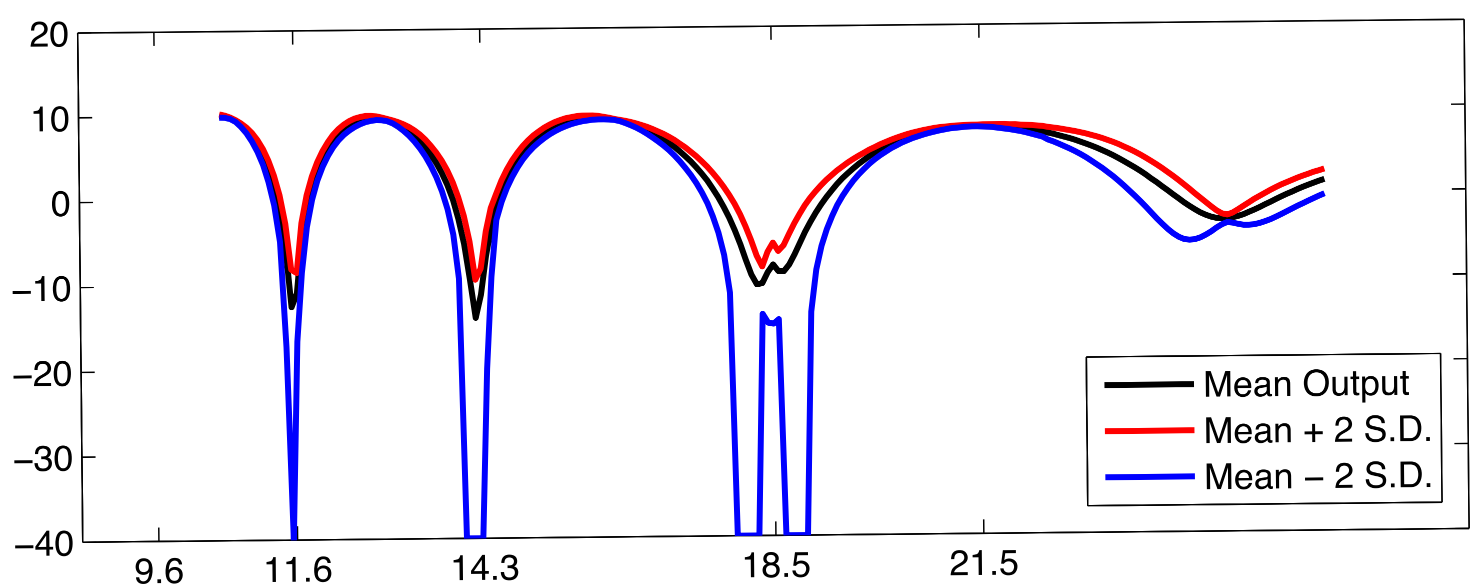
TM polarization

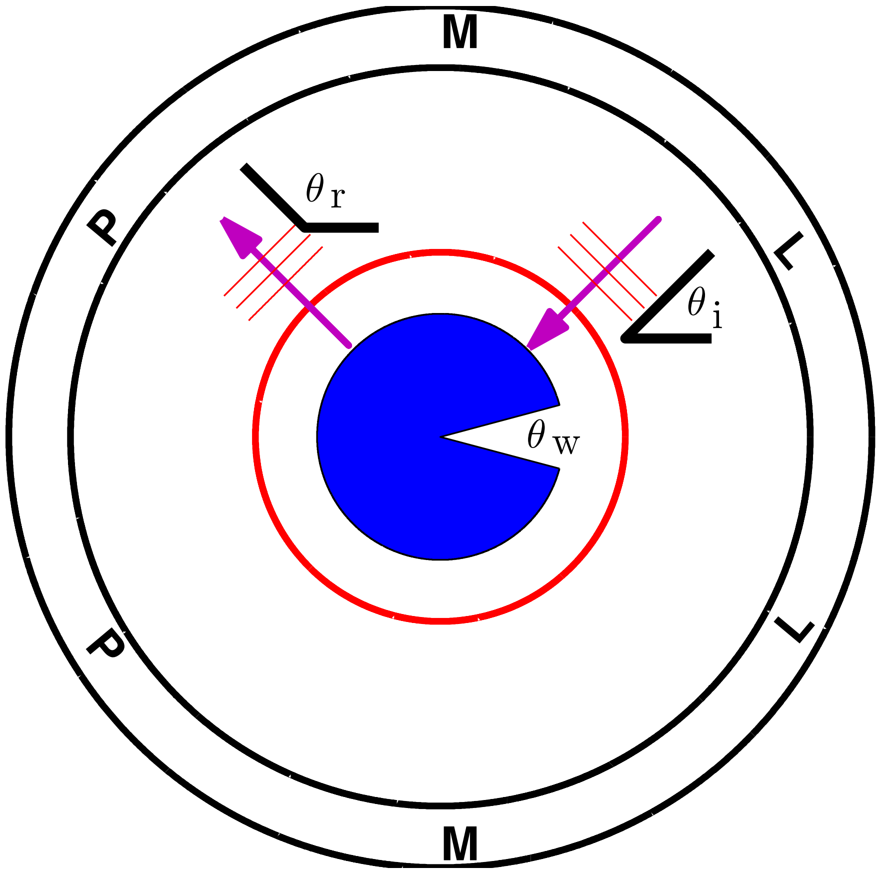
Difference in scattering is clear in fields

2D Pacman prototype for UQ

Fast evaluation over parameter space allows for rapid uncertainty quantification





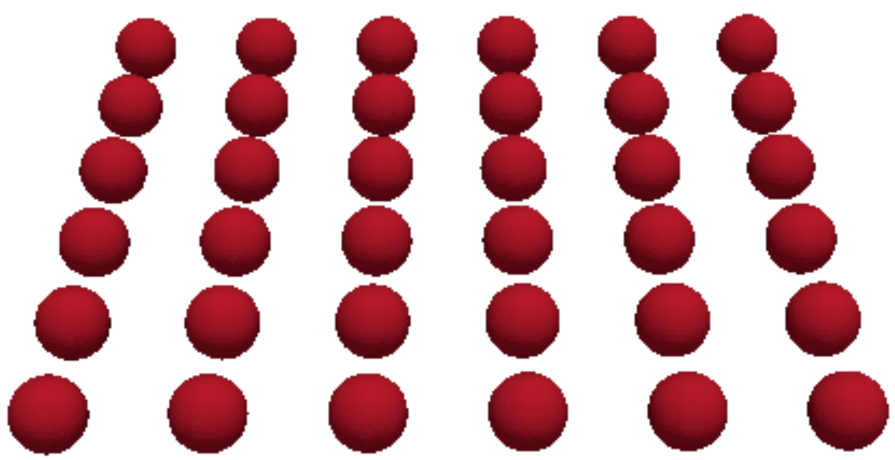


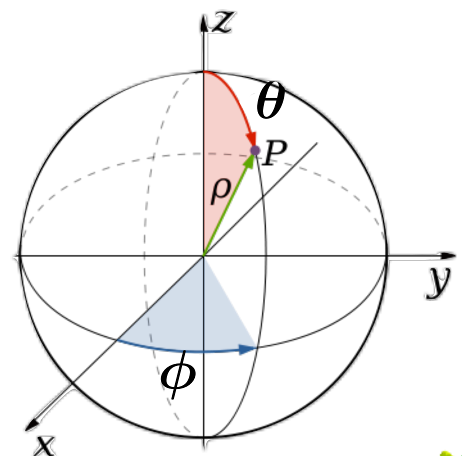
Uniformly distributed 5% randomness in gap angle

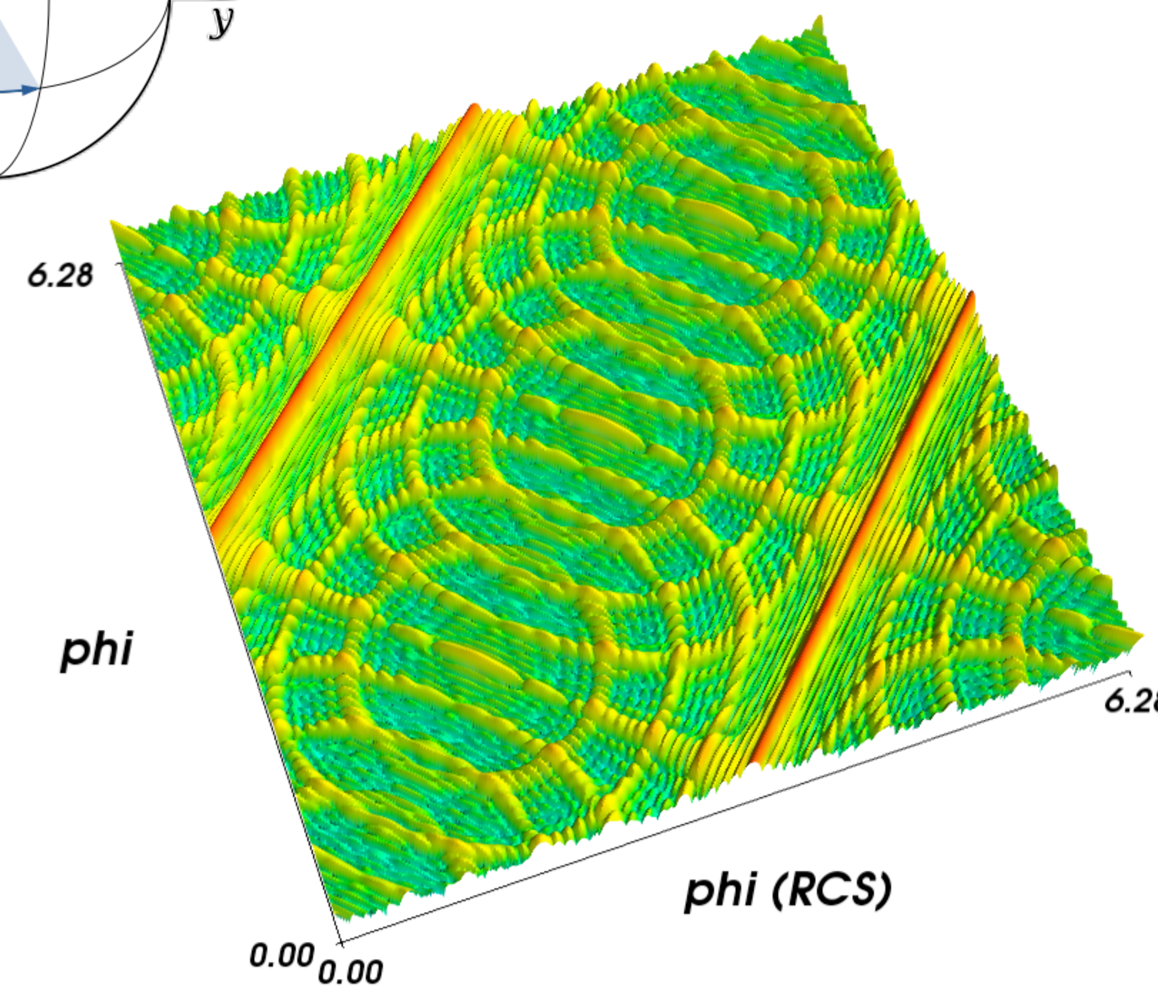
3D Multiple scattering problems

$$\phi \in [0, 2\pi]; k = 3, \theta = \pi/2$$

$$ka = 1; kd = 4$$







RB for single scatterer has 5 parameters (frequency(1), angle (2), polarization (2))

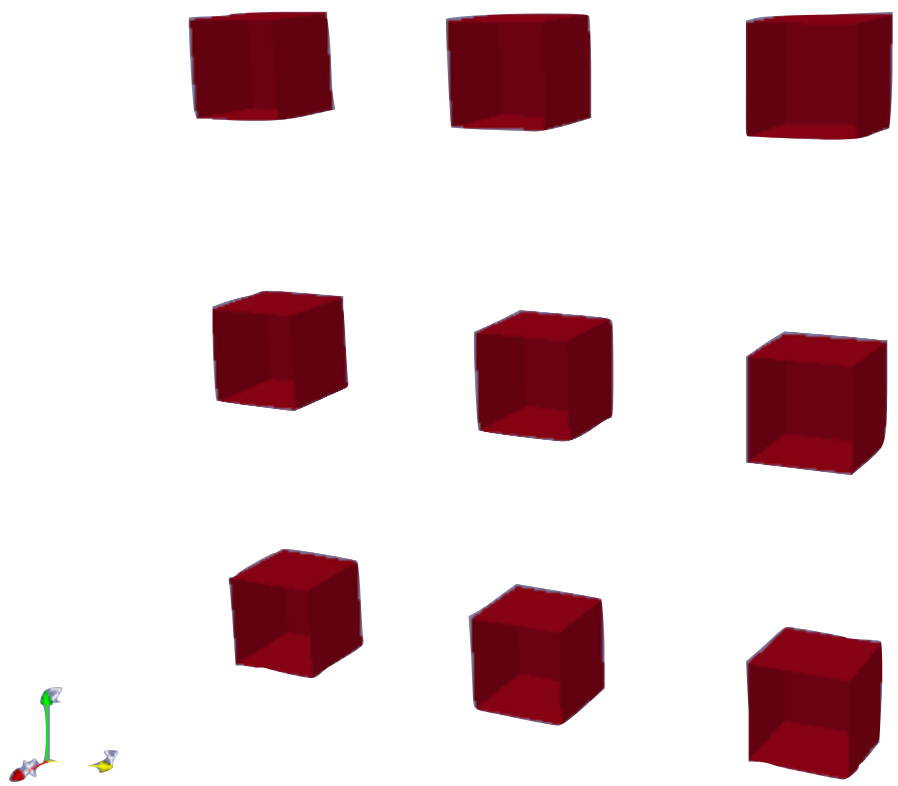
RB for interaction operator has 8 parameters (frequency(1), relative size(1), distance (2), rotation (2), polarization (2))

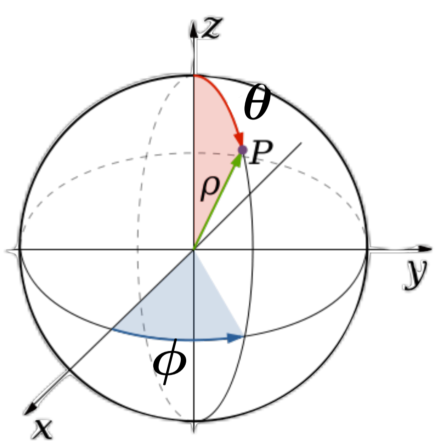
Full scattering result computed with iteration

Full RCS computed in less than 3 minutes for 36 spheres

Multiple scattering problem

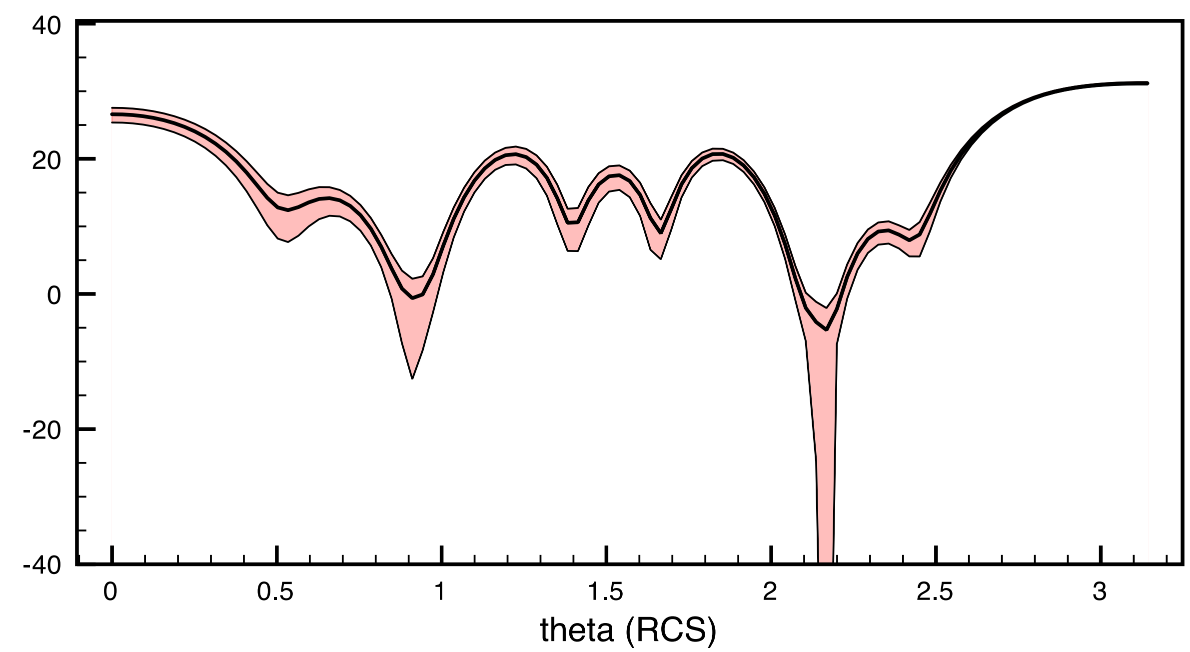
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE



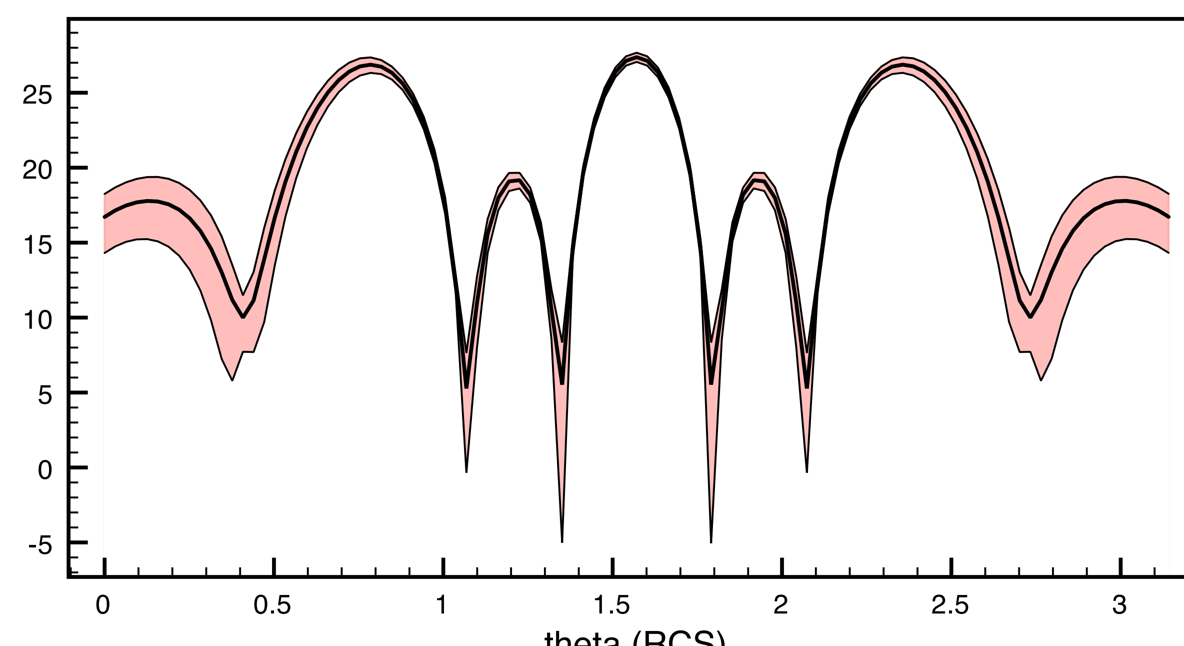


$$k = 3, \phi^i = 0, \theta^i = 0, 90$$

$$\phi^o = 0, \theta^o = 0 - 180$$



Vertical position of middle cavity uniformly distributed within [-1,1]

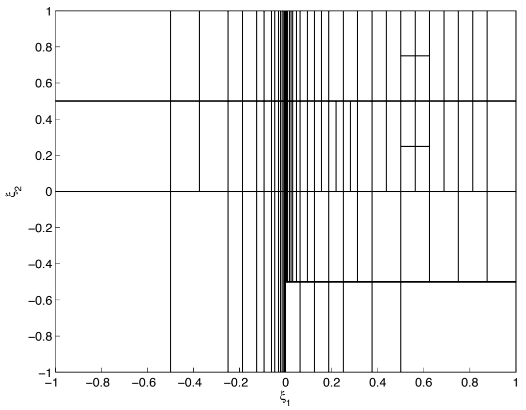


Other developments

There are naturally several other developments

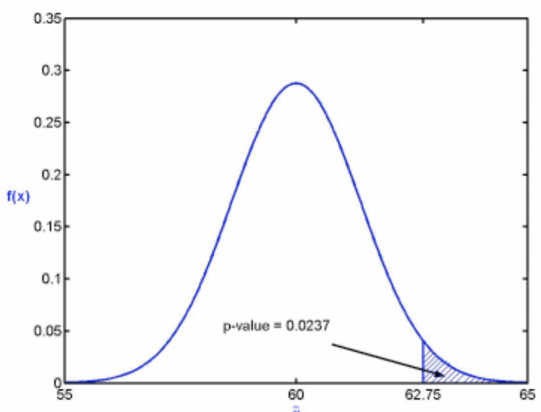
- Multi-element gPC

  X. Wan and G. E. Karniadakis, SISC 28 (2006), pp. 901-928.
  J. Foo, X. Wan and G. E. Karniadakis, JCP 227 (2008), pp. 9572-9595.



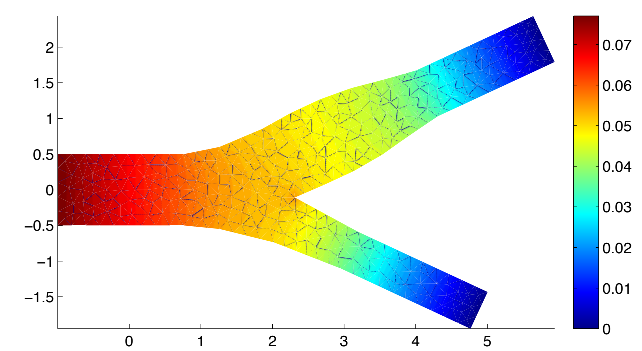
- Techniques for failure prediction

  Jing Li and D. Xiu, JCP., 2010



- UQ using reduced order modeling

  P. Chen, A. Quarteroni, G. Rozza, SAM Report 2015-03, ETHZ
  P. Chen and C. Schwab, SAM Report 2015-28, ETHZ



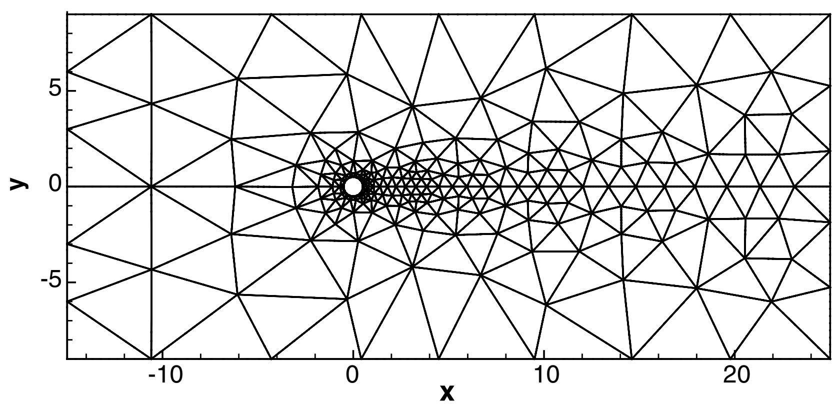
- High-dimensional interpolation and reconstruction

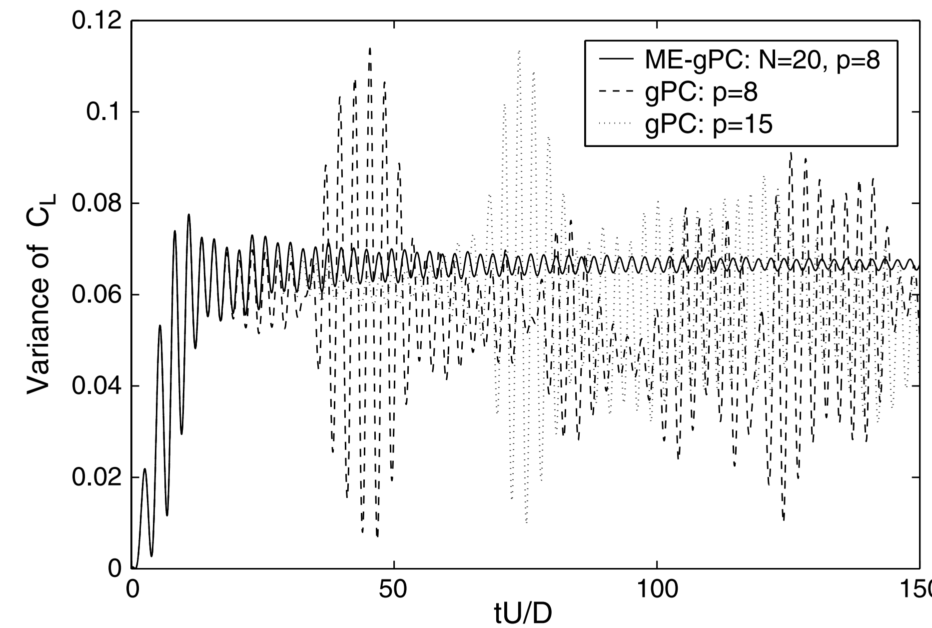
  Narayan, Xiu et al; Doostan et al

Open questions and challenges

Many challenges and interesting questions remain open

- Efficient ways to deal with long term integration



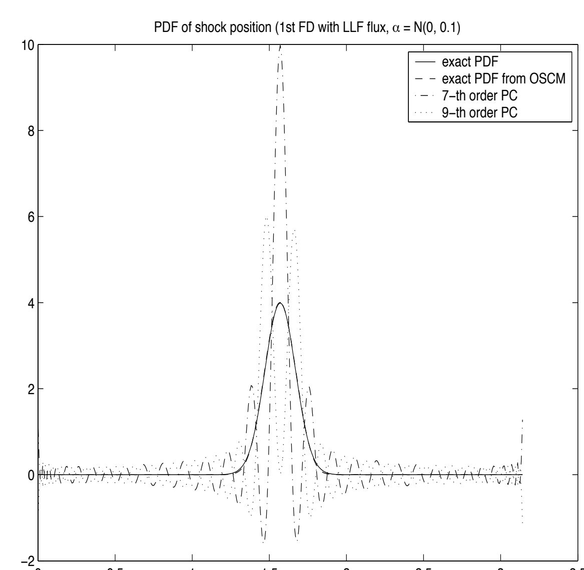


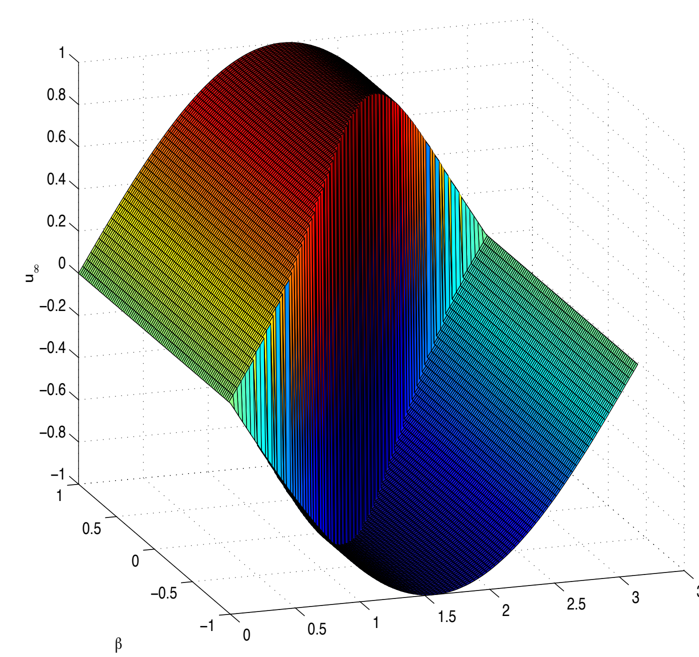
Wan et al, 2006

- Random variables with non-smooth behavior

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = \frac{\partial}{\partial x}\left(\frac{\sin^2 x}{2}\right) \qquad u(x,0) = \beta \sin x,$$

$$u_\infty(x,\beta) = \lim_{t\to+\infty} u(x,\beta,t) = \begin{cases} u^+ = \sin x, & 0 < x \le X_s \\ u^- = -\sin x, & X_s < x < \pi \end{cases}$$

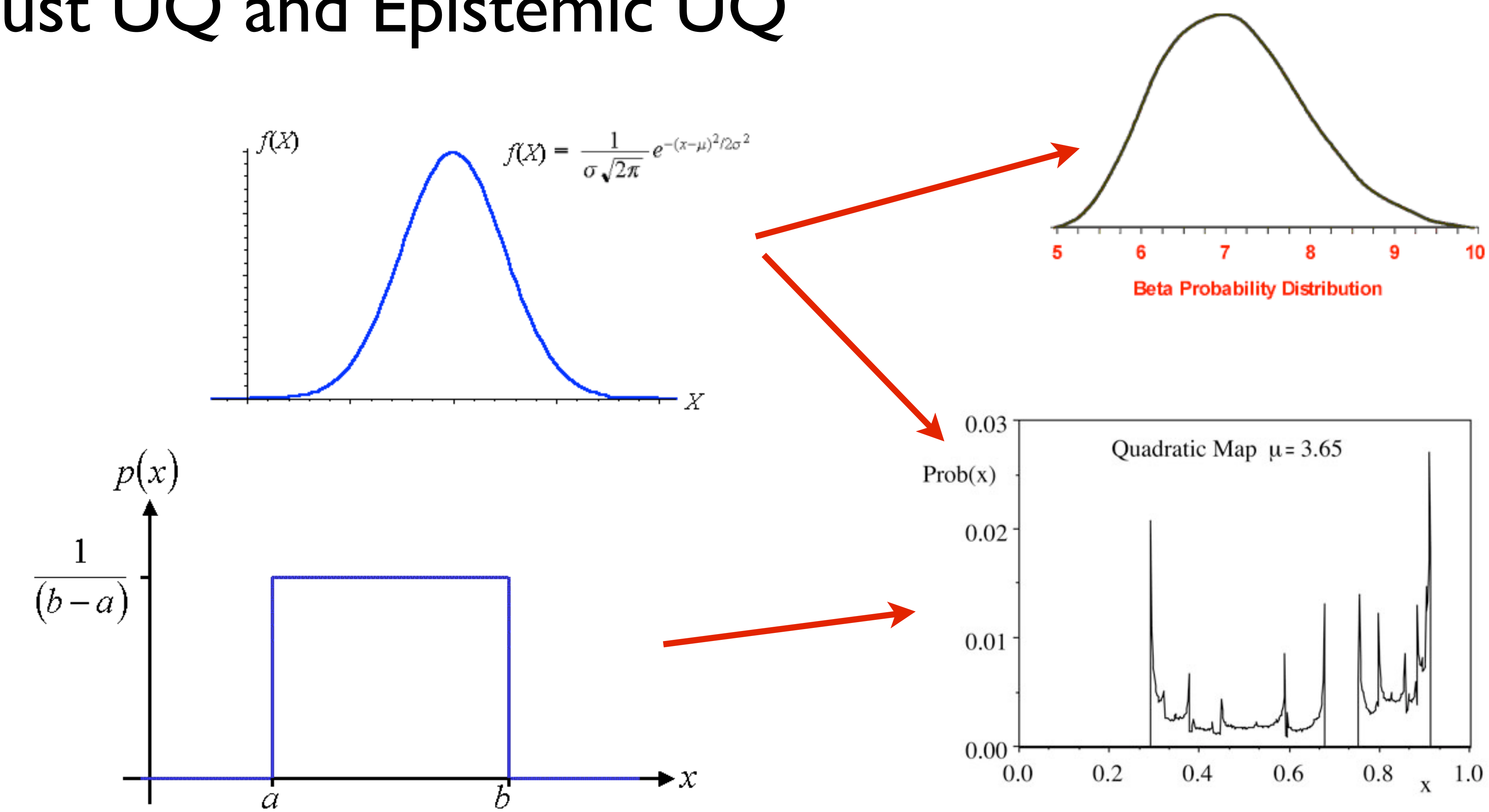




Bifurcations, transitions, hysteresis etc

Open questions and challenges

- Robust UQ and Epistemic UQ

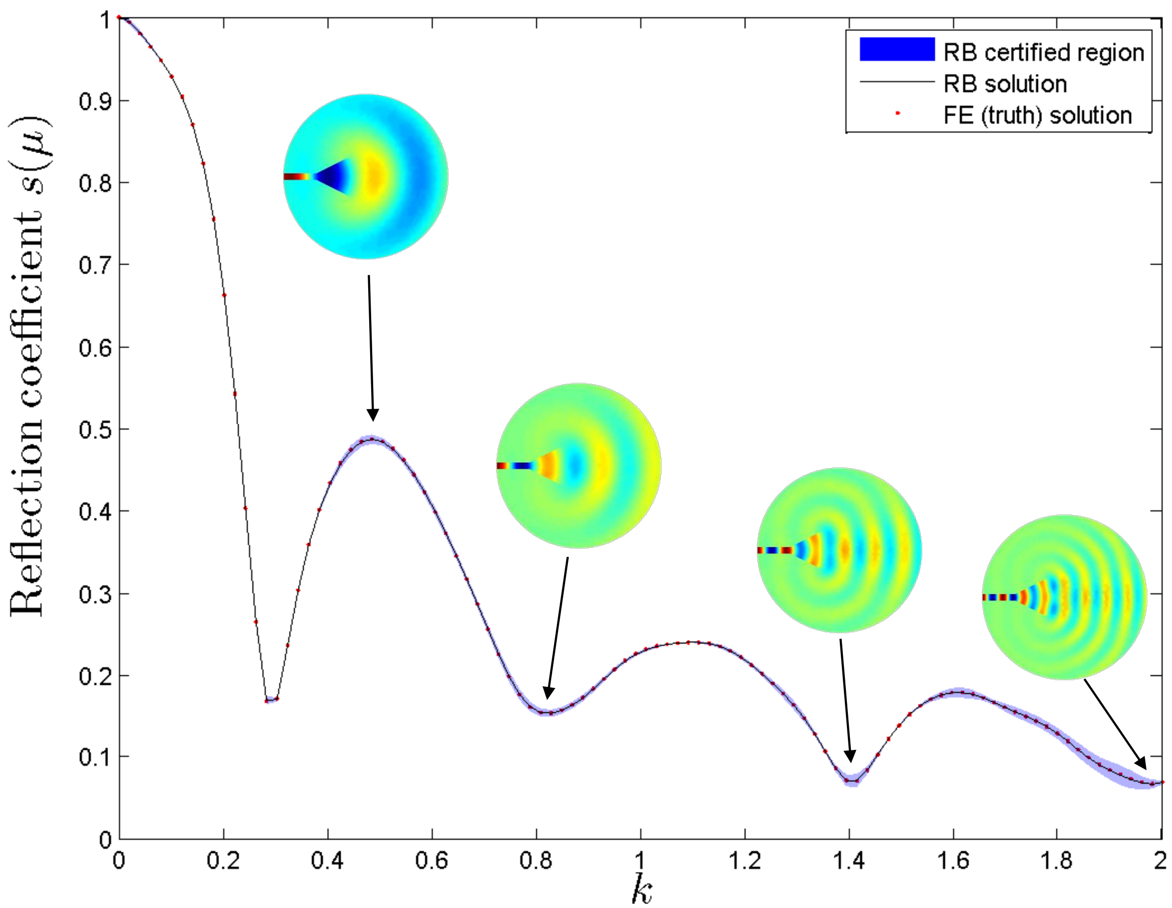


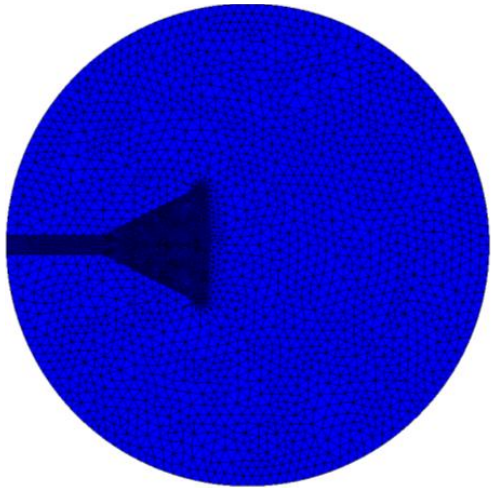
Predictions need to be robust to initial assumptions - how ?

- Error estimation, correct choice of N etc based on a priori and a posteriori error theory.

Open questions and challenges

- Design and optimization under uncertainty





Robust design
Optimization over parameter range

Willcox et al, 2010

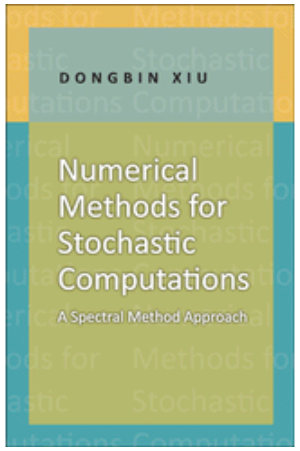
- UQ for multi-scale problems

  What is important at one scale may (not) be important at another

- UQ for very high-d problems

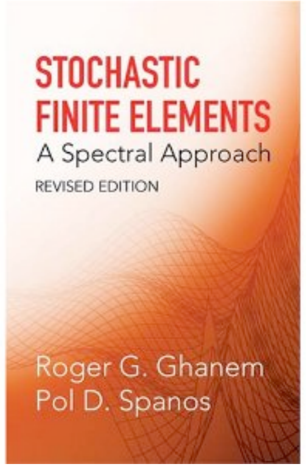
  How do we continue to push the limit ?

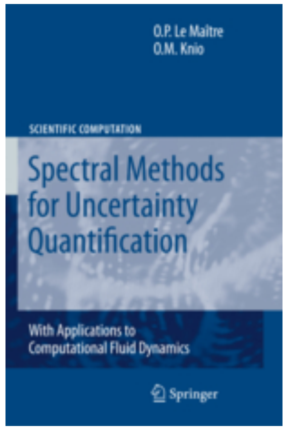
What to know more ?



D. Xiu, *Numerical Methods for Stochastic Computations: A Spectral Method Approach*, Princeton University Press, 2010.

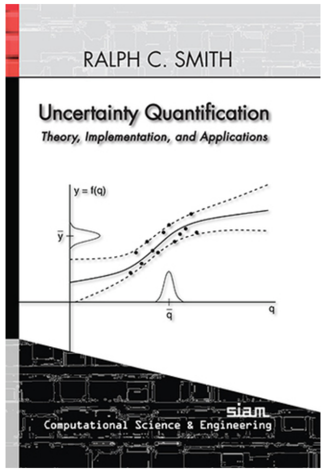
R.G. Ghamen and P.D. Spanos, *Stochastic Finite Elements: A spectral approach.* Dover Publishing, 2002.





O.P. Le Maitre and O.M. Knio, *Spectral Methods for Uncertainty Quantification*. Springer Verlag, 2010

R.C. Smith, *Uncertainty Quantification: Theory, Implementation and Applications.* SIAM CSE series, 2014.



SIAM Activity Group in UQ and SIAM Conference on UQ

UQ Community webpage: http://wwwmaths.anu.edu.au/~jakeman/index.html

UQ enabled large scale software: DAKOTA (Sandia NL): http://www.cs.sandia.gov/optimization/

References

As part of these lectures, I have plundered and pillaged

Books:

D. Xiu, *Numerical Methods for Stochastic Computations: A Spectral Method Approach*, Princeton University Press, 2010.

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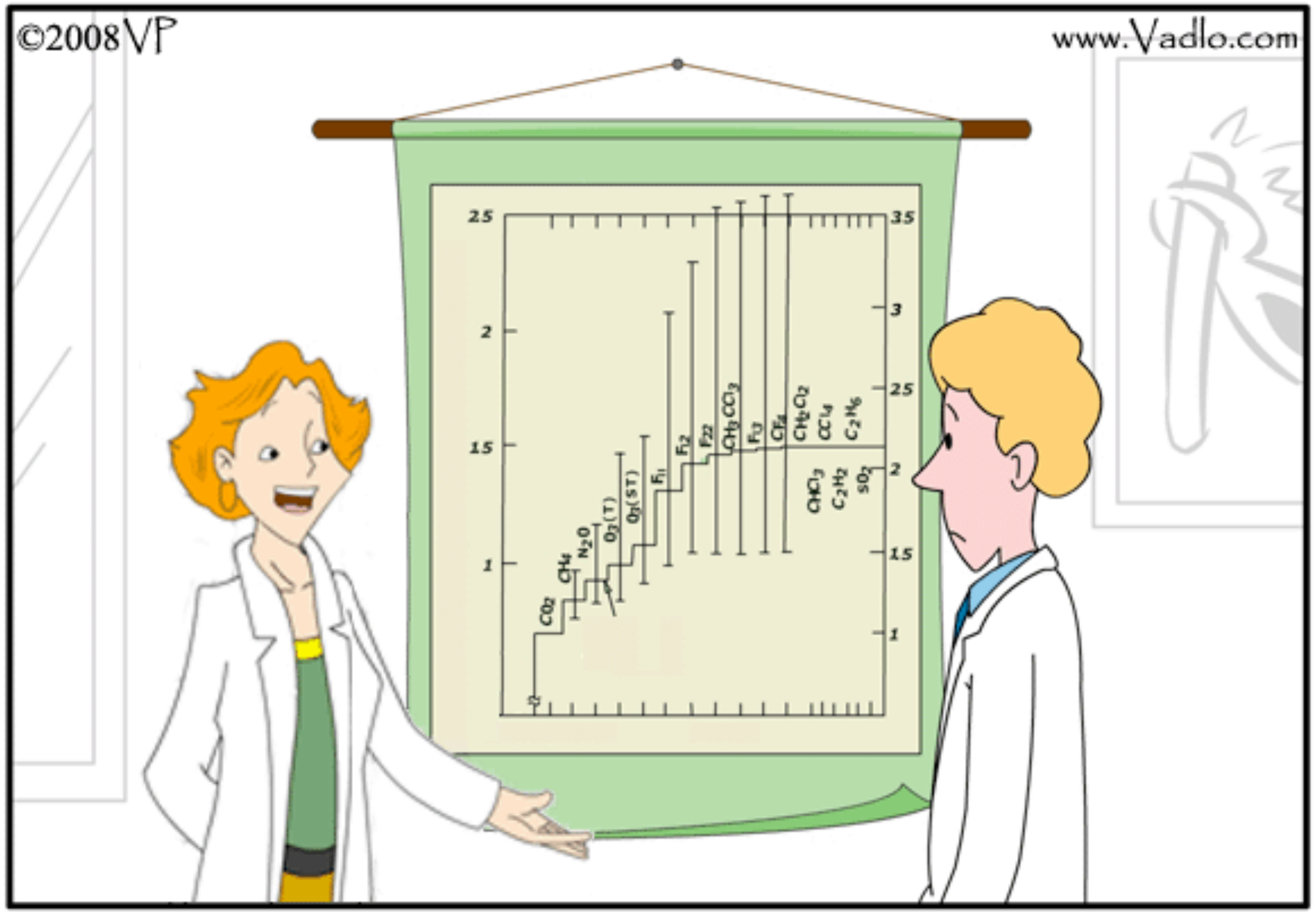

Did you really have to show the error bars?

Yes you do !

Questions or interest ?

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