Uncertainty Quantification in Simulations of Reactive Flows

Part 1: Introductory concepts

Gianluca Iaccarino
ME & iCME
Stanford University
Part I

Why Uncertainty Quantification?

...don’t believe in the psychic octopus approach to computer predictions...
Uncertainty quantification (UQ) is the science of quantitative characterization and reduction of uncertainties in applications.
Uncertainty quantification (UQ) is the science of quantitative characterization and reduction of uncertainties in applications. It tries to determine how likely certain outcomes are if some aspects of the system are not exactly known.
Why Uncertainty Quantification?
...from WikiPedia

Uncertainty quantification (UQ) is the science of quantitative characterization and reduction of uncertainties in applications. It tries to determine how likely certain outcomes are if some aspects of the system are not exactly known.

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
Why Uncertainty Quantification?

Validation

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

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**
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

Images from Trucano et al. 2002, and Romero 2008
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

Images from Trucano et al. 2002, and Romero 2008
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

...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
"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.
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. “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.
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.

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

Definitions

What are errors? Errors are associated to the translation of a mathematical formulation into a numerical algorithm and a computational code. This includes:

- round-off
- limited convergence of iterative algorithms
- implementation mistakes (bugs)

What are uncertainties? Uncertainties are associated to the specification of the input physical parameters required for performing the analysis. This includes:

- the physics
Errors vs. Uncertainties

Definitions

- What are errors? errors are associated to the *translation* of a mathematical formulation into a numerical algorithm and a computational code.
  - round-off, limited convergence of iterative algorithms)
  - implementation mistakes (bugs).

- What are uncertainties? uncertainties are associated to the specification of the input physical parameters required for performing the analysis.
  - is the physics...
Errors vs. Uncertainties

Definitions

- **What are errors?** Errors are associated to the *translation* of a mathematical formulation into a numerical algorithm and a computational code.
  - round-off, limited convergence of iterative algorithms
  - implementation mistakes (bugs)
  - is the mathematics...

- **What are uncertainties?** Uncertainties are associated to the specification of the input physical parameters required for performing the analysis.
  - is the physics...
Errors vs. Uncertainties

Definitions

- **What are errors?** Errors are associated to the *translation* of a mathematical formulation into a numerical algorithm and a computational code.
  - round-off, limited convergence of iterative algorithms
  - implementation mistakes (bugs).
  - is the mathematics...

- **What are uncertainties?** Uncertainties are associated to the specification of the input physical parameters required for performing the analysis.
Errors vs. Uncertainties

Definitions

- **What are errors?** Errors are associated to the *translation* of a mathematical formulation into a numerical algorithm and a computational code.
  - round-off, limited convergence of iterative algorithms
  - implementation mistakes (bugs).
  - is the mathematics...

- **What are uncertainties?** Uncertainties are associated to the specification of the input physical parameters required for performing the analysis.
  - is the physics...
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)
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)

▶ It is naturally defined in a probabilistic framework

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

- It is naturally defined in a probabilistic framework

- 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
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

- It is NOT naturally defined in a probabilistic framework
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

- 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...
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...

- 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
Consider a generic computational model ($y \in \mathbb{R}^d$ with $d$ large)
Consider a generic computational model \((y \in \mathbb{R}^d \text{ with } d \text{ large})\)

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
Uncertainty Quantification
Computational Framework

Consider a generic computational model \((y \in \mathbb{R}^d \text{ with } d \text{ large})\)

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
Uncertainty definition

The objective is characterize uncertainties in simulation inputs, based on available information.
Uncertainty definition

The objective is characterize uncertainties in simulation inputs, based on available information

- **Direct methods**
  - Experimental observations
  - Theoretical arguments
  - Expert opinions
  - etc.
Uncertainty definition

The objective is to characterize uncertainties in simulation inputs, based on available information.

- **Direct methods**
  - Experimental observations
  - Theoretical arguments
  - Expert opinions
  - etc.

- **Inverse methods** (Inference, Calibration)
  - determination of the statistical input parameters that represent observed data using a computational model.
Uncertainty definition

- Identification of all the explicit and hidden parameters (knobs) of the mathematical/computational model:
- Characterization of the associated level of knowledge
- The mathematical framework for propagating uncertainties is dependent on the data representation chosen
Uncertainty definition

- Identification of all the (d) explicit and hidden parameters (knobs) of the mathematical/computational model: \( y \)
Uncertainty definition

- Identification of all the (d) *explicit* and *hidden* parameters (knobs) of the mathematical/computational model: \( y \)
- Characterization of the associated level of knowledge
Uncertainty definition

- Identification of all the (d) explicit and hidden parameters (knobs) of the mathematical/computational model: \( y \)
- Characterization of the associated level of knowledge

The mathematical framework for propagating uncertainties is dependent on the data representation chosen.
Consider a generic computational model \( y \in \mathbb{R}^d \) with \( d \) large.

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.
Probabilistic Uncertainty Propagation

Perform simulations accounting for the uncertainty represented as randomness

- Define an abstract probability space \((\Omega, \mathcal{A}, \mathcal{P})\)
- Introduce uncertain input as random quantities \(y(\omega), \omega \in \Omega\)
Probabilistic Uncertainty Propagation

Perform simulations accounting for the uncertainty represented as randomness

▶ Define an abstract probability space \((\Omega, \mathcal{A}, \mathcal{P})\)
▶ Introduce uncertain input as random quantities \(y(\omega), \omega \in \Omega\)
▶ The original problem becomes stochastic with solution \(u(\omega) \equiv u(y(\omega))\)

Remark: \(y\) can affect the boundary conditions, the geometry, the forcing terms or the operator in the computational model.
Probabilistic Uncertainty Propagation

Perform simulations accounting for the uncertainty represented as randomness

- Define an abstract probability space \((\Omega, \mathcal{A}, \mathcal{P})\)
- Introduce uncertain input as random quantities \(y(\omega), \omega \in \Omega\)
- The original problem becomes stochastic with solution \(u(\omega) \equiv u(y(\omega))\)

Remark: \(y\) can affect the boundary conditions, the geometry, the forcing terms or the operator in the computational model.
Probabilistic Uncertainty Propagation

Perform simulations accounting for the uncertainty represented as randomness

- Define an abstract probability space \((\Omega, \mathcal{A}, \mathcal{P})\)
- Introduce uncertain input as random quantities \(y(\omega), \omega \in \Omega\)
- The original problem becomes stochastic with solution \(u(\omega) \equiv u(y(\omega))\)

Remark: \(y\) can affect the boundary conditions, the geometry, the forcing terms or the operator in the computational model.
Uncertainty Propagation

Intrusive vs. Non-Intrusive Methodology

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

Intrusive methods require the formulation and solution of a stochastic version of the original model.
Uncertainty Propagation

Intrusive vs. Non-Intrusive Methodology

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

Intrusive vs. Non-Intrusive Methodology

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

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

Intrusive vs. Non-Intrusive Methodology

Nonintrusive methods only require (multiple) solutions of the original (deterministic) model
+ 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
Uncertainty Propagation
Intrusive vs. Non-Intrusive Methodology

- **Nonintrusive methods** only require (multiple) solutions of the original (deterministic) model
  - 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
Consider a generic computational model \((y \in \mathbb{R}^d \text{ with } d \text{ large})\)

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
Certification & Validation

- Need to define a validation metric to compare uncertain quantities
Need to define a validation metric to compare uncertain quantities.
Certification

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

Probabilistic Uncertainty Propagation
Uncertainty = Randomness

- **Sampling Methods**: Monte Carlo, Quasi Monte Carlo, Latin Hypercube, etc.
- **Intrusive Methods**: Polynomial Chaos, Adjoint, etc.
- **Non-Intrusive Methods**: Stochastic Collocation, Response Surface, etc.
- **Optimization Methods**
Uncertainty = Randomness

Monte Carlo is your town!

► If you know how to sample... it's done
Uncertainty = Randomness
Monte Carlo is your town!

▶ If you know how to sample... it’s done

\[ \langle u \rangle = \frac{1}{N} \sum u(\xi_i) \]
Uncertainty = Randomness

Monte Carlo is your town!

▶ If you know how to sample... it’s done

▶ ...not feasible with realistic function evaluations!
Uncertainty = Randomness

Monte Carlo is your town!

- If you know how to sample... it's done
- Interpret the uncertainty as additional independent variable(s) and use approximation theory to represent the solution

...not feasible with realistic function evaluations!
Uncertainty = Randomness
Monte Carlo is your town!

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

- Interpret the uncertainty as additional independent variable(s) and use approximation theory to represent the solution

- ...not feasible with realistic function evaluations!
Uncertainty Propagation
Intrusive vs. Non-Intrusive Methodology

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

- **Intrusive methods** require the formulation and solution of a stochastic version of the original model.
The solution is expressed as a spectral expansion of the uncertain variable(s): $\xi \in \Omega$ (assumed to be Gaussian)

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

where $\psi_i(\xi)$ are Hermite polynomials and form a complete set of orthogonal basis functions $\psi_0 = 1; \psi_1 = \xi; \psi_2 = \xi^2 - 1; \psi_3 = \xi^3 - 3\xi; \ldots$ 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 $\xi$ and $h_n$ are non-zero constants.
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)

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

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

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

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

where $w(\xi)$ is the pdf of $\xi$ and $h_n$ are non-zero constants
Polynomial Chaos
Hermite Polynomials
Orthogonal Polynomials

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

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

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

where \( w(\xi) \) is the pdf of \( \xi \) 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

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.

**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

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

**Expectation of \( u \)**

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

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

**Variance of \( u \)**

\[
Var[u] = E[u^2] - (E[u])^2 = \sum_{i=0}^{\infty} u_i^2 \int_{\Omega} \psi_i^2 w(\xi) d\xi - u_0^2 = \sum_{i=1}^{\infty} u_i^2 \langle \psi_i^2 \rangle.
\]
How do we compute \( u(x, t, \xi) = \sum_{i=0}^{\infty} u_i(x, t)\psi_i(\xi) \)?
Polynomial Chaos
Stochastic Galerkin Approach

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 $i \to \infty$?
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 $i \to \infty$?

- 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
Stochastic Galerkin Approach

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 \( i \to \infty \)?

- 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
Consider the 1D linear convection equations
\[ u_t + cu_x = 0 \quad 0 \leq x \leq 1 \]
The exact solution is \( u(x, t) = u_{initial}(x - ct) \)
Consider the 1D linear convection equations

\[ u_t + cu_x = 0 \quad 0 \leq x \leq 1 \]

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

Assume the uncertainty is characterized by one parameter; let it be a Gaussian random variable \( \xi \in \Omega \)
Consider the 1D linear convection equations

\[ u_t + cu_x = 0 \quad 0 \leq x \leq 1 \]

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

Assume the uncertainty is characterized by one parameter; let it be a Gaussian 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

\( (\psi_0 = 1; \psi_1 = \xi; \psi_2 = \xi^2 - 1; \psi_3 = \xi^3 - 3\xi; \text{etc.}) \)
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
1D Linear Convection Equations - uncertainty in the initial condition

- Assume
  \[ u_{initial}(x, t = 0, \xi) = g(\xi)\cos(x) \]
- The exact solution is
  \[ u(x, t, \xi) = g(\xi)\cos(x - ct) \]
- Plug in the truncated expansion in the original PDE:
  \[ \sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \psi_i(\xi) + c \left( \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \psi_i(\xi) \right) = 0 \]
Polynomial Chaos
1D Linear Convection Equations - uncertainty in the initial condition

▶ Assume

\[ u_{\text{initial}}(x, t = 0, \xi) = g(\xi)\cos(x) \]

▶ The exact solution is

\[ u(x, t, \xi) = g(\xi)\cos(x - ct) \]

▶ Plug in the truncated expansion in the original PDE:

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

▶ Multiply by \( \psi_k(\xi) \)

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

1D Linear Convection Equations - uncertainty in the initial condition

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

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

1D Linear Convection Equations - uncertainty in the initial condition

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

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

Pulling out of the integrand the deterministic components:

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

1D Linear Convection Equations - uncertainty in the initial condition

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

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

Pulling out of the integrand the deterministic components:

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

which in compact notation is:

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + c \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \langle \psi_i \psi_k \rangle = 0 \quad \text{for } k = 0, 1, ..., P.$$
We have
\[
\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + c \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \langle \psi_i \psi_k \rangle = 0 \quad \text{for } k = 0, 1, \ldots, P.
\]
Polynomial Chaos
1D Linear Convection Equations - uncertainty in the initial condition

- We have

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

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

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

\[ \ldots \]

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

- 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 $u_0 \ldots u_P$ equations are obtained by projection of the initial condition

\[
\langle u_{\text{initial}}(x, t = 0, \xi), \psi_k \rangle = u_k(x, t = 0) = \\
= \langle g(\xi), \psi_k \rangle \cos(x) \quad k = 0, \ldots, P
\]
Polynomial Chaos
1D Linear Convection Equations - uncertainty in the initial condition

- Initial conditions for the $u_0 \ldots u_P$ equations are obtained by projection of the initial condition
  \[
  \langle u_{\text{initial}}(x, t = 0, \xi), \psi_k \rangle = u_k(x, t = 0) = \langle g(\xi), \psi_k \rangle \cos(x) \quad k = 0, \ldots, P
  \]

- The procedure is \textit{simply} an approximation of $g(\xi)$ on the polynomial basis $\psi(\xi)$
Linear Transport

Deterministic case

Initial condition
(t=0)

@ later time
(t>0)

Propagation speed (c)
Linear Transport

Uncertainty in initial conditions

Initial condition
(t=0, for various $\xi$)

@ later time
(t>0, for various $\xi$)

Propagation speed (c)
Linear Transport
Uncertainty in initial conditions

$u_i(x, t, \xi)$

Initial condition
(t=0, for various $\xi$)

@ later time
(t>0, for various $\xi$)

Propagation speed ($c$)
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

1D Linear Convection Equations - uncertainty in the transport velocity

- Assume
  
  \[ c = h(\xi) \]

- The exact solution is
  
  \[ u(x, t, \xi) = \cos(x - h(\xi)t) \]

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

1D Linear Convection Equations - uncertainty in the transport velocity

- Assume
  \[ c = h(\xi) \]

- The exact solution is
  \[ u(x, t, \xi) = \cos(x - h(\xi)t) \]

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

- Multiply by \( \psi_k(\xi) \) and integrate over the probability space \( \Omega \) – (Galerkin Projection)
  \[
  \sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \langle h(\xi) \psi_i \psi_k \rangle = 0 \quad \text{for } k = 0, 1, \ldots, P.
  \]
If we assume
\[ h(\xi) = \sum_{j=0}^{P_h} h_j \psi_j(\xi) \]

The system of equations becomes
\[
\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + \sum_{i=0}^{P} \frac{\partial u_i}{\partial x} \sum_{j=0}^{P_h} h_j \langle \psi_j \psi_i \psi_k \rangle = 0 \quad \text{for } k = 0, 1, \ldots, P.
\]

The triple product \( \langle \psi_j \psi_i \psi_k \rangle \) is non zero for \( i \neq j \)
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

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

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

- If we assume

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

- The system of equations becomes

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

- The \textit{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 \textit{non-linear} problem and leads to the long-time integration issue
Linear Transport
Uncertainty in the transport velocity

$u(x,t,\xi)$

Initial condition
$t=0$

@ later time
$t>0$, for various $\xi$

Propagation speed $c=h(\xi)$
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 Gaussian 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

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

- Plug in the governing equations

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

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

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

- 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

$$\sum_{i=0}^{P} \frac{\partial u_i}{\partial t} \langle \psi_i \psi_k \rangle + \sum_{i=0}^{P} \sum_{j=0}^{P} u_i \frac{\partial u_j}{\partial x} \langle \psi_i \psi_j \psi_k \rangle = 0$$

for $k = 0, 1, \ldots, P$.

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 $P=1$

\[
\begin{align*}
\frac{\partial u_0}{\partial t} + u_0 \frac{\partial u_0}{\partial x} + u_1 \frac{\partial u_1}{\partial x} &= 0 \\
\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_0}{\partial x} + u_0 \frac{\partial u_1}{\partial x} &= 0
\end{align*}
\]
Polynomial Chaos

1D Burgers Equations

- PC Expansion for the Burgers equations $P=1$

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

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

- PC Expansion for the Burgers equations $P=2$

$$\frac{\partial u_0}{\partial t} + u_0 \frac{\partial u_0}{\partial x} + u_1 \frac{\partial u_1}{\partial x} + 2u_2 \frac{\partial u_2}{\partial x} = 0$$

$$\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_0}{\partial x} + (u_0 + 2u_2) \frac{\partial u_1}{\partial x} + 2u_1 \frac{\partial u_2}{\partial x} = 0$$

$$\frac{\partial u_2}{\partial t} + u_2 \frac{\partial u_0}{\partial x} + u_1 \frac{\partial u_1}{\partial x} + (u_0 + 4u_2) \frac{\partial u_2}{\partial x} = 0$$
Simple example
1D Viscous Burgers

- Governing equation; note the \textit{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 \( \text{Var}[\mu] = 0.0025 \)
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 \((P = 3)\)

- 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

![Graph showing expected expansion or compression](image.png)
Only 3 terms in the PC expansion are sufficient to reproduce the MC results.
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

\[
\begin{align*}
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \\
\frac{\partial u_i}{\partial x_i} &= 0
\end{align*}
\]
Polyomial Chaos
Navier-Stokes Equations

Consider the NS equations for an incompressible fluid

\[
\frac{\partial u_i}{\partial x_i} = 0
\]

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

Assuming that the uncertainty is represented with one uncertain variable \( \xi \), the *usual* polynomial chaos expansion reads

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

\[
p(x, t, \xi) = \sum_{j=0}^{P} p^{(j)}(x, t) \psi_j(\xi)
\]
The PC expansion for the velocity plugged in the continuity
\( \partial u_i / \partial x_i = 0 \) gives

\[
\frac{\partial u_{i}^{(k)}}{\partial x_i} = 0 \quad k = 0, \ldots, P
\]
Polynomial Chaos

Navier-Stokes Equations

The PC expansion for the velocity plugged in the continuity
\( \frac{\partial u_i}{\partial x_i} = 0 \) gives

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

The momentum equation instead becomes (for each \( k \) component)

\[
\frac{\partial u_i^{(k)}}{\partial t} + \sum_{m=0}^{P} \sum_{n=0}^{P} u_j^{(m)} \frac{\partial u_i^{(n)}}{\partial x_j} \frac{\langle \psi_m \psi_n \psi_k \rangle}{\langle \psi_k \psi_k \rangle} = -\frac{1}{\rho} \frac{\partial p^{(k)}}{\partial x_i} + \mu \frac{\partial^2 u_i^{(k)}}{\partial x_j \partial x_j}
\]
Polynomial Chaos

Navier-Stokes Equations

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

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

The momentum equation instead becomes (for each $k$ component)

$$\frac{\partial u_i^{(k)}}{\partial t} + \sum_{m=0}^{P} \sum_{n=0}^{P} u_j^{(m)} \frac{\partial u_j^{(n)}}{\partial x_j} \frac{\langle \psi_m \psi_n \psi_k \rangle}{\langle \psi_k \psi_k \rangle} = -\frac{1}{\rho} \frac{\partial p^{(k)}}{\partial x_i} + \mu \frac{\partial^2 u_i^{(k)}}{\partial x_j \partial x_j}$$

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

Navier-Stokes Equations

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

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

The momentum equation instead becomes (for each $k$ component)

$$\frac{\partial u_i^{(k)}}{\partial t} + \sum_{m=0}^{P} \sum_{n=0}^{P} u_j^{(m)} \frac{\partial u_i^{(n)}}{\partial x_j} \frac{\langle \psi_m \psi_n \psi_k \rangle}{\langle \psi_k \psi_k \rangle} = -\frac{1}{\rho} \frac{\partial p^{(k)}}{\partial x_i} + \mu \frac{\partial^2 u_i^{(k)}}{\partial x_j \partial x_j}$$

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 $\xi$):

$$u(x, t, \xi) = \sum_{j=0}^{P} u^{(j)}(x, t) \psi_j(\xi)$$
Polynomial Chaos
Non-intrusive Variants

Starting from the spectral expansion (in uncertain variable $\xi$):

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

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

$$\langle u(x, t, \xi) \psi_k(\xi) \rangle = \langle \sum_{j=0}^{P} u^{(j)}(x, t) \psi_j(\xi) \psi_k(\xi) \rangle$$
Polynomial Chaos
Non-intrusive Variants

Starting from the spectral expansion (in uncertain variable $\xi$):

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

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

$$\langle u(x, t, \xi)\psi_k(\xi) \rangle = \langle \sum_{j=0}^{P} u^{(j)}(x, t)\psi_j(\xi)\psi_k(\xi) \rangle = u^{(k)}\langle \psi_k(\xi)\psi_k(\xi) \rangle$$
Starting from the spectral expansion (in uncertain variable $\xi$):

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

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

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

and therefore

$$ u^{(k)} = \frac{\langle u(x, t, \xi) \psi_k(\xi) \rangle}{\langle \psi_k(\xi) \psi_k(\xi) \rangle} $$
Polynomial Chaos
Non-intrusive Variants

Starting from the spectral expansion (in uncertain variable \( \xi \)):

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

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

\[
\langle u(x, t, \xi) \psi_k(\xi) \rangle = \langle \sum_{j=0}^{P} u^{(j)}(x, t) \psi_j(\xi) \psi_k(\xi) \rangle = u^{(k)} \langle \psi_k(\xi) \psi_k(\xi) \rangle
\]

and therefore

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

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

Polynomials are only one of the possible basis. Wavelets 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!
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
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

Further considerations:

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

\[
\begin{align*}
    u &= u_0 + \sum_{i=1}^{d} \left( \sum_{\alpha \in \mathcal{I}_i} u_{\alpha} \psi_{\alpha}(\xi_i) \right) + \sum_{i \leq i_1 < i_2 \leq d} \left( \sum_{\alpha \in \mathcal{I}_{i_1,i_2}} u_{\alpha} \psi_{\alpha}(\xi_{i_1}, \xi_{i_2}) \right) \\
    &\quad + \sum_{i \leq i_1 < \cdots < i_s \leq d} \left( \sum_{\alpha \in \mathcal{I}_{i_1,\ldots,i_s}} u_{\alpha} \psi_{\alpha}(\xi_{i_1}, \ldots, \xi_{i_s}) \right) \\
    &\quad + \cdots + \sum_{\alpha \in \mathcal{I}_{i_1,\ldots,i_d}} u_{\alpha} \psi_{\alpha}(\xi_{i_1}, \ldots, \xi_{i_d})
\end{align*}
\]
Recall that the variance is computed as

\[ \text{Var}[u] = \sum_{\alpha=1}^{P} u_{\alpha}^2 \langle \psi_{\alpha}^2 \rangle. \]
Multi-D Polynomial Chaos Methods

- Recall that the variance is computed as

\[
\text{Var}[u] = \sum_{\alpha=1}^{P} u_\alpha^2 \langle \psi_\alpha^2 \rangle.
\]

- The manipulation presented earlier allows to compute partial variances:
  - Primary effect → variable \(i\)
    \[
    \sum_{\alpha \in I_i} u_\alpha^2 \langle \psi_\alpha^2 (\xi_i) \rangle
    \]
  - Combined effects → variables \(i_1\) and \(i_2\):
    \[
    \sum_{\alpha \in I_{i_1, i_2}} u_\alpha^2 \langle \psi_\alpha^2 (\xi_{i_1}, \xi_{i_2}) \rangle
    \]
  - Combined effects → variables \(i_1, \ldots, i_s\):
    
    \[
    \ldots
    \]
Polynomial Chaos Methods

Concluding Remarks (again)

\[ u(x, t, \xi) \approx \sum_{i=0}^{p} u_i(x, t) \psi_i(\xi) \]

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:
  \[ P = \binom{P + d}{d} \]
- Non-independent uncertainties
- Approximation properties for Non-Smooth responses
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
- $M_\infty = 0.734$
- $\alpha = 2.79^\circ$
- $Re = 6.5 \times 10^6$
Classical transonic flow problem

$M_\infty = 0.734$

$\alpha = 2.79^\circ$

$Re = 6.5 \times 10^6$

Wall Pressure Distribution
Introduce/define uncertainties in the problem (NODESIM Workshop)

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

- $M_\infty = 0.734 \pm 0.005$
- $\alpha = 2.79^\circ \pm 0.1$
- $t/c = 0.1211 \pm 0.005$

Assume input distributions of the uncertainty either uniform or gaussian independent random variables
Introduce/define uncertainties in the problem (NODESIM Workshop)

- $M_\infty = 0.734 \pm 0.005$
- $\alpha = 2.79^\circ \pm 0.1$
- $t/c = 0.1211 \pm 0.005$

Assume input distributions of the uncertainty either uniform or gaussian independent random variables

Propagate the uncertainty in the simulations by performing Monte Carlo
Introduce/define uncertainties in the problem (NODESIM Workshop)

- $M_\infty = 0.734 \pm 0.005$
- $\alpha = 2.79^\circ \pm 0.1$
- $t/c = 0.1211 \pm 0.005$

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

- 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

- Input uncertainties assumed independent uniform r.v.s
Qualitatively the deterministic (not uncertain) and the mean value of the probabilistic ensemble are NOT the same....