Quantification des incertitudes en mécanique des fluides

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BACCHUS Team - INRIA Bordeaux Sud-Ouest
Associated Team AQUARIUS - Joint Team from INRIA and Stanford University

1er Février

TELECOM - ParisTech

Première rencontre GAMNI-MAIRCI: Précision et incertitudes

Team Presentation

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 and optimization
- Application in Fluid Mechanics (thermodynamics, turbulence ...)

Collaborations

- Europe: TU Delft, Arts et Métiers ParisTech, LEGI INP-Grenoble, Politecnico di Milano, CEA-Saclay, Università di Trieste, VKI, Uppsala University
- USA: Stanford University, PNNL

Projects

EU ERC Advanced Grant ADDECCO, ANR UFO, 3 submitted projects on UQ

Summary

Why uncertainty quantification ?

- Global Perspective
- Epistemic vs Aleatory uncertainties

About some classical methods

- State of the Art
- Polynomial Chaos based methods
- Specific problems in CFD

Impact on Fluid Mechanics

- Turbulence
- Thermodynamics

Innovative approach for unsteady shocked flow

- Multi-resolution finite-volume based approach

Interaction experiments/numerics

- How to set-up the first experiment on a rarefaction shock tube

Why uncertainty quantification ?

Objectives

- Improve the **Prediction** of numerical simulation
- Quality of numerical simulations → Verification and Validation (V&V)
- Use of numerical code as a reliable tool to address an **experiment**

V&V

- **Verification**: are we solving the equations correctly ?
  → Numerical analysis and tests
- **Validation**: are we solving the correct equations ?
  → Comparisons of the numerical predictions to reality
- Importance of Uncertainty Quantification
  → Estimate the **error bars** associated to given predictions
  → Evaluate the **likelihood** of a certain outcome

Some definitions

Errors vs. uncertainties

- **Errors**: associated to the translation of a mathematical formulation into a numerical algorithm
  $\rightarrow$ Round-off errors and limited convergence of certain iterative algorithms
  $\rightarrow$ 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 $\rightarrow$ **can not be reduced**
  $\rightarrow$ characterized using probabilistic approaches
  $\rightarrow$ Ex: determination of material properties or operating conditions
- **Epistemic**: potential deficiency due to a lack of knowledge
  $\rightarrow$ It can arise from assumptions introduced in the derivation of the mathematical model or from simplifications
  $\rightarrow$ **can be reduced** (for example by improving the measures)

Predictions under uncertainty

Workflow in a Deterministic simulations

- **Characterize** Geometry, initial/operating conditions, physical processes
- Formulation of a **mathematical** representation
  $\rightarrow$ Governing **equations**, **models** to capture the relevant **physical** processes
- Simplifications with respect to the real system
- Formulate a **discretized** representation
- Grid generation, **numerical methods**, **simulation** and output analysis

Introduction of UQ in numerical simulations: 3 Steps

- **Data assimilation**: ex. boundary conditions inferred from experiments
  $\rightarrow$ define random variables with a specified probability distribution functions (PDF)
- **Uncertainty propagation**: compute the PDFs of the output quantities of interest
- **Post-Processing analysis**: reliability assessments, validation metrics

The mathematical setting of the problem

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

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

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

Probability framework (on the probability space $(\Omega, \mathcal{F}, P)$):
realizations $\boldsymbol{\omega} = \{\omega_1, \ldots, \omega_d\} \in \Omega \subset \mathbb{R}$ with Ω set of outcomes, $\mathcal{F} \subset 2^\Omega$ is the σ-algebra of events, $P : \mathcal{F} \to [0, 1]$ 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** $\mu_{\mathrm{u}_i}(\mathbf{y})$ given by

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

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)

- Sampling techniques (Monte Carlo, Latin Hypercube)
- Stochastic collocation (Lagrangian interpolation)
- Probabilistic collocation (Chaos version of Lagrangian interpolation)
- (generalized-) Polynomial Chaos (gPC)

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

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

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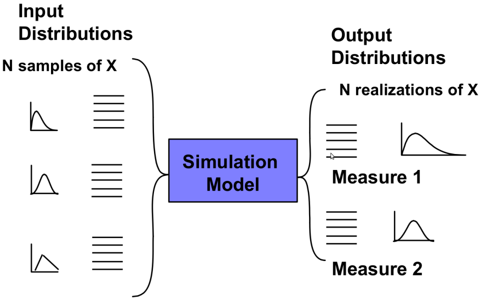
How compute this integral in an efficient way ?

First Possibility : Sampling Methods

- **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*.



Second Possibility : Quadrature Methods

Motivation

- Evaluation of **integrals** needed
  $\rightarrow$ *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
  $\rightarrow$ *Natural extension* to multiple dimensions as tensor product of 1D interpolants
  $\rightarrow$ **Curse of Dimensionality** for high dimensions, Smolyak Algorithm

- Quantities expressed as series of orthogonal polynomials on the space of random input variable

$$u(\boldsymbol{\xi}) = \sum_{k=0}^{\infty} \beta_k \Psi_k(\boldsymbol{\xi}) \tag{5}$$

  Ψ_i form an Hilbert basis of $L_2(\boldsymbol{\xi}, p(\boldsymbol{\xi}))$ in the space of the second-order random variable spanned by $\boldsymbol{\xi}$, $u(\boldsymbol{\xi}) \in L_2(\boldsymbol{\xi}, p(\boldsymbol{\xi}))$

- It is a second order random field

$$||u(\boldsymbol{\xi})||^2 = \int_{\Omega^d} u(\boldsymbol{\xi})^2 p(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} < \infty. \tag{6}$$

- The knowledge of the β_k allows to fully characterize output random variable
- Each polynomial $\Psi(\boldsymbol{\xi})$ of total degree n_o is a multivariate polynomial involving tensorization of 1D ones by a multi index m_i:

$$\Psi(\boldsymbol{\xi}) = \prod_{i=1}^{n_o} \psi_{m_i}(\xi_i). \tag{7}$$

Spectral Methods

Truncation

- In practical problems the infinite expansion has to be truncated:

$$u(\boldsymbol{\xi}) = \tilde{u}(\boldsymbol{\xi}) + \mathcal{O}_T = \sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi}) + \mathcal{O}_T, \tag{8}$$

  where $\mathcal{O}_T$ is a truncation error.
- The truncated expansion **converges** in the mean square sense as N and the polynomial order $p \to \infty$.

Generalized Polynomial Chaos

- **Optimal polynomial** expansion are built using the measure corresponding to the probability law of the random variable
- *Natural extension* to the case where random variables have different measures

	Distribution ξ	Polynomials $\psi_k(\xi)$	Support
Continuous RV	Gaussian	Hermite	$(-\infty, \infty)$
	γ	Laguerre	$[0, \infty)$
	β	Jacobi	$[a, b]$
	Uniform	Legendre	$[a, b]$
Discrete RV	Poisson	Charlier	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk	$\{0, 1, 2, \dots, n\}$
	Negative binomial	Meixner	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn	$\{0, 1, 2, \dots, n\}$

Intrusive Methods → Method of Weighted Residual

- **Define** uncertainties in the numerical problem

$$\mathcal{L}(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}); u(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}))) = \mathcal{S}(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega})), \tag{9}$$

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

- **Spectral expansion** and injection in the operator

$$\mathcal{L}\left(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}); \sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi})\right) = \mathcal{S}(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega})), \tag{10}$$

- **Projection** on the orthogonal polynomials. Obtention of a linear system to solve

$$\left\langle \mathcal{L}\left(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}); \sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi})\right), \Psi_i(\boldsymbol{\xi}) \right\rangle = \langle \mathcal{S}, \Psi_i(\boldsymbol{\xi}) \rangle \quad i = 0, 1, \ldots P \tag{11}$$

PC coefficients are coupled
Deterministic solver has to be modified

Spectral Methods: Resolution, computation of β_k

Non-intrusive Methods, Collocation Method

- **Define** uncertainties in the numerical problem

$$\mathcal{L}(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}); u(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}))) = \mathcal{S}(\boldsymbol{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega})), \tag{12}$$

  where $\mathcal{L}$ (algebraic or differential operator) and $\mathcal{S}$ are on $D \times T \times \Xi$, $\boldsymbol{x} \in D \subset \mathbb{R}^{n_d}$, with $n_d \in \{1, 2, 3\}$, $\boldsymbol{\xi}(\boldsymbol{\omega}) = \{\xi_1(\omega_1), \ldots, \xi_d(\omega_d)\} \in \Xi$ with $\Xi \subset \mathbb{R}^d$
- Coefficients obtained by **projection** on polynomial basis, *i.e.* taking inner product of output PC expansion with Ψ_k, making use of basis orthogonality

$$\beta_k = \frac{\langle u(\boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi})\rangle}{\langle \Psi_k(\boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi})\rangle}, \quad \forall k. \tag{13}$$

- The statistical moments of interest are the expected value and the variance

$$\mu(u) \approx \mu(\tilde{u}) = \beta_0, \qquad \sigma^2(u) \approx \sigma^2(\tilde{u}) = \sum_{k=1}^{P} \beta_k^2 \langle \Psi_k^2(\boldsymbol{\xi})\rangle. \tag{14}$$

- **Sensitivity analysis** based on the analysis of variance decomposition (ANOVA)

Series of deterministic computations
Deterministic solver has not to be modified (Black box)

Properties of classical methods in UQ

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

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Impact on Fluid Mechanics

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- **Thermodynamics**

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Study concerning the Model uncertainties in Thermodynamics[1]

Context: Complex compressible flows in aerodynamics

- Choice of the appropriate **thermodynamic** model (*i.e.* $p = p(\rho, T)$) $\rightarrow$ tradeoff level of **complexity/accuracy**
- For a given level $\rightarrow$ Multiple **parameter** constitutive models, different mathematical forms
- Model structure chosen by **expert judgement** $\rightarrow$ model-form uncertainty
- Model constants (**calibrated** from experimental data) not univocally determined $\rightarrow$ mixed **aleatory/epistemic** uncertainty

Thermodynamic models of increasing complexity

Soave-Redilich-Kwong

$$p_r = \frac{T_r/Z_c}{v_r - b_r} - \frac{a_r/T_r^{0.5}}{v_r(v_r + b_r)}$$

Peng-Robinson

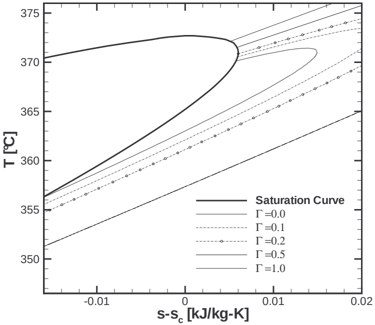
$$p_r = \frac{T_r/Z_c}{v_r - b_r} - \frac{a_r}{v_r^2 + 2b_r v_r - b_r^2}$$

Martin-Hou

$$p = \frac{RT}{v - b} + \sum_{i=2}^{5} \frac{f_i(T)}{(v - b)^i}$$

[1] *P. Cinnella, **P.M. Congedo**, V. Pediroda, L. Parussini, Sensitivity analysis of dense gas flow simulations to thermodynamic uncertainties, Physics of Fluids 23, 116101 (2011)*

Why the Need for an accurate TD model ?



Fundamental Derivative of Gas-Dynamics, Γ

- **Ideal** Gas $\rightarrow \Gamma = \frac{(\gamma+1)}{2} > 1$
- **Dense** Gas $\rightarrow \Gamma = 1 + \frac{\rho}{a}\left(\frac{\partial a}{\partial \rho}\right)_s$
- BZT fluids
  $\Gamma < 0 \rightarrow$ compression shock prohibited by 2nd law
- For Γ, **highly accurate** description of the fluid thermodynamics
- Accurate enough data only available for *simple* fluids of current use
- A few, **highly uncertain**, input data available for **BZT** fluids

Influence of TD model in Dense gas flow simulations

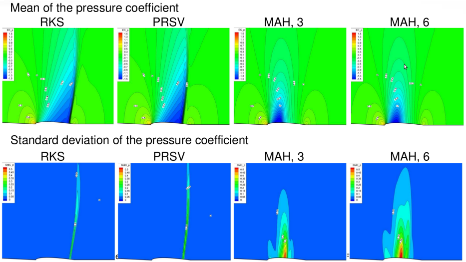
- Fluorocarbon PP10 by using three thermodynamic models
  → **Soave-Redilich-Kwong** (RKS, cubic EOS)
  → **Peng-Robinson-Stryjeck-Vera** (PRSV, cubic EOS)
  → **Martin-Hou** (MAH, 5th-order virial) + power law for ideal-gas heat capacity
- Dense gas flows over a NACA0012 airfoil with $M\infty$=0.95, aoa=0, inviscid flow
- Experimental uncertainties estimated in 3%
- Gaussian distributed input uncertainties (also checked with uniform)
- Third-order Hermite polynomials (good convergence)

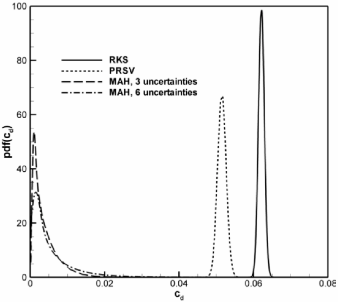
Property	p_c	T_c	Z_c	T_e
	16.2 atm	630.2 K	0.2859	467 K
Property	n	$C_{v,\infty}(T_c)\,/\,R$	ω	
	0.5255	78.37	0.4833	

Study concerning the Model uncertainties

Influence of TD model in Dense gas flow simulations

- For **simpler** models (RKS, PRSV), mean solutions very close to the deterministic ones
- For **complex** model (MAH), greater sensitivity to uncertainties
- RKS, PRSV: std(Cd) about 12% and 22% E(Cd), $E(Cd) \sim Cd_{det}$
- MAH model: std(Cd) about 100% or more then E(Cd) $\rightarrow$ **low reliability**





Model-form uncertainty overwhelms epistemic parametric uncertainty

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UQ analysis and interaction with an experiment[2]

Problem

- **Experimental** campaign to prove the existence of **non-classical** gasdynamics effects in a shock tube (FAST, being commissioned at Delft)

→ occurring in dense gas flows

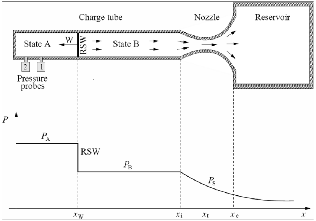


Figure: Rarefaction shock wave (RSW)

- Need for a numerical approach taking into account the source of uncertainties to ensure a **RELIABLE** shock tube experiment design
- 2 sources of uncertainties, both in the thermodynamic (TD) model and initial conditions (IC)

⇓

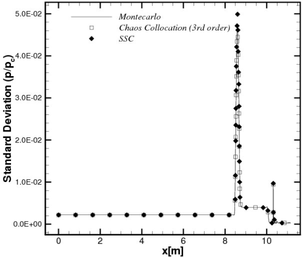
OBJECTIVE

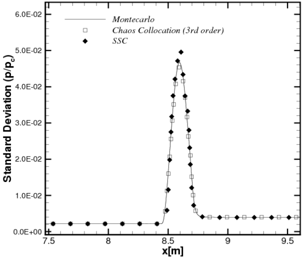
Robust conditions ensuring a RSW in the shock tube

[2] ***P.M. Congedo*** *et al., Backward uncertainty propagation method in flow problems: Application to the prediction of rarefaction shock waves, CMAME 213-216 (2012) 314-326*

Statistics validation

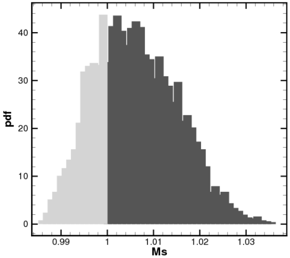
- **Comparison** between Montecarlo (MC), PC and Simplex Stochastic Collocation (SC), (unc. on TD and on IC, 8 overall)
- **Stochastic Analysis** on Rarefaction Shock Wave (RSW) properties
- Results for MC and PC very similar (difference on σ of 1.6%), no remarkable differences during time evolution, huge difference in the computational cost (3000 for MC, 256 for PC), SSC promising reduction of computational cost (35)

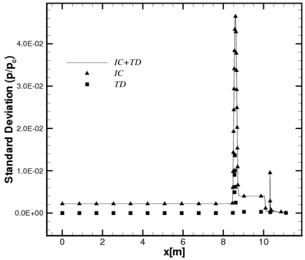


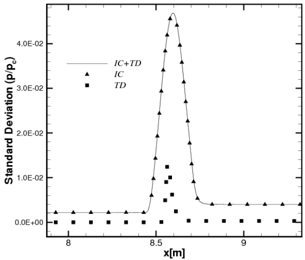


Forward propagation problem

- **Stronger** influence of uncertainty on IC with respect to uncertainty on TD
- No variations with respect to **time**
- In order to ensure the **occurrence** of a rarefaction shock wave, M_s should always be greater then 1







Probability that $M_s < 1$ is 27.8%

$\rightarrow$ Necessity for inverse analysis

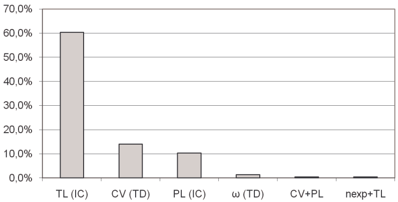
UQ analysis and interaction with an experiment (4)

Backward propagation problem

- To prove the rarefaction shock, Mach greater than 1
- Initial conditions can not be improved
- Necessity for **inverse** analysis, i.e. find the maximum **allowable** uncertainty levels on IC/TD

Procedure for inverse analysis

- **ANOVA** analysis on Montecarlo simulations most influent parameters to consider
- Find the **optimal** uncertainty bars by using PC for uncertainty estimation
- **Check** the optimal solution by means of Montecarlo

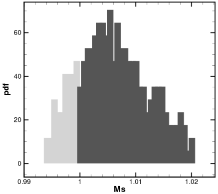


- T_L, P_L, C_V contribute for 92% to the variance, then 4 parameters considered for the inverse analysis
- Find **uncertainty bars** in order to minimize $|\mu - \sigma - 1|$
- Find uncertainty bars in order to **minimize** $|\mu - 2\sigma - 1|$

UQ analysis and interaction with an experiment (5)

First analysis, $\mu - \sigma > 1$

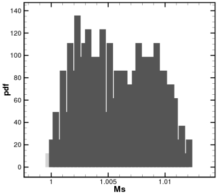
- Considering just error bar on TL (most important for ANOVA)
- For T_L of 0.04%, $\mu - \sigma$ is always more than 1 (**too** restrictive)
- By reducing uncertainty on C_v (lack of knowledge), bar errors on T_L could be **increased**
- With 1% on C_v and 0.06% on T_L, solution is robust (more **realistic** initial condition)



Probability that $M_s < 1$ is 19.1%

Second analysis, $\mu - 2\sigma > 1$

- Bar errors reduced for T_L, C_v, and P_L
- Robustness obtained for T_L 0.035%, P_L 0.1% and C_v 0.5%



- Probability that $M_s < 1$ is 0.8% instead of 27.8%
- For a very robust solution, it is necessary to reduce both sources (IC+TD) of unc.
- Important **indications** given to perform the **experience**

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Motivation for another intrusive approach[3]

gPC vs SI

Issues for classical intrusive UQ schemes (**gPC**):

1. Every problem need a specific effort (both in theoretical formulation and computational implementation)
2. The number of equation is not preserved with a stochastic representation
3. There is an intrinsic limit in the treatment of discontinuous response (adaptive techniques are demanded)

MR-SI method properties:

1. The framework is general, the implementation is easy
2. The dimensionality is in the integrals **BUT** not in the equations
3. Discontinuous responses are treated in a natural way in the framework of FV schemes

[3] *R. Abgrall et al., An adaptive scheme for solving the stochastic differential equations, MASCOT11-IMACS/ISGG Workshop, 2011*

Euler system: $\dfrac{\partial \mathbf{u}}{\partial t} + \dfrac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0$, $\mathbf{u} = \begin{Bmatrix} \rho \\ \rho u \\ e^{tot} \end{Bmatrix}$ and $\mathbf{f}(\mathbf{u}) = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ (e^{tot} + p)u \end{Bmatrix}$

Deterministic scheme ($\mathbf{u} = \mathbf{u}(x, t, \xi(\omega))$):

$$\mathbf{u}_i^{n+1}(\xi) = \mathbf{u}_i^n(\xi) - \frac{\Delta t}{\Delta x}\Big(\mathbf{F}(\mathbf{u}_{i+1}^n(\xi), \mathbf{u}_i^n(\xi)) - \mathbf{F}(\mathbf{u}_i^n(\xi), \mathbf{u}_{i-1}^n(\xi))\Big)$$

$\mathbf{u}_i^n$ is the cell average at the time t_n and $\mathbf{F}$ a numerical flux (e.g. Roe flux)

Stochastic scheme:

$$\mathbf{u}_{i,j}^{n+1} = \mathbf{u}_{i,j}^n - \frac{\Delta x}{\Delta t}\Big(\mathcal{E}(\mathbf{F}(\mathbf{u}_{i+1}^n(\xi), \mathbf{u}_i^n(\xi))|\Xi_j) - \mathcal{E}(\mathbf{F}(\mathbf{u}_i^n(\xi), \mathbf{u}_{i-1}^n(\xi))|\Xi_j)\Big)$$

$\mathbf{u}_{i,j}^n$ is the conditional expectancy of $\mathbf{u}_i$ at the time t_n

Formal analogy between physical and probabilistic space averages:

$$\mathbf{u}_i^n = \frac{1}{|\mathcal{C}_i|}\int_{\mathcal{C}_i} \mathbf{u}(x, t^n, \xi)\mathrm{d}x \rightarrow \mathbf{u}_{i,j}^n = \mathcal{E}(\mathbf{u}_i^n | \Xi_j) = \frac{1}{\mu(\Xi_j)}\int_{\Xi_j} \mathbf{u}_i^n(\xi)\mathrm{d}\mu(\xi)$$

$$\text{with} \quad \mathrm{d}\mu(\xi) = \mathrm{p}(\xi)\mathrm{d}\xi$$

where $P_{i,j}$ is the **piecewise polynomial reconstruction** of the probabilistic solution (First order (constant on every cell), Centered (2nd order), ENO, WENO)

Probabilistic discretization:

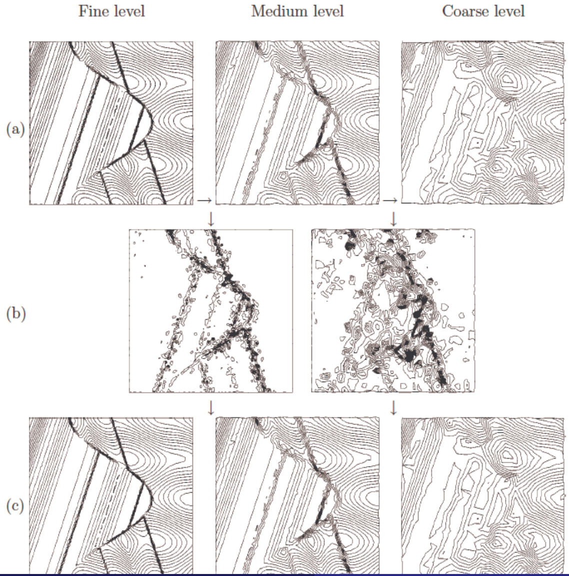
- *Tessellation* - $\Xi_j = [\xi_{j-1/2}, \xi_{j-1/2}]$ with $j = 1, \ldots, N$
- *Disjoint probability* - $\mu(\Xi_i \cap \Xi_j) = 0$
- *Fulfillment of the parameter space* - $\Xi = \bigcup_j \Xi_j$

Problems

- The SI methods suffers of the curse of dimensionality to compute integrals.
- Techniques such as Sparse Grid and/or automatic adaptive refinement algorithm for the probabilistic space are expected to reduce dramatically the overall cost $\rightarrow$ **Multiresolution framework**

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 th mesh
- A threshold ε

$$\Downarrow$$

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

Harten[4] showed that the solution of an Initial Value Problems can be expressed as a numerical schemes on the wavelets, *i.e.* interpolations errors.

We employ this framework in our SI probabilistic scheme to tackle the *curse of dimensionality*

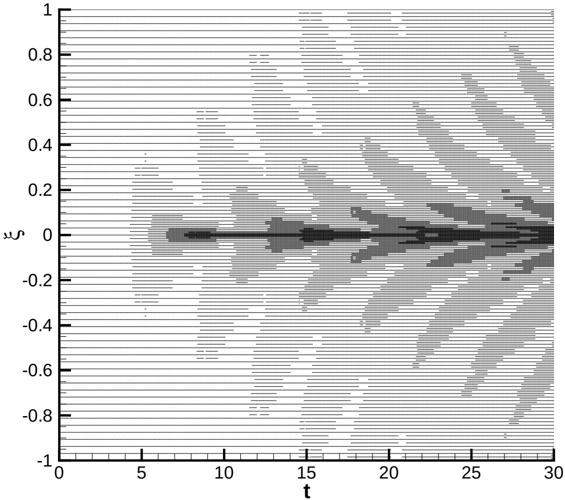
We are moving in these directions:

- An adaptive refinement in stochastical space
- A refinement/derefinement techniques by an accuracy preserving combination of interpolation/evaluation

[4] *Multiresolution algorithms for the numerical solution of hyperbolic conservation laws, Communications on Pure and Applied Mathematics, 1995*

$$
\begin{cases}
\dfrac{\mathrm{d}y_1}{\mathrm{d}t} = y_1 y_3 \\[2ex]
\dfrac{\mathrm{d}y_2}{\mathrm{d}t} = -y_2 y_3 \\[2ex]
\dfrac{\mathrm{d}y_3}{\mathrm{d}t} = -y_1^2 + y_2^2 \\[2ex]
\mathbf{y}(t=0) = (1, 0.1\xi, 0) \\
\xi = 2\omega - 1 \quad \text{with} \quad \mathcal{U}(0,1)
\end{cases}
$$

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



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

Kraichnan-Orszag model

(Some) Numerical results ($\varepsilon = 10^{-1}$, $m_L = 5$, $\Delta t = 0.05$)

Reference solution: MC with 20×10^6 points for each time step

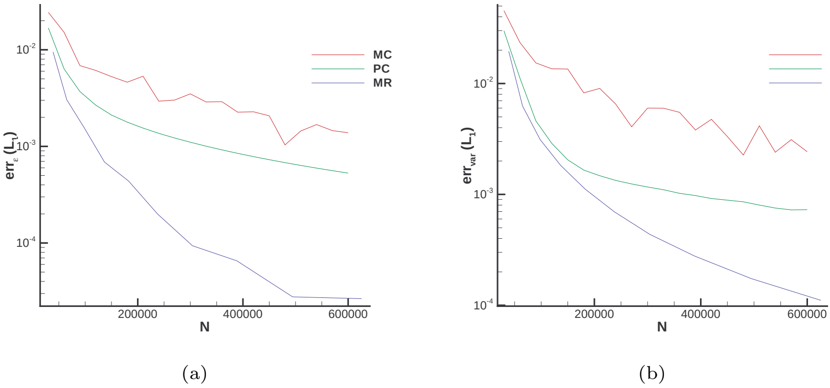


Figure: L_1 norm of the errors for the mean (a) and variance (b) for the Kraichnan-Orszag problem (y_1).

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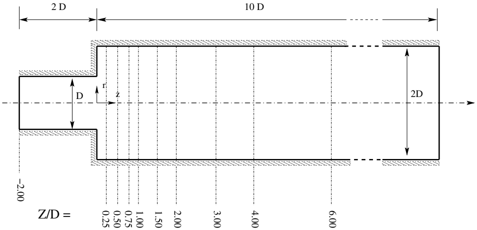
Merci pour votre attention

Experimental configuration[5]

Dellenback *et al.* AIAA J, 1987

- Turbulent flow in a pipe with an axisymmetric expansion
- Why this case : Displays recirculating flow regions and high turbulence levels
- Fluid is flowing from left to right entering the pipe with or without swirl
- Measurements by means of several probe locations downstream the expansion



[5] *P.M. Congedo et al., Numerical prediction of turbulent flows using RANS and LES with uncertain inflow conditions, under revision in IJNMF, 2012*

Flow modelling

- Incompressible flow configuration depending on Reynolds number Re and swirl number S_w at the inlet flow, that is the ratio between angular momentum flux and axial momentum flux

$$S_w = \frac{1}{R} \frac{\int_0^R r^2 \langle u_z \rangle \langle u_\theta \rangle \, dr}{\int_0^R r \langle u_z \rangle^2 \, dr} \tag{15}$$

- Two experiments performed for $Re = 30000$: a no-swirl configuration ($S_w = 0$) and a strong swirl configuration ($S_w = 0.6$)
- Navier-Stokes equations expressing mass and momentum conservation

$$\begin{cases} \dfrac{\partial u_i}{\partial x_i} = 0, \\ \\ \dfrac{\partial u_i}{\partial t} + \dfrac{\partial u_i u_j}{\partial x_j} = -\dfrac{1}{\rho} \dfrac{\partial p}{\partial x_i} + \dfrac{\partial}{\partial x_j} \left(\nu \dfrac{\partial u_i}{\partial x_j} \right), \end{cases} \tag{16}$$

For high level turbulent flows, it is not possible to perform direct numerical simulation (DNS) ⇨ RANS, LES

Which sources ?

- Measured distributions reported in literature considered as averaged distributions over a set of experimental realizations
- U_b and S_w stochastic variables described by uniform probability distribution functions (pdf) over the respective intervals
- Choice of a 2.5% variance for both U_b and S_w based on analysis of experimental set up of Dellenback *et al.*
- Inlet turbulence characteristics subject to uncertainty: extent of variation for T_i and L_t estimated from previous calculations on similar configurations

Simulations	$U_b\ (m/s)$	S_w	T_i	L_t
RANS with S_w	0.452 ± 0.0113	0.6 ± 0.015	0.006 to 0.06	$0.1\%R$ to $10\%\ R$
RANS without S_w	0.452 ± 0.0113	/	0.006 to 0.06	$0.1\%R$ to $10\%\ R$
LES with S_w	0.452 ± 0.0113	0.6 ± 0.015	/	/
LES without S_w	0.452 ± 0.0113	/	0.006 to 0.06	/

Coupling CFD and UQ

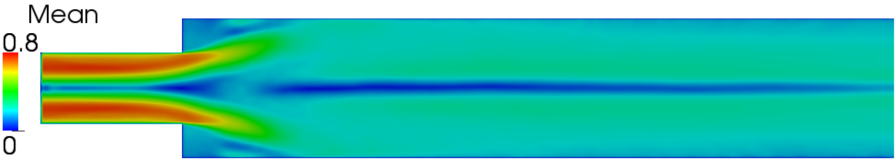
- Non-intrusive stochastic methods $\rightarrow$ Series of deterministic computations $\rightarrow$ Post-processing in order to compute solution statistics
- Grid convergence study on deterministic case allowing to retain a medium grid (1.5 million cells) for all stochastic computations
- Accuracy of the computed statistics for N uncertainties depending on polynomial chaos order p with size of stochastic DOE varying as $(p+1)^N$
- Search for trade-off between the accuracy and the overall computational cost $\rightarrow$ Comparison of maximum variance σ_{max} of time-averaged velocity magnitude and contribution (in %) of each source of uncertainty computed with $p = 2$ and $p = 3$

	σ_{max}	σ_{U_b} (%)	σ_{S_w} (%)	σ_{T_i} (%)	σ_{L_t} (%)
Flow with S_w / PC(2)	0.0146	0.81	0.50	95.9	2.31
Flow with S_w / PC(3)	0.0151	0.82	0.53	96.2	2.15
Flow without S_w / PC(2)	0.000897	9.0	/	39.9	50.7
Flow without S_w / PC(3)	0.000923	8.9	/	39.7	51.1

$\rightarrow$ **Negligible differences between 2nd and 3rd order**

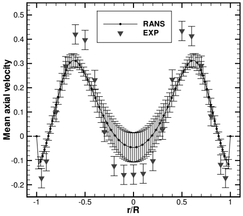
High-swirl configuration

- Computation of the mean time-averaged axial velocity using LES and PC(2) (obtained from 9 deterministic runs)
- Mean flow shows a recirculation zone occurring around the flow centerline downstream of the expansion zone

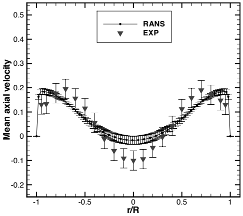


High-swirl configuration, RANS

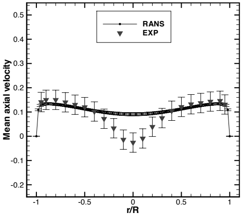
- Mean axial velocity curves systematically far from experimental distributions $\rightarrow$ Turbulent-viscosity assumption leads to inaccurate flow patterns for strong swirling flows
- Computed error bars at section $L/D = 0.75$ in back-flow region close to centerline $r/R = 0$ much larger than 2.5% inlet velocity uncertainty $\rightarrow$ strong sensitivity of the RANS approach
- Computed errors bars reduce rapidly for more downstream sections



(a) L/D=0.75



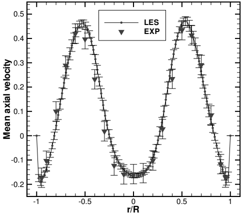
(b) L/D=1.5



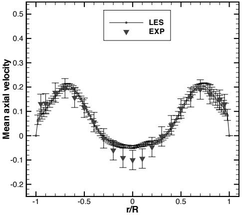
(c) L/D=4.0

High-swirl configuration, LES

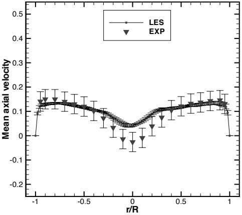
- Mean solution globally in good agreement with the measured distribution
- Numerical error bars similar to or even smaller than experimental error bars in all sections under study



(d) L/D=0.75



(e) L/D=1.5



(f) L/D=4.0

High-swirl configuration, RANS-LES

- Coefficient of variation (standard deviation divided by mean) of the axial time-averaged velocity computed at the flow centerline $r/R = 0$ for successive sections
- RANS coefficient of variation exceeds 100% at sections $L/D = 0.75$ and $L/D = 1.5$ where swirl effects are significant while it goes down to 6.6% at $L/D = 4.0$ further away from inlet
- Sensitivity of computed RANS solution to uncertain inlet conditions reduced in this flow region far from inlet while it is particularly high in first section, closest to inlet boundary where swirl effects are most significant
- LES coefficient of variation does not depart much from prescribed value on inlet conditions and remains in the same range (between 4.75% and 10.2%) along pipe centerline.

L/D	0.75	1.5	4.0
RANS	130.4	106.4	6.6
LES	4.75	10.2	8.0

Conclusions

- Uncertain mean flow properties (bulk velocity and swirl number) as well as uncertain inlet turbulence properties have been considered
- RANS and LES modelling have been analyzed through their mean flow solutions and flow variance
- Systematic comparison with experiment, taking into account both computed error bars and measurement errors
- Contributions of uncertainties to global variance have also been examined
- RANS modeling of the high-swirl case found to strongly amplify the uncertainty on the inlet turbulence intensity, particularly so when computing the axial velocity distributions
- LES approach found to consistently provide numerical results within the measurement error $\rightarrow$ weak sensitivity to the inlet uncertainties