Uncertainty Quantification in Simulations of Reactive Flows

Part 1: Introductory concepts

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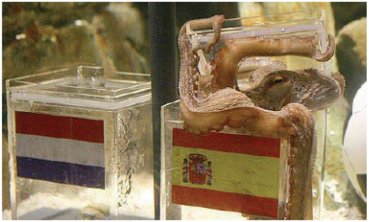
Outline

1. Why Uncertainty Quantification?
2. Definitions
3. Computations Under Uncertainty
4. Probabilistic Uncertainty Propagation
5. Examples
6. Extra material . . .

Part I

Why Uncertainty Quantification?

...don't believe in the psychic octopus approach to computer predictions...



Why Uncertainty Quantification?

...from WikiPedia

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An example would be to predict the acceleration of a human body in a head-on crash with another car: even if we exactly knew the speed, small differences in the manufacturing of individual cars, how tightly every bolt has been tightened, etc, will lead to different results that can only be predicted in a statistical sense. [...]

Why Uncertainty Quantification?

Decision Making

- UQ is critical in identifying the confidence in an outcome
- Provides basis for **certification** in high-consequence decisions

Why Uncertainty Quantification?

Validation

- UQ is a fundamental component of model validation
- Required to identify the effect limited knowledge in inputs of the simulations

Experiments

Simulations

Why Uncertainty Quantification?

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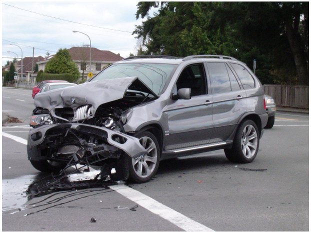
Controlled tests



Real World

Why Uncertainty Quantification?

A simplistic view

- In spite of the wide spread use of simulations it remains difficult to provide objective confidence levels
- One of the objective of UQ is to add error bars

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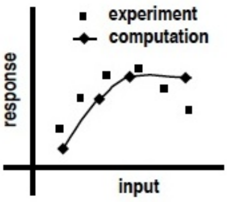

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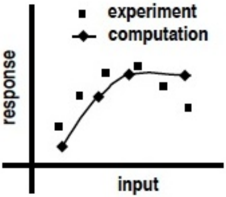

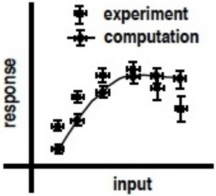

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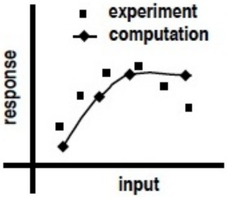
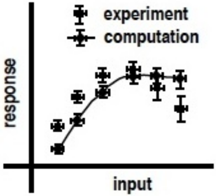
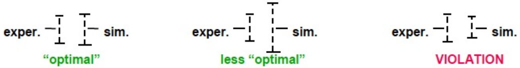




...but also the precise notion of validated model



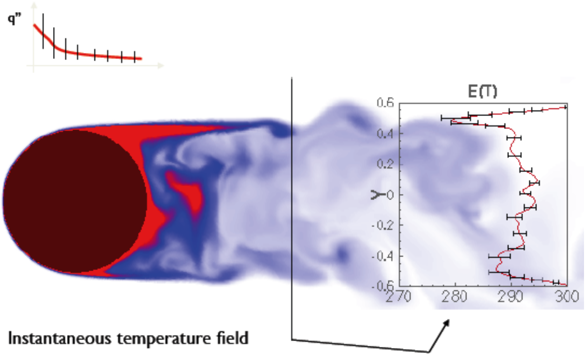
Images from Trucano et al. 2002, and Romero 2008

Why Uncertainty Quantification?

Error Bars

The objective is to replace the subjective notion of confidence with a mathematical rigorous measure

Unsteady turbulent heat convection with uncertain wall heating



Costantine & Iaccarino, AIAA-2009-0975

Part II

Definitions

"As we know there are known knowns.
There are things we know we know.
We also know there are known unknowns.
That is to say, we know there are some things we do not know.
But there are also unknown unknowns,
The ones we don't know we don't know."

D. Rumsfeld, Feb. 12, 2002, Department of Defense news briefing

Verification and Validation

Definitions

The American Institute for Aeronautics and Astronautics (AIAA) has developed the “Guide for the Verification and Validation (V&V) of Computational Fluid Dynamics Simulations” (1998)

What is V&V?

- Verification: The process of determining that a model implementation accurately represents the developer’s conceptual description of the model.
- Validation: The process of determining the degree to which a model is an accurate representation of the real world for the intended uses of the model

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  "are we solving the equations *correctly*?" – it is an exercise in *mathematics*
- Validation: ~~The process of determining the degree to which a model is an accurate representation of the real world for the intended uses of the model~~
  "are we solving the *correct* equations?" – it is an exercise in *physics*

Errors vs. Uncertainties

Definitions

The AIAA "Guide for the Verification and Validation (V&V) of CFD Simulations" (1998) defines

- errors as recognisable deficiencies of the models or the algorithms employed
- uncertainties as a potential deficiency that is due to lack of knowledge.

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Well...

- The definitions are not very *precise*
- Do not clearly distinguish between the *mathematics* and the *physics*.
- What is the relation with V&V?

Errors vs. Uncertainties

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  - round-off, limited convergence of iterative algorithms)
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Uncertainties

Aleatory: it is the physical variability present in the system or its environment.

- It is not strictly due to a lack of knowledge and cannot be reduced (also referred to as variability, stochastic uncertainty or **irreducible uncertainty**)

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- Examples are: material properties, operating conditions manufacturing tolerances, etc.

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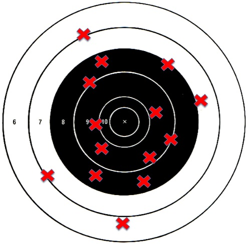
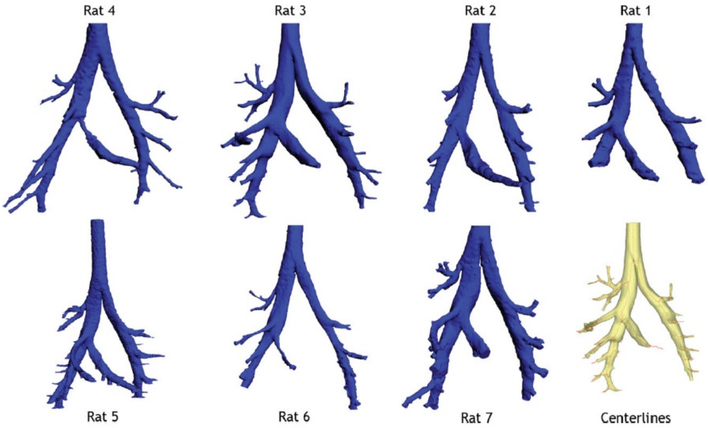
- Examples are: material properties, operating conditions manufacturing tolerances, etc.
- In mathematical modeling it is also studied as noise



Aleatory Uncertainty

Natural variance

Patient-to-patient differences



Courtesy of de Backer et al, 2009

Aleatory Uncertainty

Flight conditions

Difference between measured (balloon) and expected (Global Reference Atmospheric Model) temperature in the earth atmosphere

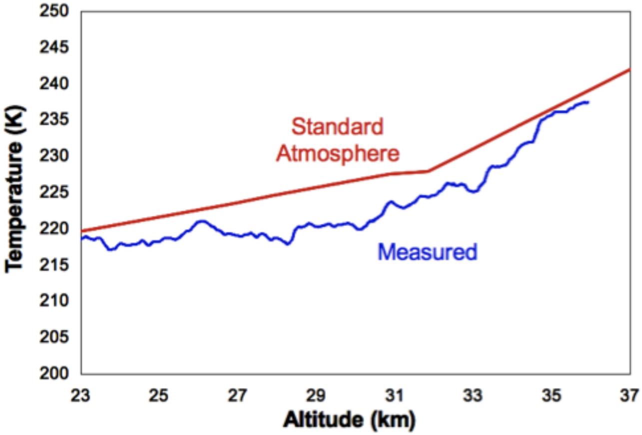


Image from Smart et al. 2003

Uncertainties

Epistemic: it is a potential deficiency that is due to a lack of knowledge

- It can arise from assumptions introduced in the derivation of the mathematical model (it is also called **reducible uncertainty** or incertitude)

- Examples are: turbulence model assumptions or surrogate chemical models

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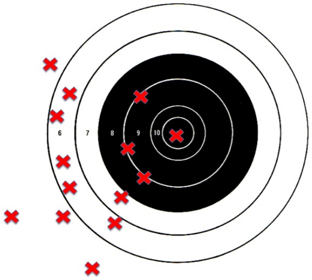
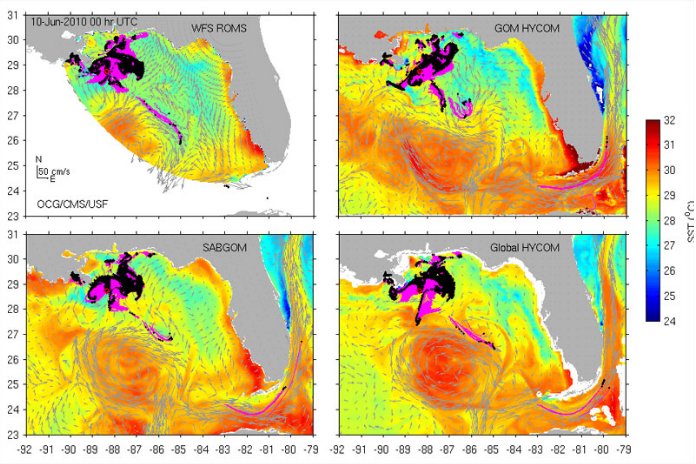
- It is NOT naturally defined in a probabilistic framework
- Can lead to strong bias of the predictions



Epistemic Uncertainty

Model uncertainty

Deepwater Horizon oil tracking forecast

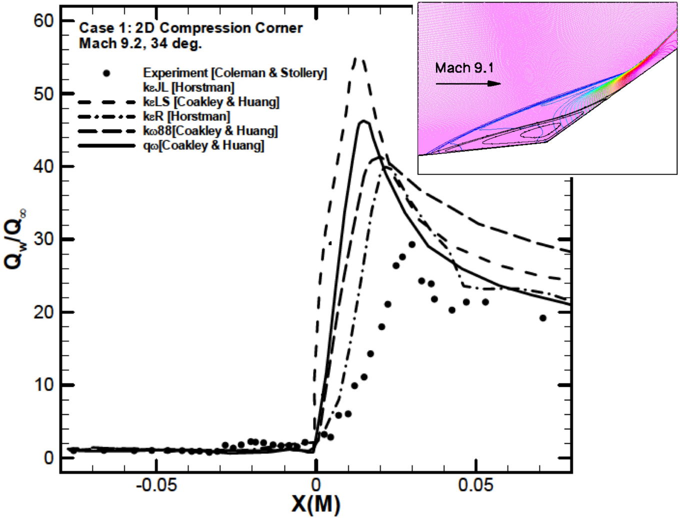


Source: University of Texas Institute of Geophysics

Epistemic Uncertainty

Model uncertainty

Predictions of heat flux over a compression ramp



Source: Roy et al, 2007

Summary

Not all uncertainties created equal..

- Uncertainties relate to the physics of the problem of interest! not to the errors in the mathematical description/solution...

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Not all uncertainties created equal..

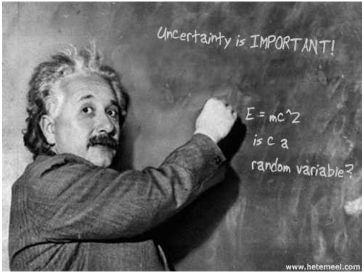
- Uncertainties relate to the physics of the problem of interest! not to the errors in the mathematical description/solution...
- Reducible vs. Irreducible Uncertainty
  - Epistemic uncertainty can be reduced by increasing our knowledge, e.g. performing more experimental investigations and/or developing new physical models.
  - Aleatory uncertainty cannot be reduced as it arises naturally from observations of the system. Additional experiments can only be used to better characterize the variability.

Part III

Computations Under Uncertainty
=
Predictive Simulations

"The significant problems we face cannot be solved
at the same level of thinking we were at when we created them."

A. Einstein



Uncertainty Quantification

Computational Framework

Consider a generic computational model ($\boldsymbol{y} \in \Re^d$ with d large)

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How do we handle the uncertainties?

1. Uncertainty definition: characterize uncertainties in the inputs
2. Uncertainty propagation: perform simulations accounting for the identified uncertainties
3. Certification: establish acceptance criteria for predictions

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  - Theoretical arguments
  - Expert opinions
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- Direct methods
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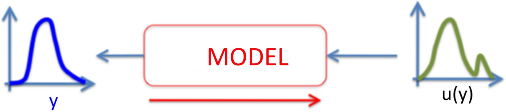
  - etc.
- Inverse methods (Inference, Calibration)
  - determination of the statistical input parameters that represent observed data using a computational model



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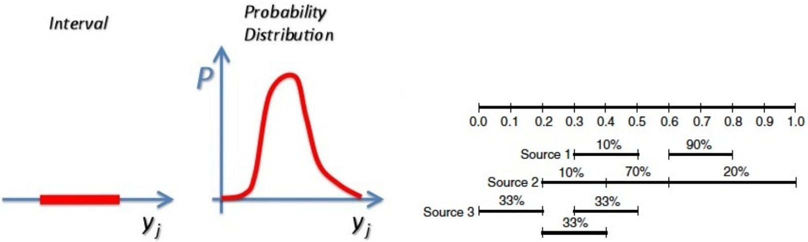
- Characterization of the associated level of knowledge



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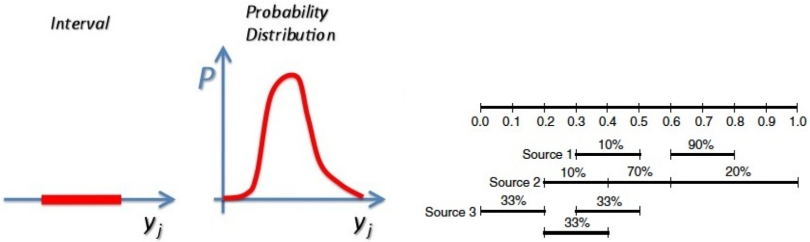

- The mathematical framework for propagating uncertainties is dependent on the data representation chosen

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Probabilistic Uncertainty Propagation

Perform simulations accounting for the uncertainty represented as randomness

- Define an abstract probability space $(\Omega, \mathcal{A}, \mathcal{P})$
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Remark: $\boldsymbol{y}$ can affect the boundary conditions, the geometry, the forcing terms or the operator in the computational model.

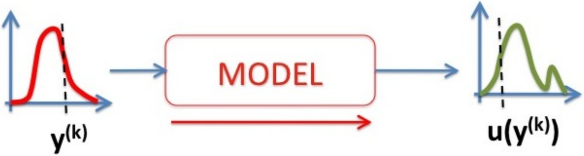
Uncertainty Propagation

Intrusive vs. Non-Intrusive Methodology

Uncertainty Propagation

Intrusive vs. Non-Intrusive Methodology

- Nonintrusive methods only require (multiple) solutions of the original (deterministic) model



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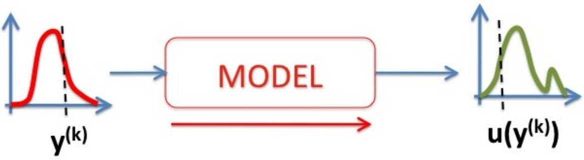
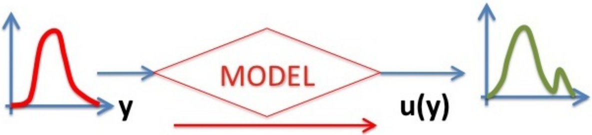


- Intrusive methods require the formulation and solution of a stochastic version of the original model



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  - + Simple extension of the "conventional" simulation paradigm
  - + Embarrassingly parallel: solutions are independent
  - + Conceptually very simple
- Intrusive methods require the formulation and solution of a stochastic version of the original model
  - + Exploit the mathematical structure of the problem
  - + Leverage theoretical & algorithmic advancements
  - + Are largely (or entirely) deterministic

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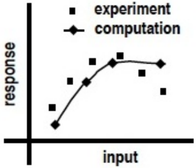
Certification & Validation



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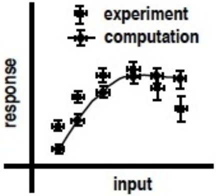
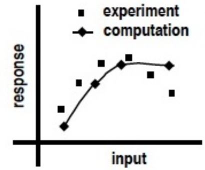


- Need to define a validation metric to compare *uncertain* quantities

Certification & Validation



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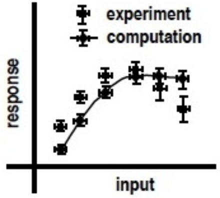

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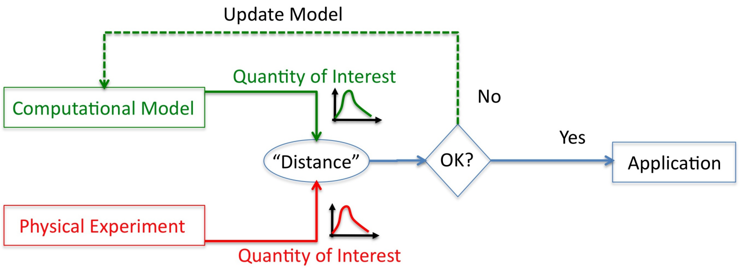
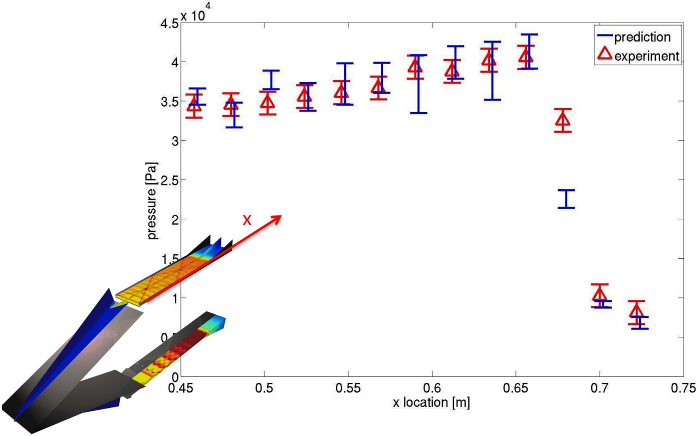


Certification

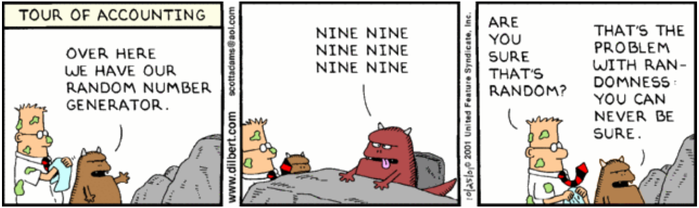
- Quantification of the confidence in the validation process
- Breakdown of the uncertainty sources



Hypersonic air-breathing vehicle - HyShot II

Part IV

Probabilistic Uncertainty Propagation



Uncertainty = Randomness

- Sampling Methods: Monte Carlo, Quasi Monte Carlo, Lati Hypercube, etc.
- Intrusive Methods: Polynomial Chaos, Adjoints, etc.
- Non-Intrusive Methods: Stochastic Collocation, Response Surface, etc.
- Optimization Methods

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Monte Carlo is your town!

- If you know how to sample... it's done

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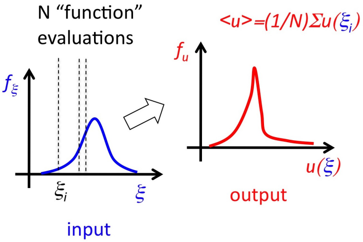

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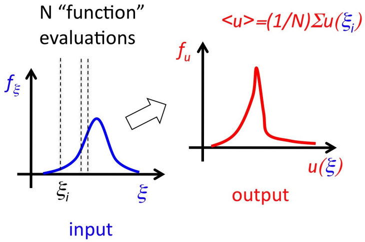

- ...not feasible with realistic function evaluations!

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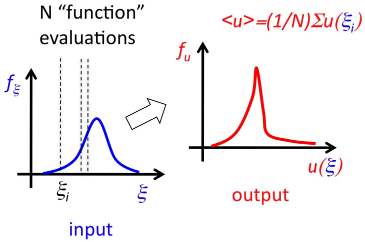

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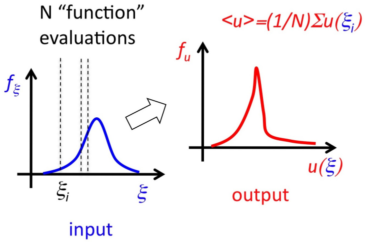

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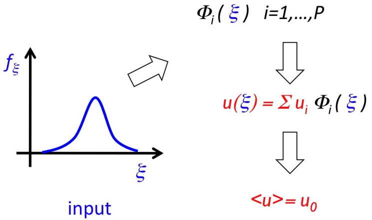

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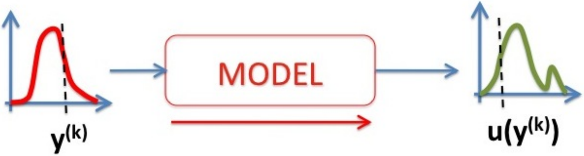
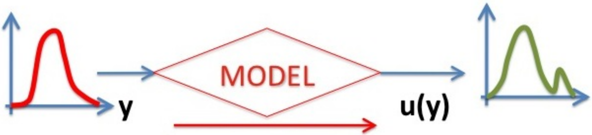


- Intrusive methods require the formulation and solution of a stochastic version of the original model



Polynomial Chaos

Stochastic Galerkin Approach

The solution is expressed as a spectral expansion of the *uncertain* variable(s): $\xi \in \Omega$ (assumed to be Gaussian)

$$u(x,t,\xi) = \sum_{i=0}^{\infty} \underbrace{u_i(x,t)}_{\textit{deterministic}} \underbrace{\psi_i(\xi)}_{\textit{stochastic}}$$

Polynomial Chaos

Stochastic Galerkin Approach

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$$u(x,t,\xi) = \sum_{i=0}^{\infty} \underbrace{u_i(x,t)}_{\text{deterministic}} \underbrace{\psi_i(\xi)}_{\text{stochastic}}$$

The $\psi_i(\xi)$ are Hermite polynomials and form a complete set of orthogonal basis functions

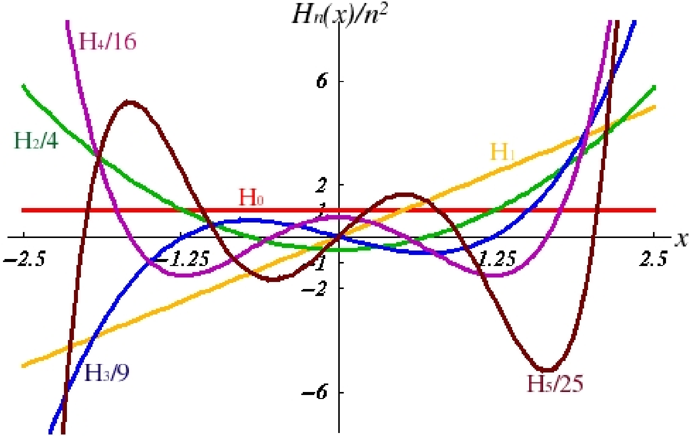
$\psi_0 = 1$; $\psi_1 = \xi$; $\psi_2 = \xi^2 - 1$; $\psi_3 = \xi^3 - 3\xi$; etc.

$\langle \psi_n \psi_m \rangle = \int_\Omega \psi_n(\xi)\psi_m(\xi) w(\xi) d\xi = h_n \delta_{n,m}$

where $w(\xi)$ is the pdf of ξ and h_n are non-zero constants

Polynomial Chaos

Hermite Polynomials



Polynomial Chaos

Hermite Polynomials

Orthogonal Polynomials

$$\langle \psi_n \psi_m \rangle = \int_\Omega \psi_n(\xi)\psi_m(\xi) w(\xi) d\xi = h_n \delta_{n,m}$$

$$E[\psi_0] = \int_\Omega \psi_0(\xi) w(\xi) d\xi = 1$$

$$E[\psi_k] = \int_\Omega \psi_k(\xi) w(\xi) d\xi = 0, k > 0$$

where $w(\xi)$ is the pdf of ξ and h_n are non-zero constants

Polynomial Chaos

Stochastic Galerkin Approach

If we can compute $u(x,t,\xi) = \sum_{i=0}^{\infty} u_i(x,t)\psi_i(\xi)$ we can evaluate directly the moments

Polynomial Chaos

Stochastic Galerkin Approach

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Expectation of u

$$E[u] = \int_\Omega u w(\xi) d\xi = \int_\Omega \left(\sum_{i=0}^{\infty} u_i \psi_i \right) w(\xi) d\xi =$$

$$u_0 \int_\Omega \psi_0(\xi) w(\xi) d\xi + \sum_{i=1}^{\infty} u_i \int_\Omega \psi_i(\xi) w(\xi) d\xi = u_0 = E[u]$$

Polynomial Chaos

Stochastic Galerkin Approach

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$$E[u] = \int_{\Omega} uw(\xi)d\xi = \int_{\Omega}\left(\sum_{i=0}^{\infty} u_i\psi_i\right) w(\xi)d\xi =$$

$$u_0 \int_{\Omega} \psi_0(\xi)w(\xi)d\xi + \sum_{i=1}^{\infty} u_i \int_{\Omega} \psi_i(\xi)w(\xi)d\xi = u_0 = E[u]$$

Variance of u

$$Var[u] = E[u^2] - (E[u])^2 = \sum_{i=0}^{\infty} u_i^2 \int_{\Omega} \psi_i^2 w(\xi)d\xi - u_0^2 = \sum_{i=1}^{\infty} u_i^2 \langle \psi_i^2 \rangle.$$

Polynomial Chaos

Stochastic Galerkin Approach

How do we compute $u(x,t,\xi) = \sum_{i=0}^{\infty} u_i(x,t)\psi_i(\xi)$?

Polynomial Chaos

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How do we compute $u(x, t, \xi) = \sum_{i=0}^{\infty} u_i(x, t)\psi_i(\xi)$?

More precisely how do we compute $u_i(x, t)$ for $i \to \infty$?

Polynomial Chaos

Stochastic Galerkin Approach

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More precisely how do we compute $u_i(x, t)$ for $i \to \infty$?

- We truncate the series $u(x, t, \xi) \approx \sum_{i=0}^{P} u_i(x, t)\psi_i(\xi)$
- We substitute the expression $u(x, t, \xi) = \sum_{i=0}^{\infty} u_i(x, t)\psi_i(\xi)$ in the governing PDE and perform a Galerkin projection operation

Polynomial Chaos

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Polynomial Chaos

1D Linear Convection Equations

- Consider the 1D linear convection equations

$$u_t + cu_x = 0 \quad 0 \leq x \leq 1$$

- The exact solution is $u(x, t) = u_{initial}(x - ct)$

Polynomial Chaos

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where $\psi_i(\xi)$ are (1D) Hermite polynomials
($\psi_0 = 1$; $\psi_1 = \xi$; $\psi_2 = \xi^2 - 1$; $\psi_3 = \xi^3 - 3\xi$; etc.)

Polynomial Chaos

1D Linear Convection Equations - uncertainty in the initial condition

- Assume
$$u_{initial}(x, t = 0, \xi) = g(\xi)cos(x)$$
- The exact solution is
$$u(x, t, \xi) = g(\xi)cos(x - ct)$$

Polynomial Chaos

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- Assume

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- Plug in the truncated expansion in the original PDE:

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t}\psi_i(\xi) + c\left(\sum_{i=0}^{P} \frac{\partial u_i}{\partial x}\psi_i(\xi)\right) = 0$$

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- Multiply by $\psi_k(\xi)$

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t}\psi_i(\xi)\cdot\psi_k(\xi)+c\left(\sum_{i=0}^{P} \frac{\partial u_i}{\partial x}\psi_i(\xi)\right)\cdot\psi_k(\xi) = 0 \quad \text{for } k = 0, 1, ..., P$$

Polynomial Chaos

1D Linear Convection Equations - uncertainty in the initial condition

- Integrate over the probability space Ω – (Galerkin Projection) - for each $k = 0, 1, ..., P$

$$\int_\Omega \sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \psi_i(\xi) \cdot \psi_k(\xi) w(\xi) d\xi + \int_\Omega c \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \psi_i(\xi) \cdot \psi_k(\xi) w(\xi) d\xi = 0$$

Polynomial Chaos

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Pulling out of the integrand the *deterministic* components:

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \int_{\Omega} \psi_i(\xi) \psi_k(\xi) w(\xi) d\xi + c \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \int_{\Omega} \psi_i(\xi) \psi_k(\xi) w(\xi) d\xi = 0$$

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which in compact notation is:

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + c \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \langle \psi_i \psi_k \rangle = 0 \qquad \text{for } k = 0, 1, ..., P.$$

Polynomial Chaos

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Polynomial Chaos

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- The orthogonality property $\langle \psi_i \psi_k \rangle = \delta_{ik} h_k$ implies

$$\frac{\partial u_0}{\partial t} + c\frac{\partial u_0}{\partial x} = 0$$

$$\vdots$$

$$\frac{\partial u_P}{\partial t} + c\frac{\partial u_P}{\partial x} = 0$$

- We obtain a system of $P+1$ uncoupled & deterministic eqns.

Polynomial Chaos

1D Linear Convection Equations - uncertainty in the initial condition

- Initial conditions for the $u_0 \dots u_P$ equations are obtained by projection of the initial condition

$$\langle u_{initial}(x, t = 0, \xi), \psi_k \rangle = u_k(x, t = 0) =$$

$$= \langle g(\xi), \psi_k \rangle cos(x) \quad k = 0, \dots, P$$

Polynomial Chaos

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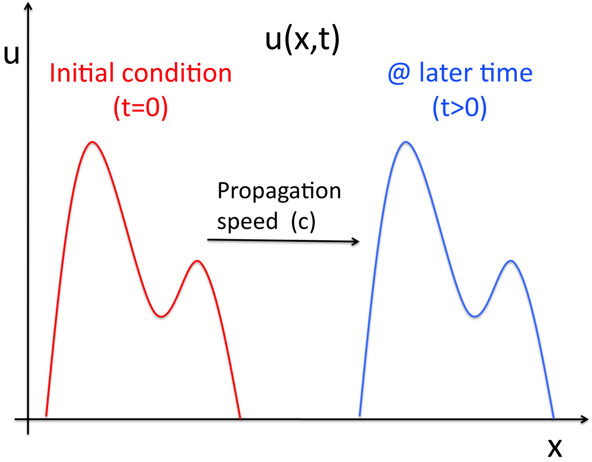
$$= \langle g(\xi), \psi_k \rangle cos(x) \quad k = 0, \ldots, P$$

- The procedure is *simply* an approximation of $g(\xi)$ on the polynomial basis $\psi(\xi)$

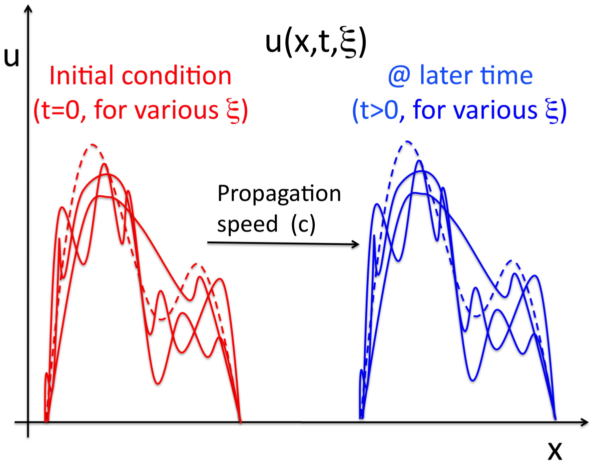
Linear Transport

Deterministic case



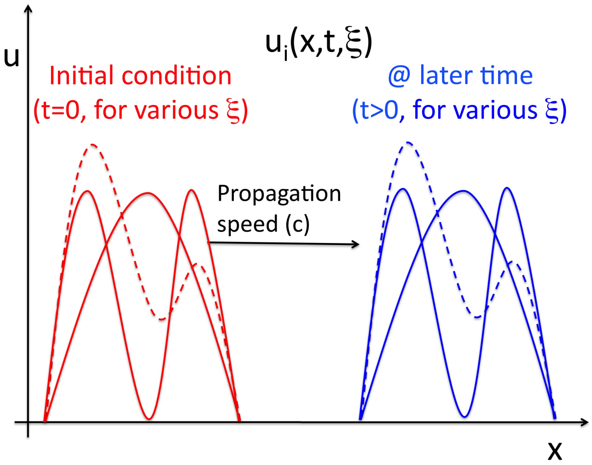
Linear Transport

Uncertainty in initial conditions



Linear Transport

Uncertainty in initial conditions



Polynomial Chaos

1D Linear Convection Equations - uncertainty in the transport velocity

- Assume
$$c = h(\xi)$$
- The exact solution is
$$u(x, t, \xi) = cos(x - h(\xi)t)$$

Polynomial Chaos

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- Plug in the truncated expansion is the original PDE:
$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t}\psi_i(\xi) + h(\xi)\left(\sum_{i=0}^{P} \frac{\partial u_i}{\partial x}\psi_i(\xi)\right) = 0$$

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- Multiply by $\psi_k(\xi)$ and integrate over the probability space Ω – (Galerkin Projection)

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t}\langle\psi_i\psi_k\rangle + \sum_{i=0}^{P} \frac{\partial u_i}{\partial x}\langle h(\xi)\psi_i\psi_k\rangle = 0 \qquad \text{for } k = 0, 1, ..., P.$$

Polynomial Chaos

1D Linear Convection Equations - uncertainty in the transport velocity

- If we assume

$$h(\xi) = \sum_{j=0}^{P_h} h_j \psi_j(\xi)$$

- The system of equations becomes

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \sum_{j=0}^{P_h} h_j \langle \psi_j \psi_i \psi_k \rangle = 0 \qquad \text{for } k = 0, 1, ..., P.$$

- The *triple* product $\langle \psi_j \psi_i \psi_k \rangle$ is non zero for $i \neq j$

Polynomial Chaos

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- The *triple* product $\langle \psi_j \psi_i \psi_k \rangle$ is non zero for $i \neq j$
- We obtain a system of $P + 1$ coupled & deterministic eqns.

Polynomial Chaos

1D Linear Convection Equations - uncertainty in the transport velocity

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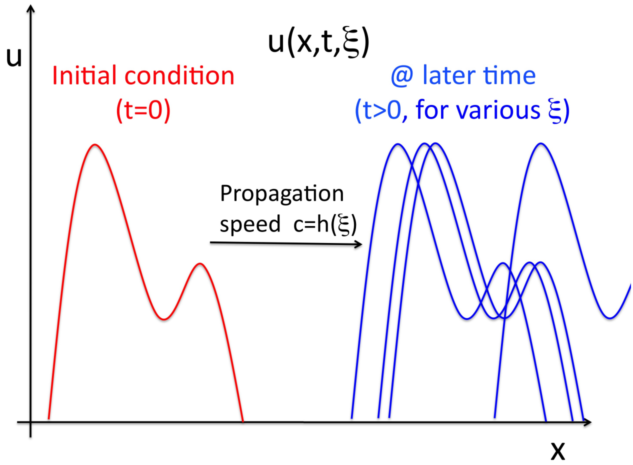
- The *triple* product $\langle \psi_j \psi_i \psi_k \rangle$ is non zero for $i \neq j$
- We obtain a system of $P + 1$ coupled & deterministic eqns.
- This is a much tougher non-linear problem and leads to the long-time integration issue

Linear Transport

Uncertainty in the transport velocity



Polynomial Chaos

1D Burgers Equations

- Consider the 1D Burgers equations

$$u_t + uu_x = 0 \quad 0 \leq x \leq 1$$

- Assume the uncertainty is characterized by one parameter; let it be a Guassian random variable $\xi \in \Omega$
- Consider a (truncated) spectral expansion of the solution in the *random* space

$$u(x,t,\xi) = \sum_{i=0}^{\infty} u_i(x,t)\psi_i(\xi) \approx \sum_{i=0}^{P} u_i(x,t)\psi_i(\xi)$$

where $\psi_i(\xi)$ are (1D) Hermite polynomials
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Polynomial Chaos

1D Burgers Equations

- *Plug* in the governing equations

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t}\psi_i(\xi) + \left(\sum_{j=0}^{P} u_j\psi_j(\xi)\right)\left(\sum_{i=0}^{P} \frac{\partial u_i}{\partial x}\psi_i(\xi)\right) = 0$$

Polynomial Chaos

1D Burgers Equations

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- Multiply by $\psi_k(\xi)$ and integrate over the probability space Ω – (Galerkin Projection)

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t}\langle\psi_i\psi_k\rangle + \sum_{i=0}^{P}\sum_{j=0}^{P} u_i\frac{\partial u_j}{\partial x}\langle\psi_i\psi_j\psi_k\rangle = 0 \qquad \text{for } k = 0, 1, ..., P.$$

- We obtain a system of $P+1$ coupled & deterministic equations (independently of the type of uncertainty)

Polynomial Chaos

1D Burgers Equations

PC expansion for the Burgers equations

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + \sum_{i=0}^{P} \sum_{j=0}^{P} u_i \frac{\partial u_j}{\partial x} \langle \psi_i \psi_j \psi_k \rangle = 0 \qquad \text{for } k = 0, 1, ..., P.$$

Double/Triple products are “numbers”

$$\langle \psi_i \psi_j \rangle = \delta_{ij} i!$$

$$\langle \psi_i \psi_j \psi_k \rangle = \begin{cases} 0 & \text{if } i+j+k \text{ is odd or } \max(i,j,k) > s \\ \frac{i!j!k!}{(s-i)!(s-j)!(s-k)!} & \text{otherwise} \end{cases}$$

and $s = (i+j+k)/2$

Polynomial Chaos

1D Burgers Equations

- PC Expansion for the Burgers equations P=1

$$
\begin{aligned}
\frac{\partial u_0}{\partial t} + u_0 \frac{\partial u_0}{\partial x} + u_1 \frac{\partial u_1}{\partial x} &= 0 \\
\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_0}{\partial x} + u_0 \frac{\partial u_1}{\partial x} &= 0
\end{aligned}
$$

Polynomial Chaos

1D Burgers Equations

- PC Expansion for the Burgers equations P=1

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\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_0}{\partial x} + u_0 \frac{\partial u_1}{\partial x} &= 0
\end{aligned}
$$

- PC Expansion for the Burgers equations P=2

$$
\begin{aligned}
\frac{\partial u_0}{\partial t} + u_0 \frac{\partial u_0}{\partial x} + u_1 \frac{\partial u_1}{\partial x} + 2u_2 \frac{\partial u_2}{\partial x} &= 0 \\
\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_0}{\partial x} + (u_0 + 2u_2) \frac{\partial u_1}{\partial x} + 2u_1 \frac{\partial u_2}{\partial x} &= 0 \\
\frac{\partial u_2}{\partial t} + u_2 \frac{\partial u_0}{\partial x} + u_1 \frac{\partial u_1}{\partial x} + (u_0 + 4u_2) \frac{\partial u_2}{\partial x} &= 0
\end{aligned}
$$

Simple example
1D Viscous Burgers

- Governing equation; note the *modified* convective flux:

$$\frac{1}{2}(1-u)\frac{\partial u}{\partial x} = \mu\frac{\partial^2 u}{\partial u^2}$$

- Exact solution

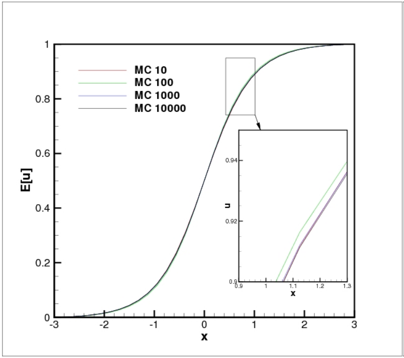
$$u(x) = \frac{1}{2}\left[1 + tanh\left(\frac{x}{4\mu}\right)\right]$$

- Assume uncertainty in the viscosity - Gaussian r.v. with $E[\mu] = 0.25$ and $Var[\mu] = 0.0025$

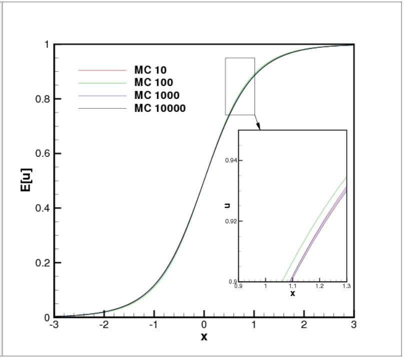
Monte Carlo Sampling

1D Viscous Burgers

Expectation of the solution:



Computed solution (32 points)

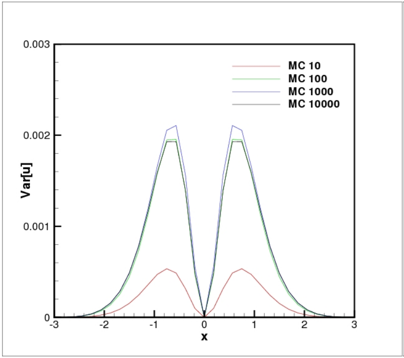


Exact solution

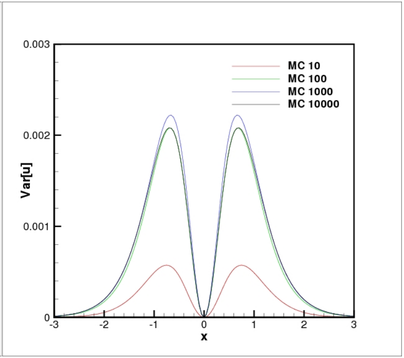
Monte Carlo Sampling

1D Viscous Burgers

Variance of the solution:



Computed solution (32 points)

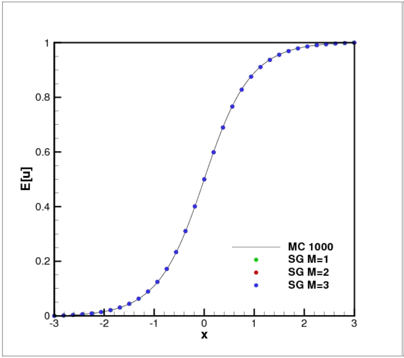


Exact solution

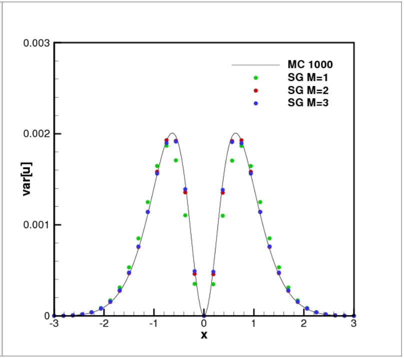
Polynomial Chaos

1D Viscous Burgers

Statistics of the solution:



Expectation

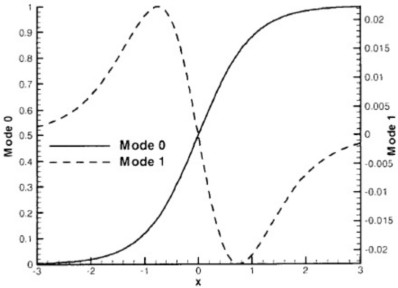


Variance

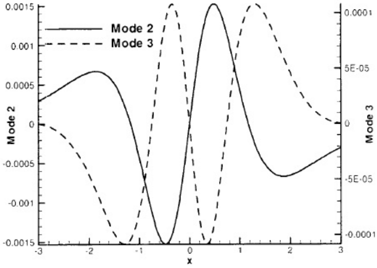
Polynomial Chaos

1D Viscous Burgers

Polynomial chaos modes of the solution ($P = 3$)



Coefficients “0” and “1”



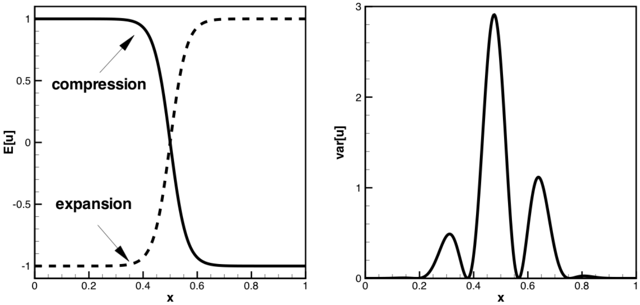
Coefficients “2” and “3”

- Mode “0” is the mean (as expected)
- Mode “1” is dominant with respect to the others (u_1^2 closely approximates the variance)

1D Burgers Equations

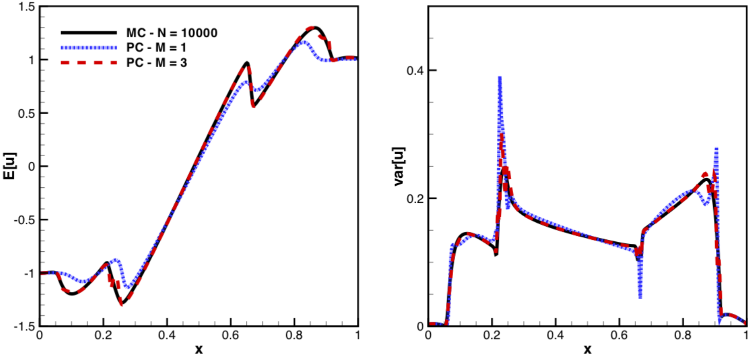
Uncertainty Propagation

- Uncertainty in the initial conditions
  - Expected expansion or compression (mean value of the initial condition)
  - Non-uniform variance
  - Objective: Compare Monte Carlo solutions (reference) to PC solutions



1D Burgers Equations

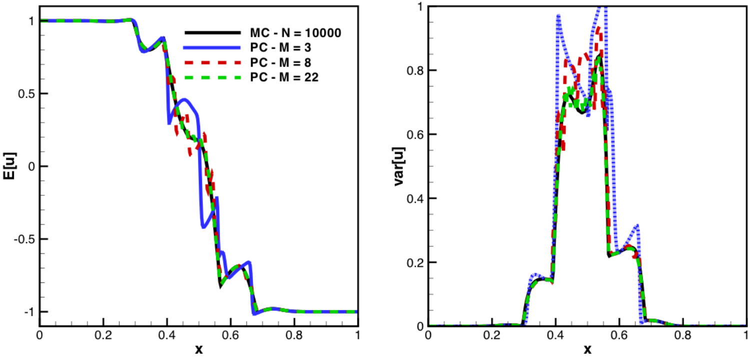
Uncertainty Propagation - Expansion



- Only 3 terms in the PC expansion are sufficient to reproduce the MC results

1D Burgers Equations

Uncertainty Propagation - Compression



- Even with 22 terms in the PC expansion, the results do not reproduce precisely the MC estimates

Polynomial Chaos

Navier-Stokes Equations

Consider the NS equations for an incompressible fluid

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j}$$

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Assuming that the uncertainty is represented with one uncertain variable ξ, the *usual* polynomial chaos expansion reads

$$u_i(x,t,\xi) = \sum_{j=0}^{P} u_i^{(j)}(x,t)\psi_j(\xi)$$

$$p(x,t,\xi) = \sum_{j=0}^{P} p^{(j)}(x,t)\psi_j(\xi)$$

Polynomial Chaos

Navier-Stokes Equations

The PC expansion for the velocity plugged in the continuity ($\partial u_i / \partial x_i = 0$) gives

$$\frac{\partial u_i^{(k)}}{\partial x_i} = 0 \quad k = 0, \ldots, P$$

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We obtain $P + 1$ equations for the velocity-mode vectors and $P + 1$ constraints.

- Not dissimilar from deterministic system
- Can be solved by projection and results in a coupled system of $3 \times (P + 1)$ momentum-like equations with $P + 1$ constraints.

Polynomial Chaos

Non-intrusive Variants

Starting from the spectral expansion (in uncertain variable ξ):

$$u(x,t,\xi) = \sum_{j=0}^{P} u^{(j)}(x,t)\psi_j(\xi)$$

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We can multiply left and right and side for $\psi_k(\xi)$ and integrate

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and therefore

$$u^{(k)} = \frac{\langle u(x,t,\xi)\psi_k(\xi)\rangle}{\langle\psi_k(\xi)\psi_k(\xi)\rangle}$$

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Computing the integrals $\langle u\phi_k\rangle$ requires sampling for example and therefore the solution of the original problem!

Concluding...

Polynomial Chaos

- The use of polynomial expansions transform the *original* stochastic problem into a more complex deterministic problem
- Polynomials are only one of the possible basis. wavelet are another popular choice.
- This forces us to interpret the resulting mathematical structure with potential enormous gains w.r.t. non-intrusive approaches

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- Polynomials are only one of the possible basis. wavelet are another popular choice.
- This forces us to interpret the resulting mathematical structure with potential enormous gains w.r.t. non-intrusive approaches
- It also forces you to rewrite codes!
- Non-intrusive variants can provide similar information (equivalent only in the linear case) and just require the evaluation of integrals!

Polynomial Chaos Methods

Concluding Remarks

Explicit representation of the quantity of interest u in terms of the uncertainty

$$u(x,t,\xi) \approx \sum_{i=0}^{P} u_i(x,t)\psi_i(\xi)$$

Accomplishments:

- Only need to solve deterministic problems
- Simple computations of the statistics of u
- Exponential convergence behavior

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Further considerations:

- Extensions to Multiple Uncertain Variables (Dimensions): $\xi_1, \xi_2, \ldots, \xi_d$
- Approximation properties for Non-Smooth responses

Polynomial Chaos Methods

Extension to multiple dimensions

- Consider d independent identically distributed random variables $\xi_1, \xi_2, \ldots, \xi_d$
- The PCE representation is written as:

$$u(x, t, \xi_1, \xi_2, \ldots, \xi_d) \approx \sum_{\alpha=0}^{\mathcal{P}} u_\alpha(x, t) \Psi_\alpha(\xi_1, \xi_2, \ldots, \xi_d)$$

  where Ψ_i is a multivariate polynomial obtained as tensor product of univariate polynomials

$$\Psi_\alpha(\xi_1, \xi_2, \ldots, \xi_d) = \psi_{\alpha_1}(\xi_1) \times \psi_{\alpha_2}(\xi_2) \times \cdots \times \psi_{\alpha_d}(\xi_d)$$

- The Galerkin procedure applies as before.

Multi-D Polynomial Chaos Methods

- In Multi-D in addition to the standard statistics (expectation. variance, etc.) it is useful to compute the relative importance of one variable with respect to the others
- One option is to compute the contribution of each variable to the variance (ANOVA decomposition)
- Consider the following manipulation

$$
u = u_0 + \sum_{i=1}^{d} \left(\sum_{\alpha \in \mathcal{I}_i} u_\alpha \Psi_\alpha(\xi_i) \right) + \sum_{i \le i_1 < i_2 \le d} \left(\sum_{\alpha \in \mathcal{I}_{i_1, i_2}} u_\alpha \Psi_\alpha(\xi_{i_1}, \xi_{i_2}) \right)
$$

$$
+ \sum_{i \le i_1 < \ldots i_s \le d} \left(\sum_{\alpha \in \mathcal{I}_{i_1, \ldots, i_s}} u_\alpha \Psi_\alpha(\xi_{i_1}, \ldots, \xi_{i_s}) \right)
$$

$$
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$$

Multi-D Polynomial Chaos Methods

- Recall that the variance is computed as

$$Var[u] = \sum_{\alpha=1}^{\mathcal{P}} u_\alpha^2 \langle \Psi_\alpha^2 \rangle.$$

Multi-D Polynomial Chaos Methods

- Recall that the variance is computed as

$$Var[u] = \sum_{\alpha=1}^{\mathcal{P}} u_\alpha^2 \langle \Psi_\alpha^2 \rangle.$$

- The manipulation presented earlier allows to compute partial variances:
  - Primary effect $\rightarrow$ variable i

$$\sum_{\alpha \in \mathcal{I}_i} u_\alpha^2 \langle \Psi_\alpha^2(\xi_i) \rangle$$

  - Combined effects $\rightarrow$ variables i_1 and i_2:

$$\sum_{\alpha \in \mathcal{I}_{i_1, i_2}} u_\alpha^2 \langle \Psi_\alpha^2(\xi_{i_1}, \xi_{i_2}) \rangle$$

  - Combined effects $\rightarrow$ variables $i_1, \ldots, i_s$:

$$\ldots$$

Polynomial Chaos Methods

Concluding Remarks (again)

$$u(x,t,\xi) \approx \sum_{i=0}^{\mathcal{P}} u_i(x,t)\psi_i(\xi)$$

Advantages:

- Only need to solve deterministic problems
- Simple computations of the statistics of u
- Exponential convergence behavior
- Useful sensitivity information extracted with minimal effort

Polynomial Chaos Methods

Concluding Remarks (again)

$$u(x,t,\xi) \approx \sum_{i=0}^{\mathcal{P}} u_i(x,t)\psi_i(\xi)$$

Advantages:

- Only need to solve deterministic problems
- Simple computations of the statistics of u
- Exponential convergence behavior
- Useful sensitivity information extracted with minimal effort

Disadvantages

- Many uncertainties (exponential increase in cost)
- Cardinality of the PCE:

$$\mathcal{P} = \frac{(P+d)!}{P!d!}$$

- Non-independent uncertainties
- Approximation properties for Non-Smooth responses

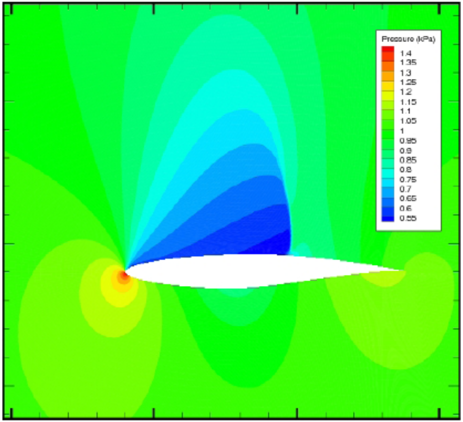
Part V

Examples

Fluid Dynamics of High Speed Flows

RAE 2822 Airfoil

- *Classical* transonic flow problem
- $M_\infty = 0.734$
- $\alpha = 2.79^o$
- $Re = 6.5 \times 10^6$



Pressure field

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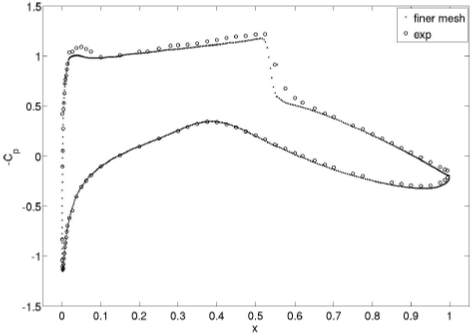

Wall Pressure Distribution

Fluid Dynamics of High Speed Flows

RAE 2822 Airfoil

- Introduce/define uncertainties in the problem (NODESIM Workshop)
  - $M_\infty = 0.734 \pm 0.005$
  - $\alpha = 2.79^o \pm 0.1$
  - $t/c = 0.1211 \pm 0.005$

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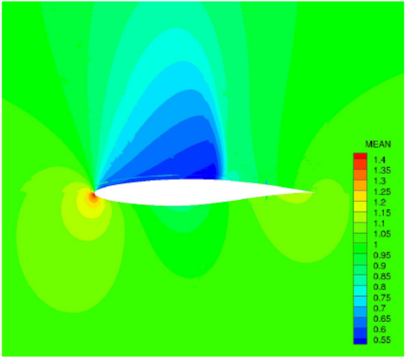
- Assume input distributions of the uncertainty either uniform or gaussian independent random variables
- Propagate the uncertainty in the simulations by performing Monte Carlo
- Analyze the results in terms of probability distribution of the output of interest (pressure distribution, lift, etc.)

Fluid Dynamics of High Speed Flows

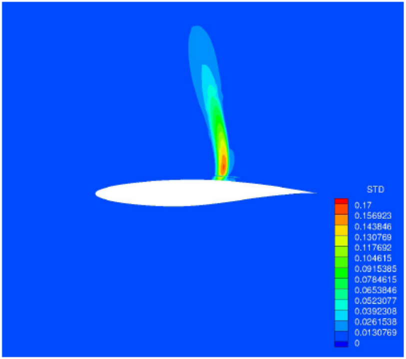
RAE 2822 Airfoil

- Resulting combined uncertainty

Mean Pressure



Pressure variance

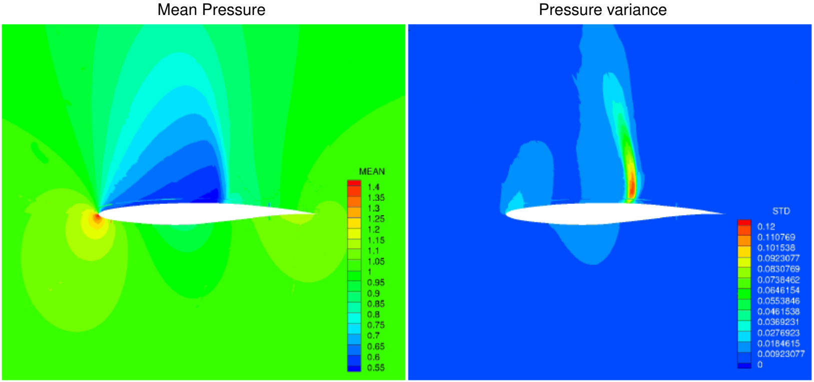


- Input uncertainties assumed independent uniform r.v.s

Fluid Dynamics of High Speed Flows

RAE 2822 Airfoil

- Resulting combined uncertainty

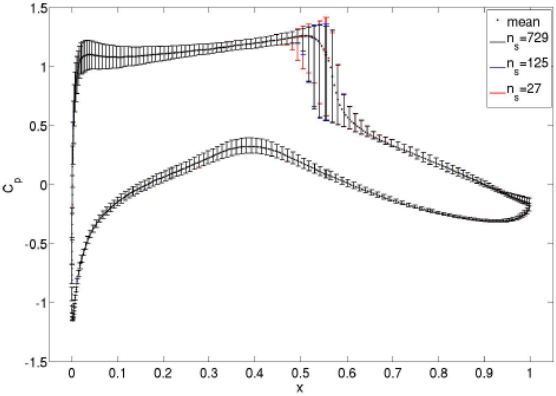


- Input uncertainties assumed independent gaussian r.v.s

Fluid Dynamics of High Speed Flows

RAE 2822 Airfoil

- Resulting combined uncertainty on wall pressure distribution



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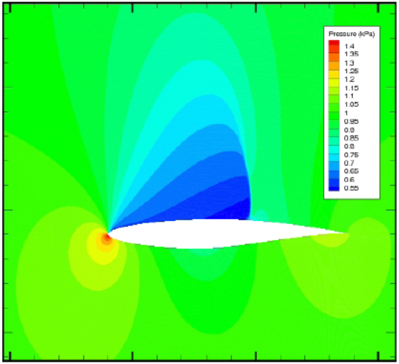
Fluid Dynamics of High Speed Flows

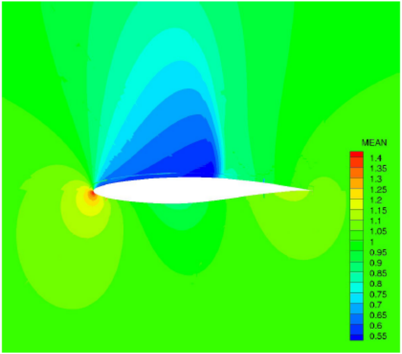
RAE 2822 Airfoil

- Qualitatively the deterministic (not uncertain) and the mean value of the probabilistic ensemble are NOT the same....

Deterministic



Mean Value



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