

# Quantification of Uncertainty in Numerical simulation of Fluid Flows

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March 28

*MaiMoSine, Grenoble*  
**Workshop on Validation, Verification and UQ**



- 1 Introduction
- 2 UQ definitions
- 3 Mathematical setting
- 4 Some methods for solving UQ propagation problems
- 5 Problems in Fluid Mechanics
- 6 Some highlights from a new method

- Virtual Prototyping (VP) → key technology for industry to respond to the challenges of designing sustainable products, environmental challenges and cost effectiveness
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- Managing the design process in light of these uncertainties is the key to robust design
- Introducing the probabilistic nature of the uncertainties in the simulation is highly challenging, as the whole process transforms the resolution of deterministic physical conservation laws, to non-deterministic methods, governed by stochastic partial differential equations (SPDE)
- As a consequence, predicted quantities, such as loads, lift, ....., are represented by a probability density function (pdf), providing a domain of confidence, associated to the considered uncertainties

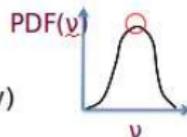
# Meaning of quantifying uncertainties in the numerical simulation

## EDP modèle

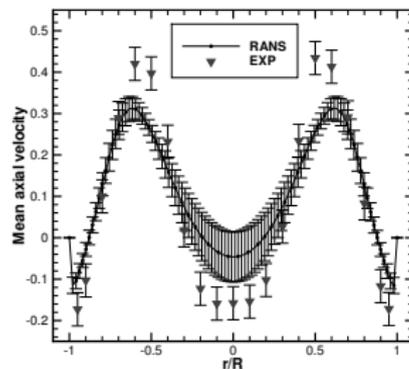
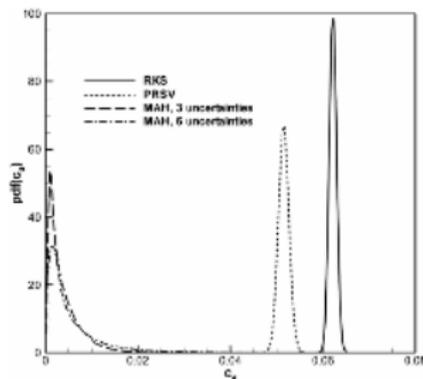
$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} + S(x)$$

## + INCERTITUDE

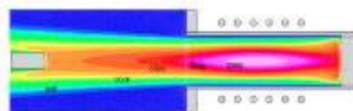
Paramètres de l'équation  
(Ex. propriétés physiques  $\nu$ )



**OBJECTIF :**  
SOLUTION  
STATISTIQUE  
DE L'EDP



# Three pillars for predictive engineering simulations



Computations

Verification

Validation

$$\sigma_e = \frac{(n_e q_e)^2}{p_e} D_e$$

Theory

$$D_e = \frac{1}{3} \rho_e T_e M_b [\phi_e^{\Omega}, \phi_e^{\Omega}]_e$$

Experiments



- Computation cannot be truly predictive without the coupling to theory and experiments...
- This coupling is precisely the verification and validation process!

- ⇒
- **Verification:** Is the computational method implemented correctly?
  - **Validation :** Are we solving the right equations?
  - **Uncertainty Quantification** is the end-to-end study of the reliability of scientific predictions

- Uncertainty identification: Data (e.g., operational uncertainties, geometrical variability); Model (e.g., physical model approximations, grid dependence, convergence)
- Uncertainty categorization (Epistemic) or Irreducible (Aleatory) Reducible

- Uncertainty identification: Data (e.g., operational uncertainties, geometrical variability); Model (e.g., physical model approximations, grid dependence, convergence)
- Uncertainty categorization (Epistemic) or Irreducible (Aleatory) Reducible
- Uncertainty quantification: Statistical description of input uncertainties (e.g., mean value and standard deviation); Distribution type (defined by a probability density function pdf-)
- Uncertainty propagation: Probabilistic definition of the output quantities; (Applying methods such as Monte Carlo Simulation; Methods of Moments; Polynomial Chaos,...)
- Uncertainty analysis: Analysis of variance (ANOVA); Allocation of output uncertainty to specific sources; Identify the factors that contribute most to risk

## Errors vs. uncertainties

- **Errors:** associated to the translation of a mathematical formulation into a numerical algorithm
  - Round-off errors and limited convergence of certain iterative algorithms
  - Implementation mistakes (bugs) or usage errors
- **Uncertainties:** associated to the choice of the physical models and to the specification of the input parameters

## Uncertainty Classification

- **Aleatory:** not strictly due to a lack of knowledge → **can not be reduced**
  - characterized using probabilistic approaches
  - Ex: determination of material properties or operating conditions
- **Epistemic:** potential deficiency due to a lack of knowledge
  - It can arise from assumptions introduced in the derivation of the mathematical model or from simplifications
  - **can be reduced** (for example by improving the measures)

- Epistemic uncertainties are a property of the models applied in the analysis, including the choices made by the modeler
- The aleatory uncertainties are a strict property of the system being analyzed

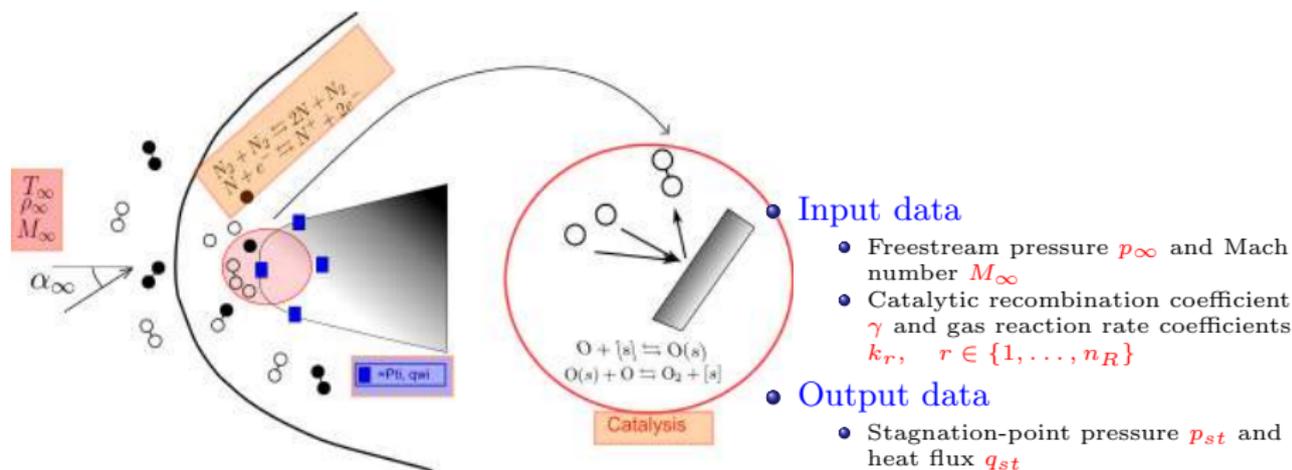
- Epistemic uncertainties are a property of the models applied in the analysis, including the choices made by the modeler
- The aleatory uncertainties are a strict property of the system being analyzed
- Different ways of treatment and quantification
- Methods for handling epistemic uncertainties generally place some type of bounds on the resulting output uncertainty, largely based on (subjective) estimates of error and input uncertainty levels.

## Introduction of UQ in numerical simulations: 3 Steps

- **Data assimilation**: (ex. conditions inferred from experiments) define a random vector  $\xi = (\xi_1, \dots, \xi_N)$  that parametrizes uncertain input data with a specified PDF  $p_\xi$
- **Uncertainty propagation**: data uncertainty propagate into the forward model so that the output quantities of interest (QOIs) are random  
→ compute statistics of the QOI
- **Post-Processing analysis**: reliability assessments, validation metrics

## How taking into account experimental uncertainties and observations in the numerical simulation

- Forward problem
- Backward problem

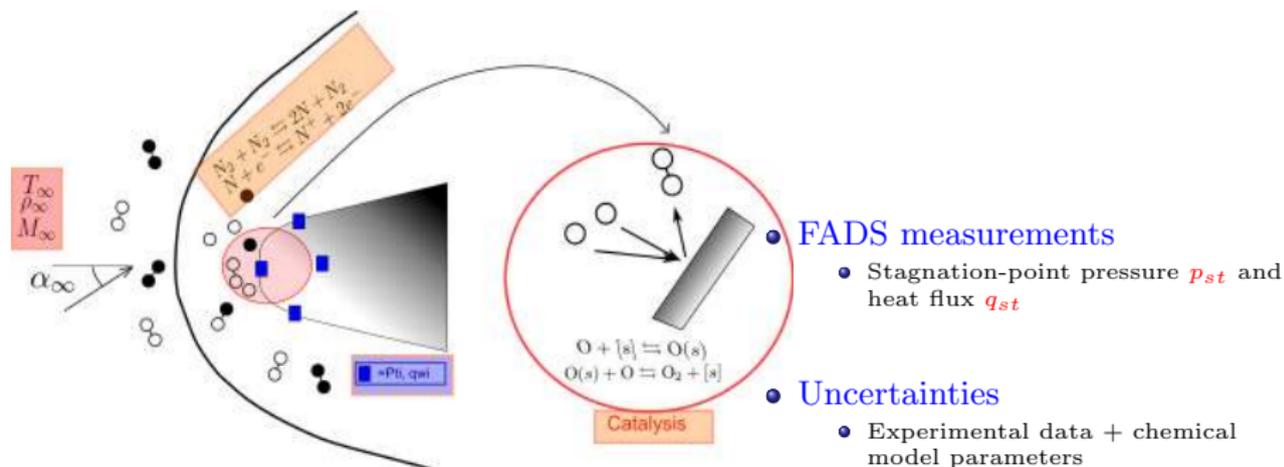


- CFD code

⇒ Sources of uncertainties

- Unknown:  $p_\infty \sim \mathcal{U}(16.3, 24.3)$  and  $M_\infty \sim \mathcal{U}(13.7, 17.3)$
- Arrhenius gas reaction rate coefficients
- Epistemic uniform uncertainty on  $\gamma \sim \mathcal{U}(0.001, 0.002)$

# Inverse problem example



- Investigation of one point of the trajectory of the EXPERT vehicle  
( $p_\infty = 20.3$ ,  $T_\infty = 245.5$ ,  $M_\infty = 15.5$ )

⇒ **Objective:** determine uncertainties on freestream conditions  $p_\infty$  and  $M_\infty$  from the FADS data

Let the output of interest  $u(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}))$  be governed by the equation:

$$\mathcal{L}(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}); u(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}))) = \mathcal{S}(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega})), \quad (1)$$

where  $\mathcal{L}$  (algebraic or differential operator) and  $\mathcal{S}$  are on  $D \times T \times \Xi$ ,  $\mathbf{x} \in D \subset \mathbb{R}^{n_d}$ , with  $n_d \in \{1, 2, 3\}$ ,  $\boldsymbol{\xi}(\boldsymbol{\omega}) = \{\xi_1(\omega_1), \dots, \xi_d(\omega_d)\} \in \Xi$  with parameters space  $\Xi \subset \mathbb{R}^d$

Probability framework (on the probability space  $(\Omega, \mathcal{F}, P)$ ):

realizations  $\boldsymbol{\omega} = \{\omega_1, \dots, \omega_d\} \in \Omega \subset \mathbb{R}$  with  $\Omega$  set of outcomes,  $\mathcal{F} \subset 2^\Omega$  is the  $\sigma$ -algebra of events,  $P : \mathcal{F} \rightarrow [0, 1]$  is a probability measure.

The objective of uncertainty propagation is to find the **probability distribution** of  $u(\mathbf{y}, \boldsymbol{\xi})$  and its **statistical moments**  $\mu_{u_i}(\mathbf{y})$  given by

$$\mu_{u_i}(\mathbf{y}) = \int_{\Xi} u(\mathbf{y}, \boldsymbol{\xi})^i f_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}. \quad (2)$$

**How compute this integral in an efficient way ?**

Actually two kind of methodologies exist:

- *Intrusive*: the method requires intensive modifications of the numerical code  
NOTE: the number of equations is not preserved!
- *Non-intrusive*: No modifications of the deterministic scheme are demanded (the CFD code is a black-box)
  
- Deterministic Methods (moments, perturbation ...)
- Sampling techniques (Monte Carlo, Latin Hypercube)
- Stochastic collocation (Lagrangian interpolation)
- Probabilistic collocation (Chaos version of Lagrangian interpolation)
- (generalized-) Polynomial Chaos (gPC)
- Surrogate modelling

The gPC can be intrusive (Galerkin projection) or non-intrusive.

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$$\mathcal{L}(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}); u(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}))) = \mathcal{S}(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega})), \quad (3)$$

where  $\mathcal{L}$  (algebraic or differential operator) and  $\mathcal{S}$  are on  $D \times T \times \Xi$ ,  $\mathbf{x} \in D \subset \mathbb{R}^{n_d}$ , with  $n_d \in \{1, 2, 3\}$ ,  $\boldsymbol{\xi}(\boldsymbol{\omega}) = \{\xi_1(\omega_1), \dots, \xi_d(\omega_d)\} \in \Xi$  with parameters space  $\Xi \subset \mathbb{R}^d$

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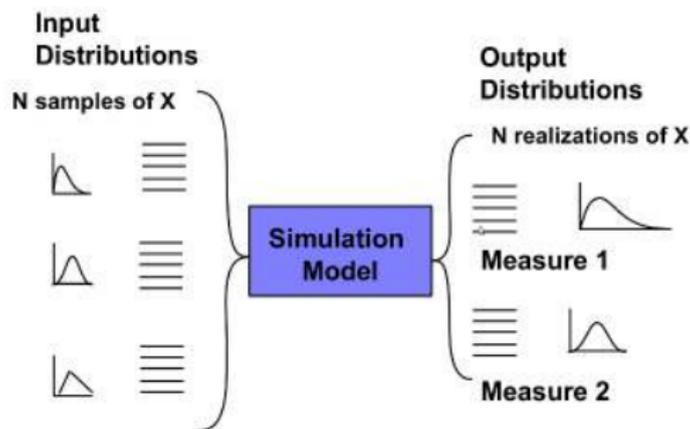
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**How compute this integral in an efficient way ?**

- **Repeated** simulations with a proper selection of the input values
- Results **collected** to generate a statistical characterization of the outcome  
→ Efficient Monte Carlo (MC), pseudo-MC (Latin hypercube) or quasi-MC
- Sampling is **not the most efficient** UQ method, but it is *easy* to implement, *robust*, and *transparent*.



### Motivation

- Evaluation of **integrals** needed  
→ *Natural* to employ conventional numerical integration techniques

### How ?

- Quadratures based on **Newton-Cotes** formulas for equally spaced abscissas
- **Stochastic Collocation**: Gaussian quadrature, *i.e.* the Gauss-Legendre integration formula based on Legendre polynomials  
→ *Natural extension* to multiple dimensions as tensor product of 1D interpolants  
→ **Curse of Dimensionality** for high dimensions, Smolyak Algorithm

[Wiener 38; Cameron & Martin 47; Ghanem & Spanos 91]

Every QOI  $u$  can be expanded in a convergent series of the form

$$u(\boldsymbol{\xi}) \approx u^{\text{PC}}(\boldsymbol{\xi}) = \sum_{\alpha=0}^P u_{\alpha} \Psi_{\alpha}(\boldsymbol{\xi}),$$

- $P = (n_{\boldsymbol{\xi}} + N_0)!/n_{\boldsymbol{\xi}}!N_0!$ , **No**: expansion degree
- $\{\Psi_{\alpha}\}_{\alpha=0,\dots,P}$  polynomial functions orthogonal w.r.t  $p_{\boldsymbol{\xi}}$
- correspondence between  $p_{\boldsymbol{\xi}}$  and  $\{\Psi_{\alpha}\}$
- $\{u_{\alpha}\}_{\alpha=0,\dots,P}$  : deterministic spectral coefficients

Determination of  $\{u_{\alpha}\}$  by a **non-intrusive spectral method** (NISP)

$$u_{\alpha} = \|\Psi_{\alpha}\|^{-2} \int u(\boldsymbol{\xi}) \Psi_{\alpha}(\boldsymbol{\xi}) \approx \|\Psi_{\alpha}\|^{-2} \sum_{i=1}^n u(\mathbf{x}, t, \boldsymbol{\xi}_i) \Psi_{\alpha}(\boldsymbol{\xi}_i) \omega_i$$

$(\boldsymbol{\xi}_i, \omega_i)$  quadrature formulae points and weights  $\rightarrow$  **deterministic code used as a black box**

From PC expansions of QOIs [Crestaux, Le Maitre & Martinez 09]

- derivation of **means** and **variances**

$$E(u^{\text{PC}}) = u_0, \quad \text{Var}(u^{\text{PC}}) = \sum_{\alpha=1}^P u_{\alpha}^2(\mathbf{x}) \langle \Psi_i^2 \rangle$$

- estimation of sensitivity information using the analysis of variance (ANOVA) decomposition
  - **Sobol first order indices**  $\{S_i\}_{i=1, \dots, n_{\xi}}$  determining the contribution to the variance of the  $i^{\text{th}}$  random parameter to the QOI  $u$
  - **Sobol total order indices**  $\{S_{T,i}\}_{i=1, \dots, n_{\xi}}$  determining the contribution of the  $i^{\text{th}}$  random parameter to the QOI  $u$  including interactions with other parameter  $j \in \{1, \dots, n_{\xi}\}, j \neq i$

## Sampling

- **Strengths:** Simple and reliable, convergence rate is dimension-independent
- **Weaknesses:**  $\sqrt{N}$  convergence  $\rightarrow$  expensive for accurate tail statistics

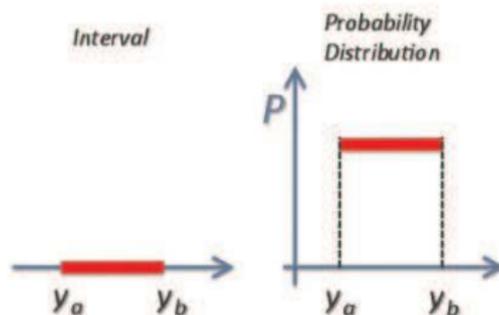
## Stochastic expansions

- **Strengths:** functional representation, exponential convergence rates
- **Problems**
  - $\Rightarrow$  Discontinuity  $\rightarrow$  Gibbs phenomena
  - $\Rightarrow$  Singularity  $\rightarrow$  divergence in moments
  - $\Rightarrow$  Scaling to large  $n$   $\rightarrow$  exponential growth in number of simulation

- Second order probability
- **Interval valued probability**
- Evidence Theory
- ...

Minimal statement of knowledge: the input  $y$  is bounded  $y \in [y_a, y_b]$ .

- **Nothing is known** expect that input uncertainties vary in some intervals
- Different than a random variable with a uniform probability: one true value vs. every outcome has the **same probability** of occurring



- Treating intervals in a **probabilistic framework**
  1. **Substitute** intervals with uniform r.v.s
  2. **Propagate** uncertainty using any of the probabilistic UQ methods
  3. Discard the probabilistic information and **compute the support** of the output
    - **Very costly** and requires precise evaluation of the tail distribution of the output quantity

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    - **Very costly** and requires precise evaluation of the tail distribution of the output quantity
- Formulate the problem as a **two-optimization** problems, focused on the **bounds** of the output quantity in the space of the possible input
  - **Worst case** scenario analysis

Consider  $n_{\xi_1}$  **epistemic** random variables and  $n_{\xi_2}$  **aleatory** random variables. Using **interval analysis** in a mixed aleatory/epistemic uncertainty framework reduces to solve the following problems

$$\min_{\xi_1(\omega) \subset \mathbb{R}^{n_{\xi_1}}} \mu'_{u_i}(\mathbf{x}, t) \quad \text{and} \quad \max_{\xi_1(\omega) \subset \mathbb{R}^{n_{\xi_1}}} \mu'_{u_i}(\mathbf{x}, t) \quad (5)$$

with

$$\mu'_{u_i}(\mathbf{x}, t) = \int_{\Xi_2} u(\mathbf{x}, t, \xi_2)^i f_{\xi}(\xi_2) d\xi_2, \quad (6)$$

We are interested in a method that directly address the computation of 5 and 6 by **minimizing** the computational cost.

## High number of uncertainties

- Use of different types of (sparse) numerical quadratures, sparse tensor products, adaptive methods
- **Problem reduction via ANOVA (or others) analysis and predominant uncertainties**

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## Discontinuous Flows (Compressible with shocks)

- **Develop adapted bases: multi-resolution or multi-elements gPC**
- Semi-intrusive multi-resolution stochastic method

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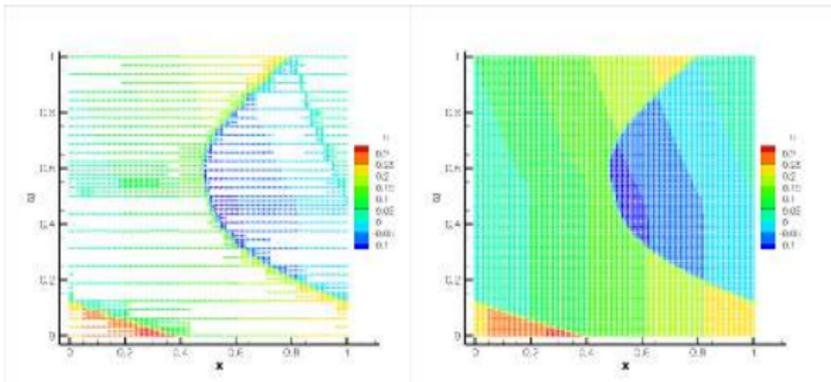
## Coupling numerics/physics

- Use of observations in the model calibrations
- **Use of UQ tools in order to perform predictive numerical experiments**

# Main Idea

Adaptive refinement/derefinement of the whole surface

Major issue in **UQ+CFD** → Number of CFD runs



**Classical methods:**

$$N = N_x \times N_t \times N_\xi$$

Remark:  $N_\xi$  is constant

**Evaluations ratio:**

The number of effective evaluations in the physical/stochastic space can be reduced

$$\eta = \eta(t) = \frac{N_{\text{Adaptive}}}{N_{\text{Full}}}$$

**Need for an intrusive approach**

→ Coupled strategy in physical/stochastic spaces

→ Semi-Intrusive Method (No additional equations)

*Weak Coupling* (Fixed CFD and physical mesh)

**Aim:** Increase/Decrease points for selected locations of the spatial-time space

$$N_\xi = N_\xi(x, t)$$

# Motivation and background

Towards a UQ framework for unsteady compressible flow problems

## AIM

Building a generalized UQ framework for systems with discontinuous responses affected by a moderate number of uncertainties

## Desired properties

- Generalized non-intrusive/intrusive framework
- Capability to manage whatever form of pdf (discontinuous, time varying)
- Easy implementation even in the intrusive form: semi-intrusive approach (*i.e.* for complex code/problems the deterministic scheme is fixed!)
- Efficient memory usage (the grids are  $T \times \Omega \times \Xi$ ,  $\Omega \subset \mathcal{R}^n$ ,  $\Xi \subset \mathcal{R}^d$ )
- Lower computational cost (with respect equivalent approaches)

# The main idea

From Harten to the spatial-TE algorithm

## Harten framework (essential elements)

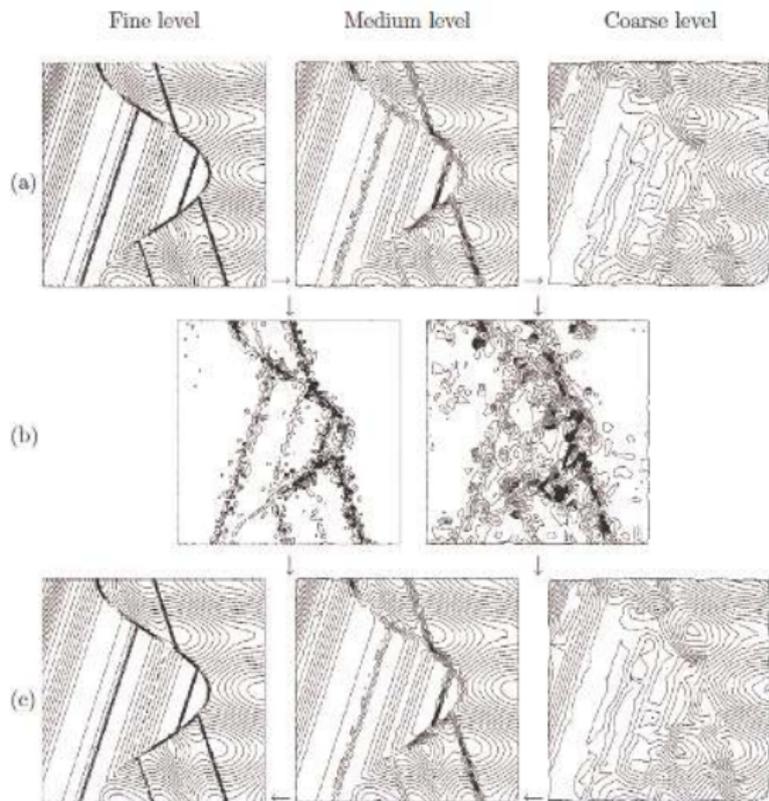
- 1 Hierarchical representation of the information between different resolution levels
- 2 Truncation of the non-essential information
- 3 Advancing between different time steps employing a CFL-like condition (in the physical space), *i.e.* you can predict a mesh from the previous time step

## The spatial-TE algorithm

- From the coarsest level to the finest
- Same truncation criterion of Harten
- Generalized time advancing strategy efficient in the combined physical/stochastic space. **Discontinuities in the responses could arise from the physical space, bifurcation in stochastic space or discontinuous (variation) of the pdf**

# Classical Multiresolution framework

*Abgrall and Harten, Multiresolution Representation in Unstructured Meshes, SIAM Journal on Numerical Analysis, 1998*



What we need:

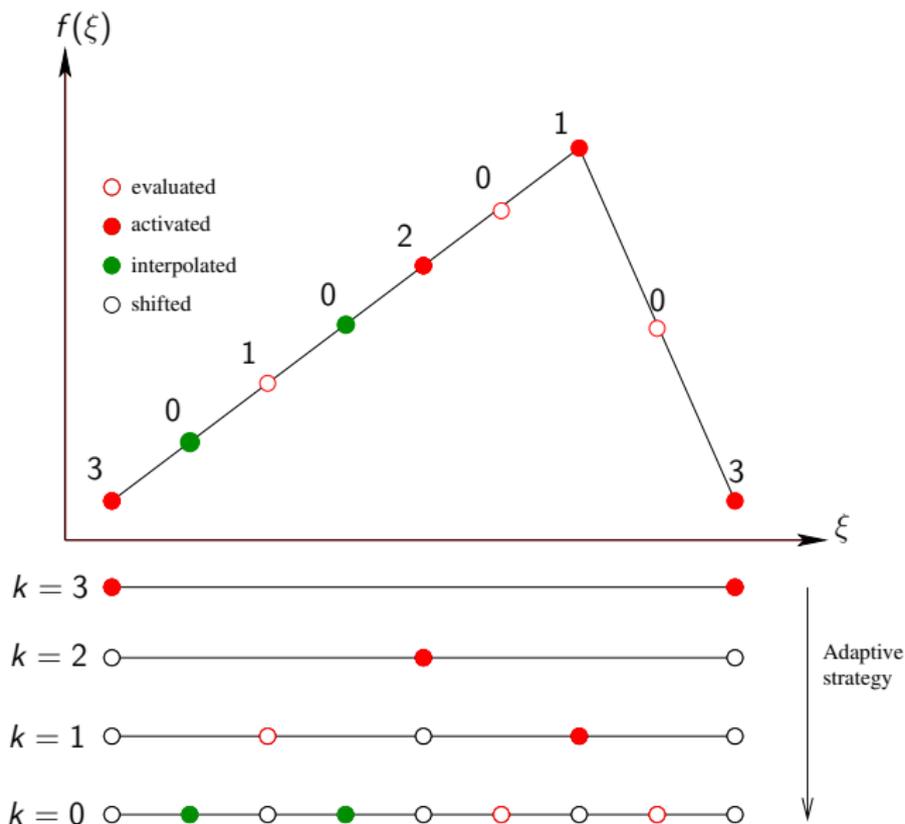
- A set of nested grid
- An interpolation operator
- A well resolved solution on the mesh
- A threshold  $\varepsilon$

↓

$$\|u^0 - \hat{u}^0\| \leq C\varepsilon,$$

# TE strategy

A constructive example

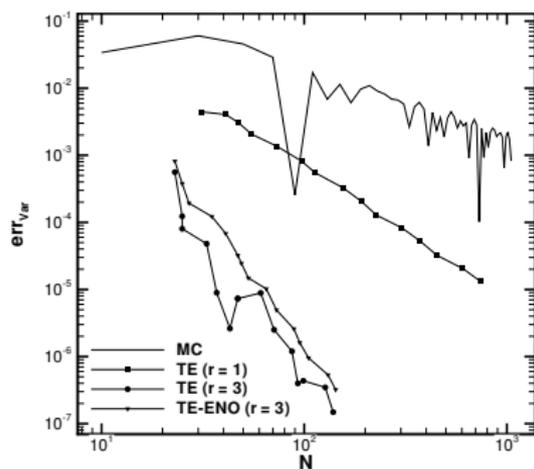


# Numerical results

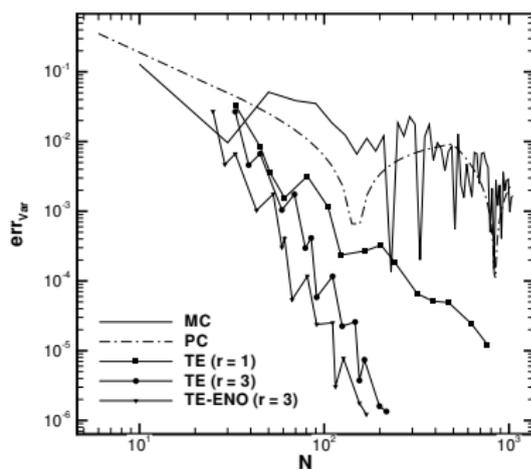
A steady (analytical) function

$$f_1 = f_1(\xi) = \sin(2\xi^2\pi)$$

$$f_2 = \begin{cases} \sin(2\xi^2\pi) & \text{if } \xi \leq 11/20 \\ \sin(2\xi^2\pi) + 1 & \text{otherwise.} \end{cases}$$



(c)



(d)

Figure: Relative error on the variance:  $f_1$  (c) and  $f_2$  (d)

# Kraichnan-Orszag model

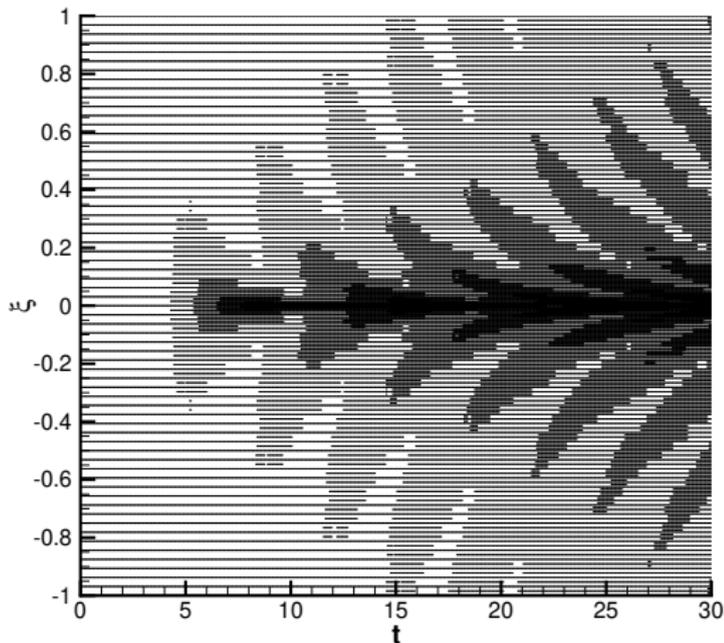
Actually a stiff problem in UQ

$$\begin{cases} \frac{dy_1}{dt} = y_1 y_3 \\ \frac{dy_2}{dt} = -y_2 y_3 \\ \frac{dy_3}{dt} = -y_1^2 + y_2^2 \end{cases}$$

$$\mathbf{y}(t=0) = (1, 0.1\xi, 0)$$

$$\xi = 2\omega - 1 \quad \text{with } \mathcal{U}(0, 1)$$

Numerical solution: RK4 with  
 $\Delta t = 0.05$  (600 time steps)

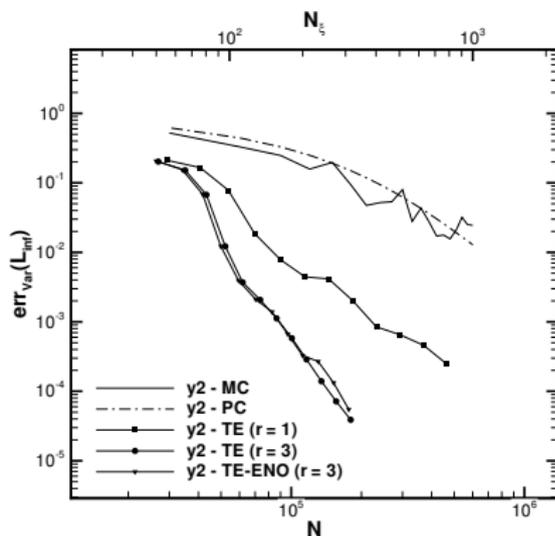
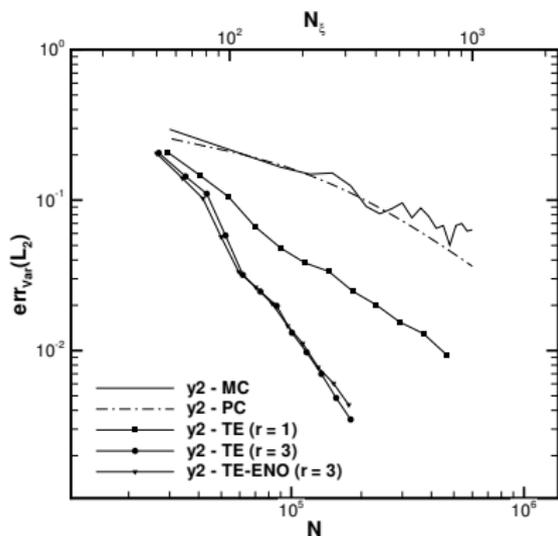


The classical intrusive PC fails to converge after  $t = 8$

# Numerical results

A non-linear vectorial ODE system: Kraichnan-Orszag

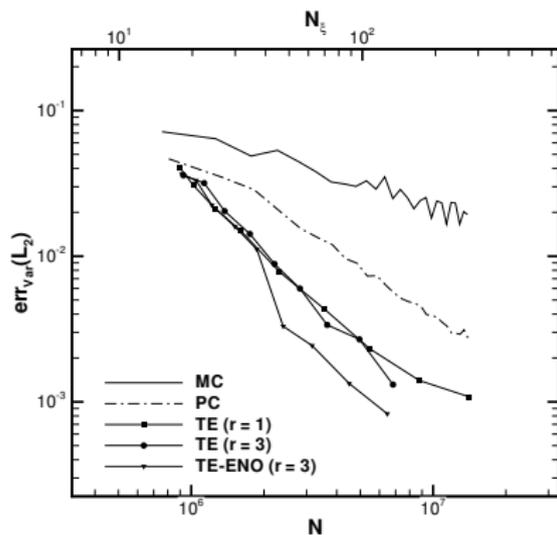
$$\left\{ \begin{array}{l} \text{err}_{\mu^m}|_{L_p} = \|\mu^m(t) - \mu_{\text{ref}}^m(t)\|_{L_p} = \left( \frac{1}{N_t} \sum_{i=1}^{N_t} \left| \frac{\mu_i^m(t) - \mu_{\text{ref},i}^m(t)}{\mu_{\text{ref},i}^m(t)} \right|^p \right)^{1/p} \\ \text{err}_{\mu^m}|_{L_\infty} = \|\mu^m(t) - \mu_{\text{ref}}^m(t)\|_{L_\infty} = \max_i \left| \frac{\mu_i^m(t) - \mu_{\text{ref},i}^m(t)}{\mu_{\text{ref},i}^m(t)} \right|, \end{array} \right.$$



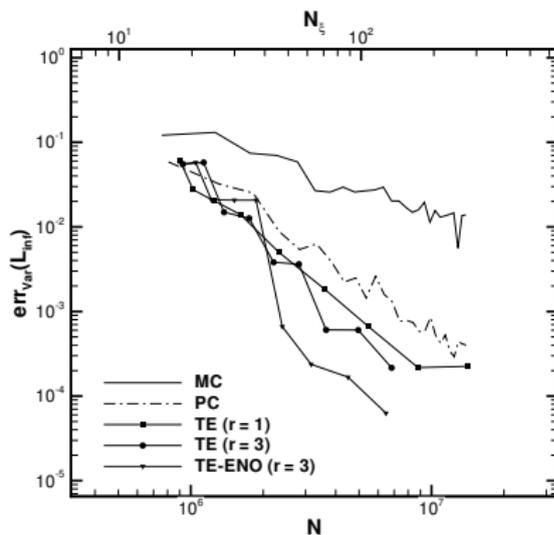
# Numerical results

A non-linear PDE case: the inviscid Burgers equation (Uncertain IC)

$$\begin{cases} \frac{\partial u(x, t, \xi)}{\partial t} + \frac{\partial f(u(x, t, \xi))}{\partial x} = 0 \\ u(x, 0, \xi) = u_0(x, \xi) = \sin(x\pi\xi) \end{cases}$$



(c)



(d)

## Conclusions

- Generalized framework for UQ
- Easy implementation starting from existing deterministic codes
- Good accuracy compared to classical techniques (MC and PC)

## Work in progress

- Extension to two and three dimensional stochastic spaces
- Application to multidimensional physical codes
- Point-value and Cell-averages comparison (in a real battle)

## Staff

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## Main activities

- Efficient and Flexible numerical methods for UQ
  - Semi-intrusive approach for unsteady discontinuous functions
  - Computation and decomposition of High-Order statistics
  - Bayesian methods (inverse problem, model calibration, ...)

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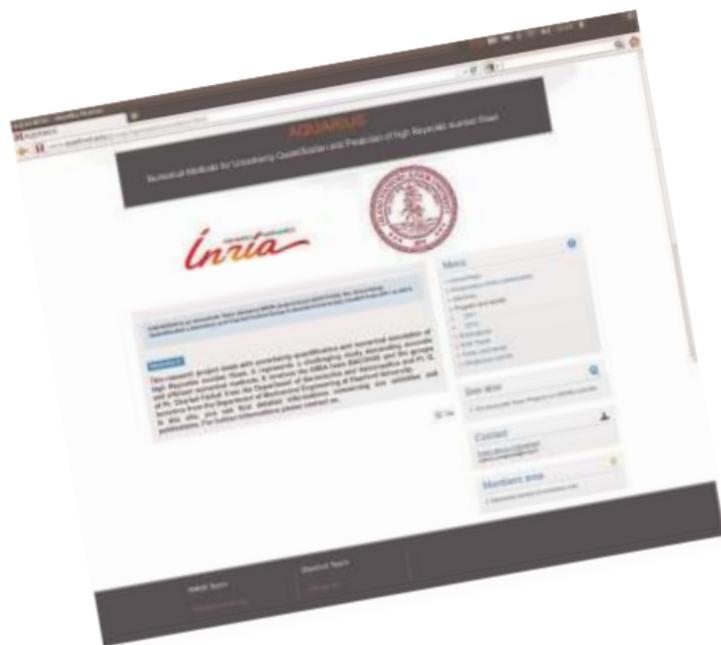
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  - Computation and decomposition of High-Order statistics
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- Methods for robust design optimization
  - Efficient strategy using response surface and stochastic dimension reduction
  - Simplex<sup>2</sup> Method
  - HR-Simplex

## Staff

- BACCHUS Team, INRIA Bordeaux Sud-Ouest, Leader: **R. Abgrall**
- AQUARIUS Team, Joint Team with UQ Lab (Stanford University)  
Leaders: **P.M. Congedo**, **G. Iaccarino**

## Main activities

- Efficient and Flexible numerical methods for UQ
  - Semi-intrusive approach for unsteady discontinuous functions
  - Computation and decomposition of High-Order statistics
  - Bayesian methods (inverse problem, model calibration, ...)
- Methods for robust design optimization
  - Efficient strategy using response surface and stochastic dimension reduction
  - Simplex<sup>2</sup> Method
  - HR-Simplex
- Application in Fluid Mechanics (Real-gas flows, Tsunami, Multiphase flows)



<http://www.stanford.edu/group/uq/aquarius/index3.html>