Uncertainty Management and Quantification in Industrial Analysis and Design

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The Role of Uncertainties in VP

- Uncertainty quantification and management has been recognized in the last few years as a major component of Virtual Prototyping and risk management in industrial design

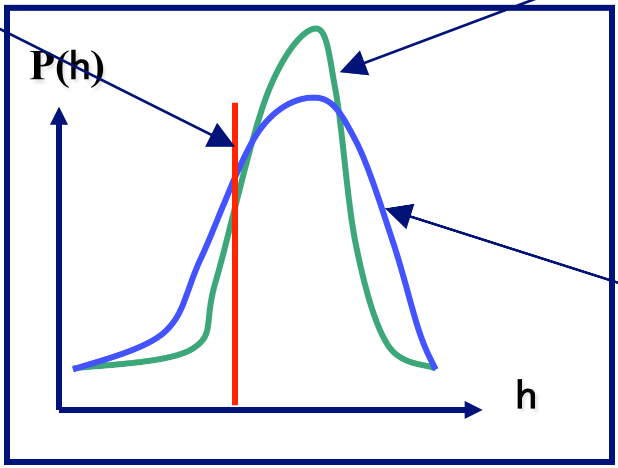
- Introducing the probabilistic nature of the uncertainties in the simulation software systems, is a highly challenging undertaking, as the whole process transforms the resolution of deterministic physical conservation laws, to *non-deterministic methods*, governed by *stochastic* partial differential equations (SPDE)

- As a consequence, predicted quantities, such as loads, lift, drag, efficiencies, temperatures, …., are now represented by a *probability density function* (pdf), providing a domain of confidence, associated to the considered uncertainties, introducing hereby a fundamental shift in paradigm for the whole of the VP methodology.

- What is required to bring this new technology and approach to industrial level?

NON-deterministic simulations

Result of deterministic CFD simulations for mean value of measured uncertainty parameter as input



pdf of non-deterministic CFD simulations for given pdf of uncertainty parameter as input

pdf of deterministic CFD simulations for randomly sampled uncertainty parameter as input

The Global Picture: Risk and Uncertainty Management

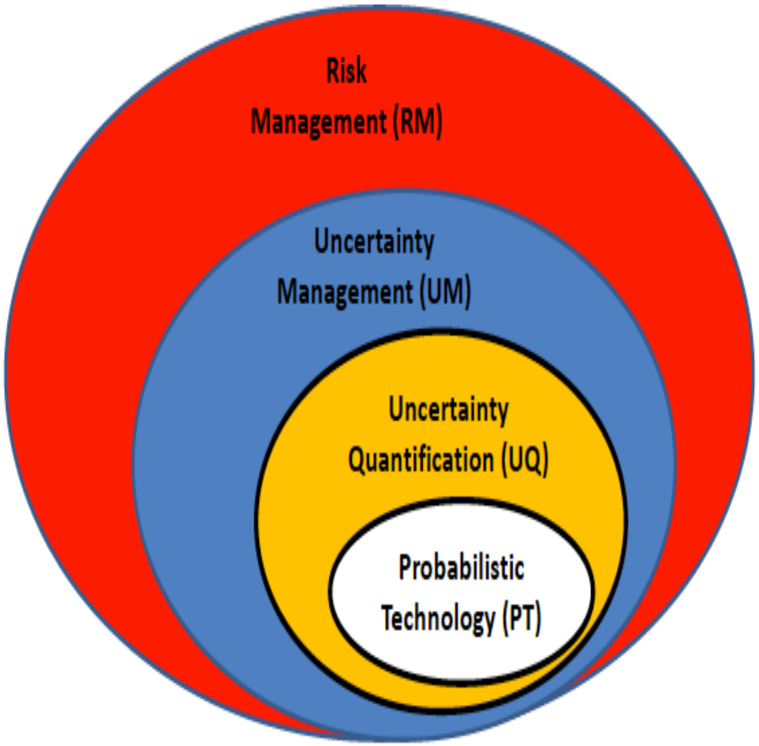
- Risk is considered here as the possibility of not matching the design targets, suffering damage, failure or loss of the system as well as the occurrence of any non-desirable event
- Risk management covers therefore the evaluation of all uncertainties affecting the design, development and operation of the system, including uncertainties on cost and delivery timings

Risk management (RM) has therefore to rely on *Uncertainty Management (UM),* which includes

- *Uncertainty Quantification (UQ) and*
- *Robust design methodologies (RDM) taking into account uncertainties*

Uncertainty Quantification

The area of ***Uncertainty Quantification*** covers the following activities



- **Uncertainty identification:** *Data (e.g., operational uncertainties, geometrical variability); Model (e.g., physical model approximations, grid dependence, convergence)*

- **Uncertainty categorization** *Reducible (Epistemic) or Irreducible (Aleatory)*

- **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*

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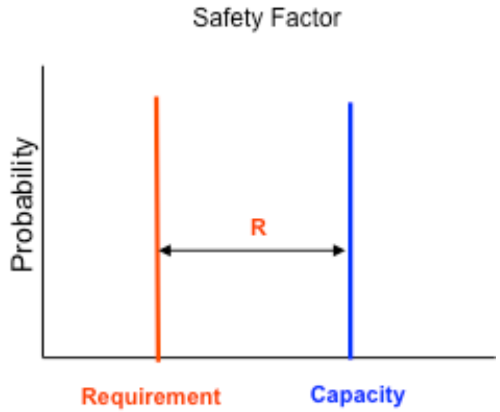
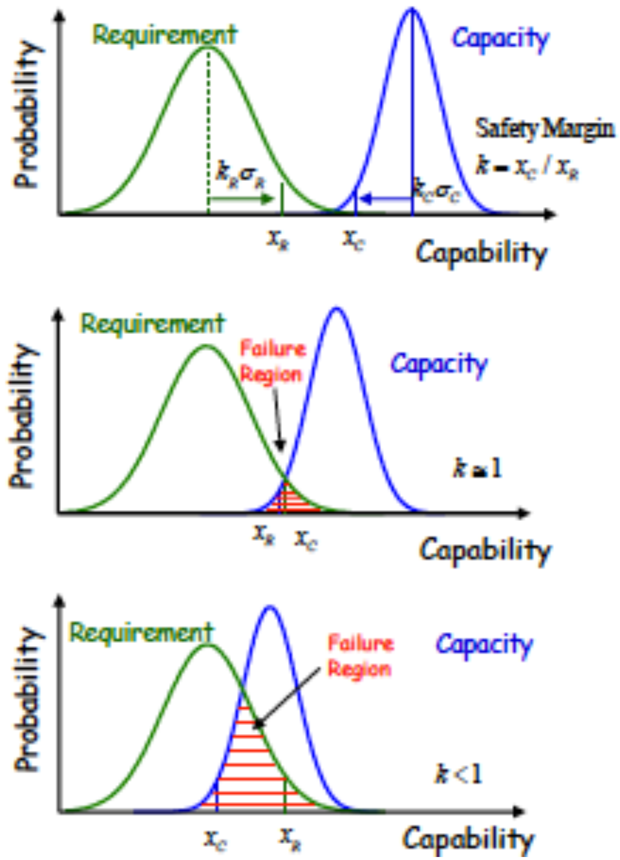
From UM to UQ, from Green et al (2008)

Uncertainty Quantification and Safety Factors

- A traditional approach to risk management is the introduction of safety factors, or safety margins, comparing the resistance of a system (which we can term as its *capacity*), compared to the estimated loads (termed in general as *requirement*).
- In the traditional and still current practice, a deterministic value is estimated for the load x_R and a value is provided, as best as possible, for the maximum capacity $x_{C.}$ On basis of which a *safety margin* $k=x_{R/}x_C$ is imposed on the system.
- On the other hand, taking into account uncertainties and their pdf's, (right figures) allows ranges (under the form of pdf's) for requirements (loads) and capacity (resistance) to be evaluated in a rational way, allowing to define a failure region where the two pdf's overlap. Full safety, taking into account the known uncertainties, is obtained for k>1.
- If k>1, upper right figure, the design is perfectly safe; while when k≅1, a certain risk factor will exist. In case k<1, a large failure region exists, which would lead to a catastrophic design, of course to be rejected.

Safety Factors





Ideal

Troublesome

Hopeless

From: Lawrence L.Green, Lecture on Advanced Uncertainty Analysis, NASA/NIASummer Design Institute on Uncertainty, August 4, 2011

Errors and uncertainties

- In the aerospace community a clear difference between the concepts of *uncertainty* and *error* is made
- In the AIAA G-077-1998 guidelines the
  - uncertainty is "a potential deficiency in any phase or activity of the modeling process that is due to the lack of knowledge",
  - the error is "a recognizable deficiency in any phase or activity of the modeling process that is not due to the lack of knowledge".
- Following Oberkampf et al. (2003) and Trucano et al. (2006), in computational science and engineering the uncertainty has technically two distinct meanings:
  - The first one is the ***aleatory*** uncertainty, known also as *irreducible* uncertainty, associated with the inherent randomness of the modeled physical system and its environment.
  - The second one is the ***epistemic*** uncertainty, called also *reducible* uncertainty, and is caused by the lack of knowledge or information regarding the system and its environment.

Uncertainty Categorization

- ***Epistemic uncertainties*** are globally generated by numerical errors due to discretization approximations and grid dependences, as well as lack of knowledge associated to the imperfect physical models, such as turbulence, combustion or multiphase models

- They are considered as **reducible uncertainties**, since they could be reduced through increased understanding and research, or more relevant physical data, and are globally related to the lack of knowledge about the appropriate value to use for the considered quantity

- The important consequence is that *epistemic uncertainties have a fixed, but poorly known, value in the analysis*. For instance, the elastic modulus for a composite material in a specific component is fixed but its value can be unknown or poorly known; the turbulent viscosity in a CFD simulation is known to be subject to the many approximations attached to turbulence models

Uncertainty Categorization

- On the other hand, ***aleatory uncertainties*** are related to the inherent randomness of the system being analyzed, such as variability of operational conditions, geometrical randomness from the manufacturing process, which cannot be reduced by further data

- *Hence, epistemic uncertainties are a property of the models applied in the analysis, including the choices made by the modeler; while the aleatory uncertainties are a strict property of the system being analyzed*

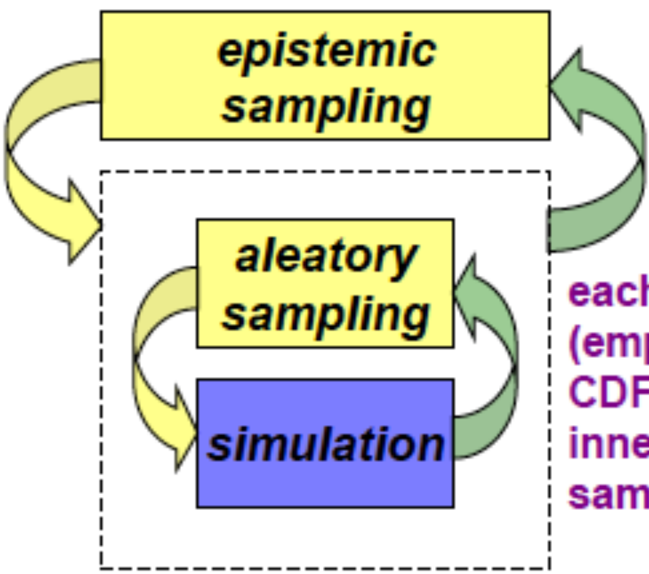
- The methods for handling epistemic uncertainties generally place some type of bounds on the resulting output uncertainty, largely based on (subjective) estimates of error and input uncertainty levels. It is indeed difficult to provide objective estimates of the numerical errors, or of the error associated to the weaknesses of a given turbulence model
  - As an example, since the transonic flow over an aircraft wing, contains many physical effects, such as shock-boundary interactions, separation, tip effects and vortices, the sensitivity of a turbulence model to each of these effects can be widely different, making it a subjective task to assess the associated error margins

Probability Box: Epistemic and aleatory uncertainties

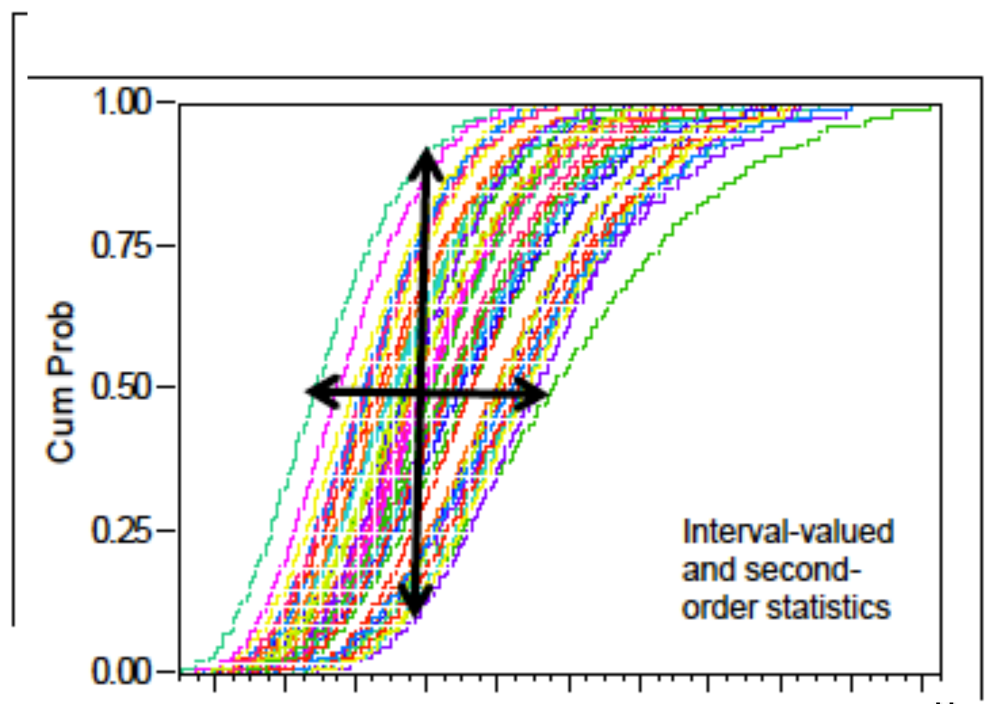
Nested sampling technique which combines epistemic and aleatory uncertainty

- Frequently used in UQ studies and regulatory analyses
- For each outer loop sample of epistemic (interval) variables, run an inner loop UQ study over aleatory (probability) variables

50 outer loop samples
→ 50 CDF traces



each discrete (empirical) CDF: 100 inner loop samples



Identification of uncertainties

This has to rely on the experience and expert knowledge of designers and experimentalists

Identified uncertainties

- Operational conditions: Inlet or exit flow conditions
- Geometrical uncertainties
  - Tip clearance
  - Fabrication tolerances on geometry; Leading edge, TE; blade shapes
  - Blade inlet or outlet angles
  - Roughness
- Modeling uncertainties, such as turbulence models
- Numerical error sources (grid effects, numerical dissipation)

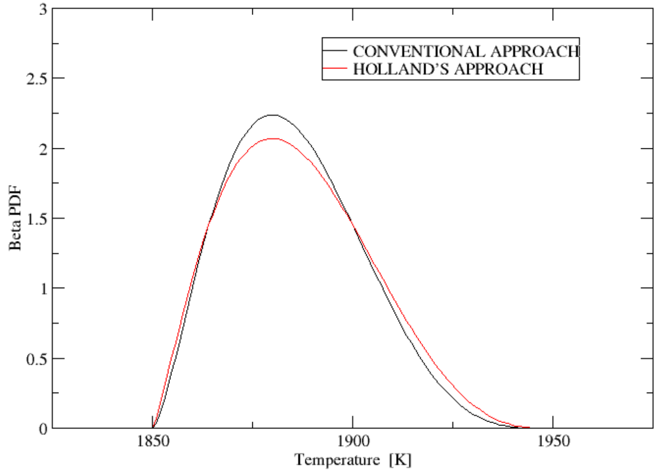
Quantification of uncertainties

A statistical description of the uncertainties is required

- If only max; min and most likely values are known, another utility is available to fit a beta pdf distribution

Example of Beta distribution

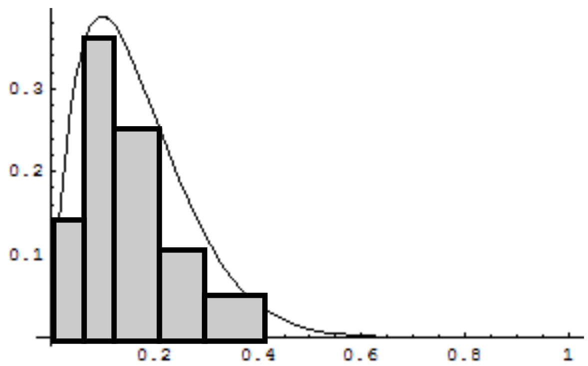
- Gas turbine inlet temperature
  - the most likely temperature: m = 1880 K
  - the minimum temperature: a = 1850 K
  - the maximum temperature: b = 1950 K



Holland's approach	p	q	Mean temperature [K]	Standard deviation [K]
Holland (2002)	2.286	4	1886.4	17.82
Present	2.2857143	4	1886.3636365	17.821

Quantification of uncertainties

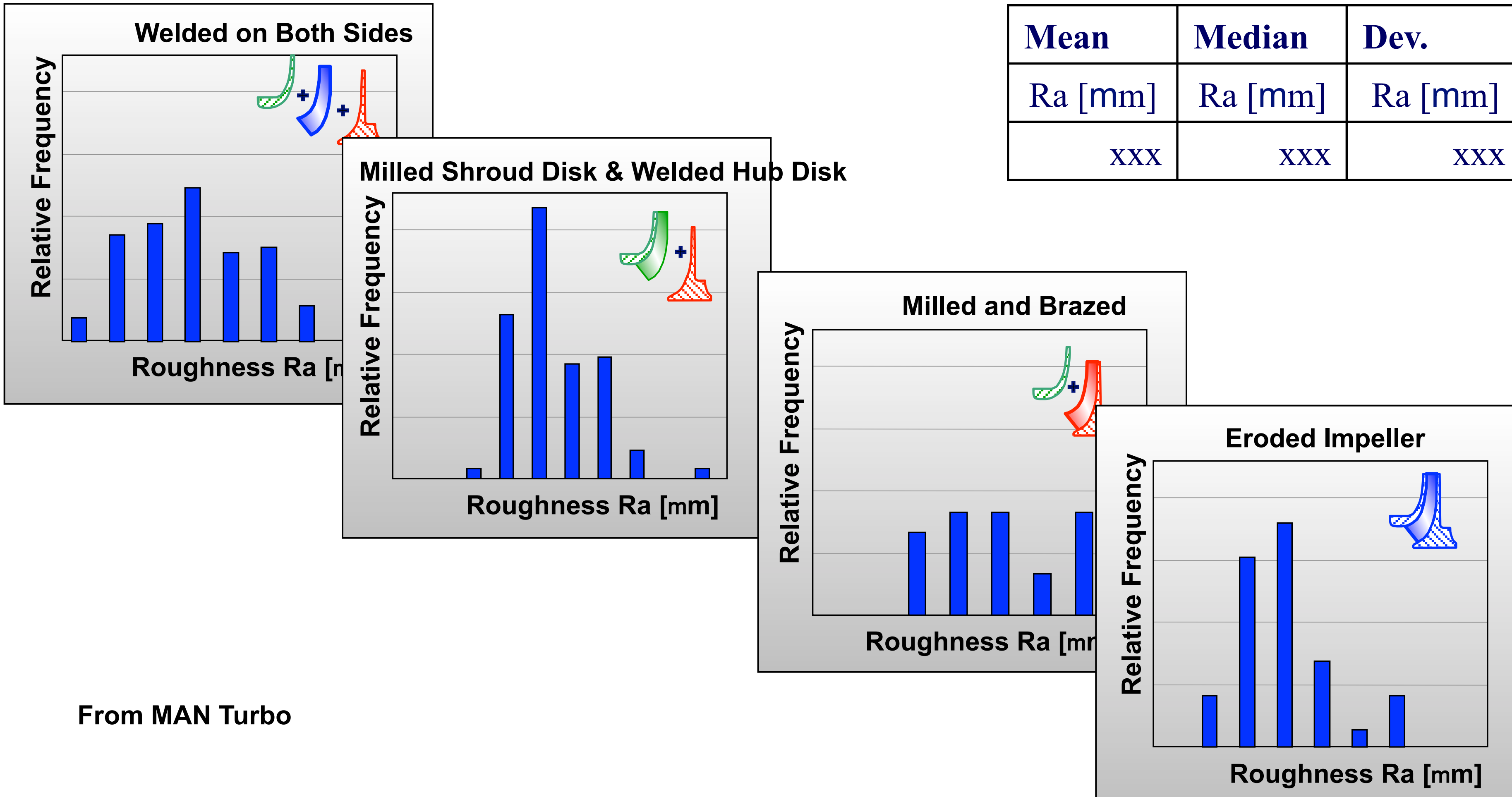
- If empirical statistical distribution data are available, a utility is available to fit a best pdf



- Example of roughness, (from MAN Turbo)

Wall Roughness as Uncertainty Parameter

Distribution of measured samples

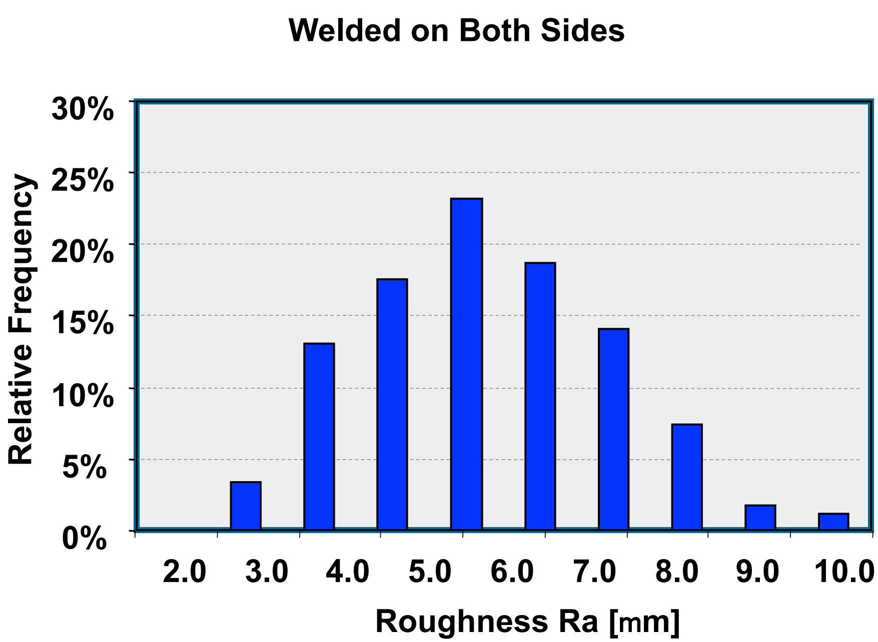


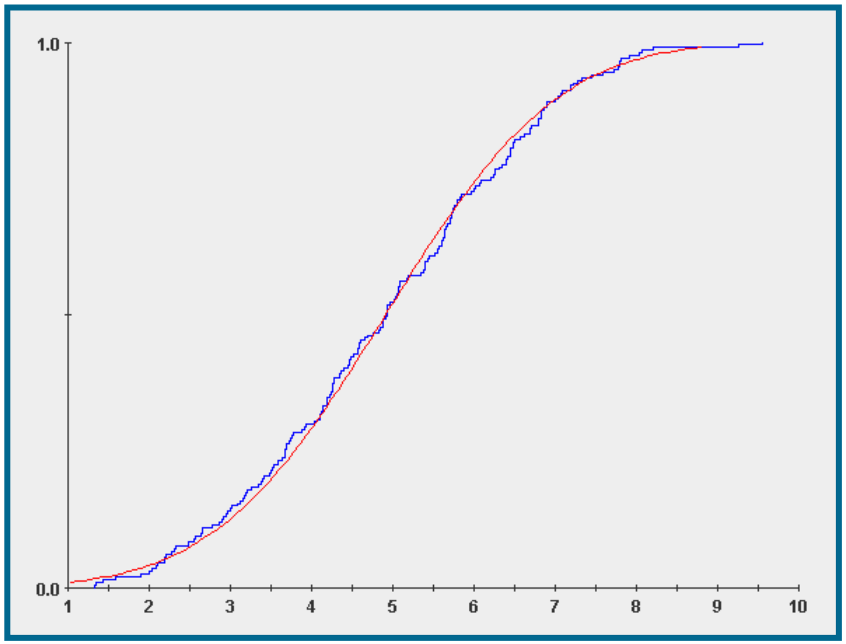
Mean	Median	Dev.
Ra [mm]	Ra [mm]	Ra [mm]
xxx	xxx	xxx

From MAN Turbo

Estimation of Probability Density Functions

Measured distribution





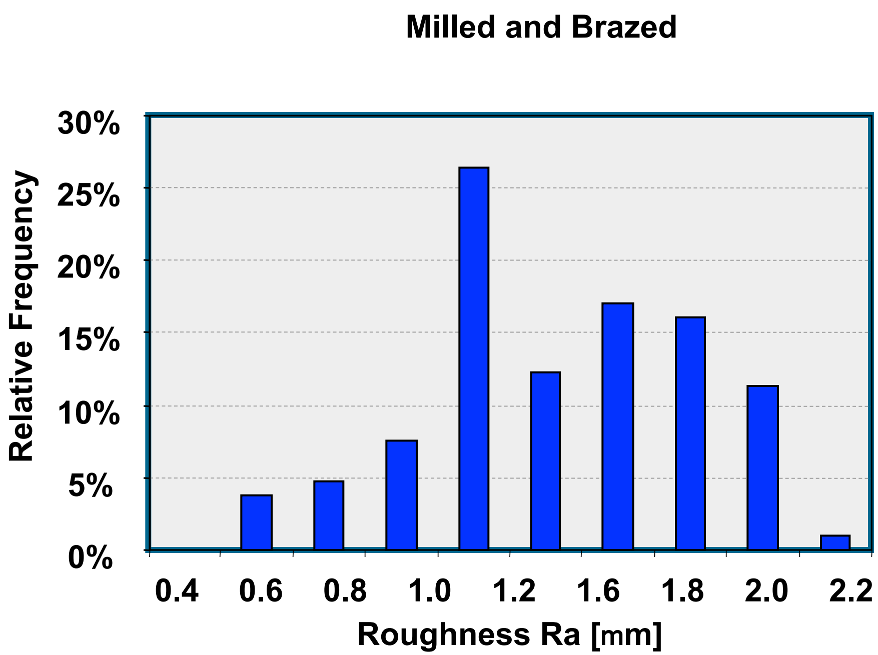
Mean	Median	Dev.
Ra [mm]	Ra [mm]	Ra [mm]
4.92	4.94	1.67

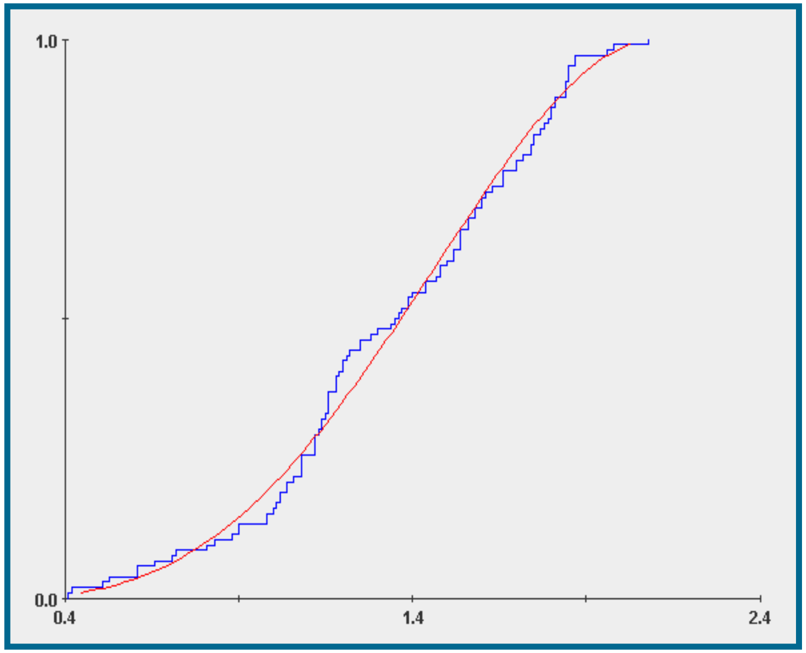
Best Fit: Normal Distribution
KS = 0.9354129891900814
-NLL = 1.9292891405798975

From MAN Turbo

Estimation of Probability Density Functions

Measured distribution





Mean	Median	Dev.
Ra [mm]	Ra [mm]	Ra [mm]
1.34	1.36	0.38

Best Fit: Beta Distribution
KS = 0.572224943817288
-NLL = 0.413899158143873

From MAN Turbo

Propagation of the uncertainties

- Innovative mathematical and algorithmic methods have to be developed for the treatment of differential equations containing stochastic input parameters and model parameters

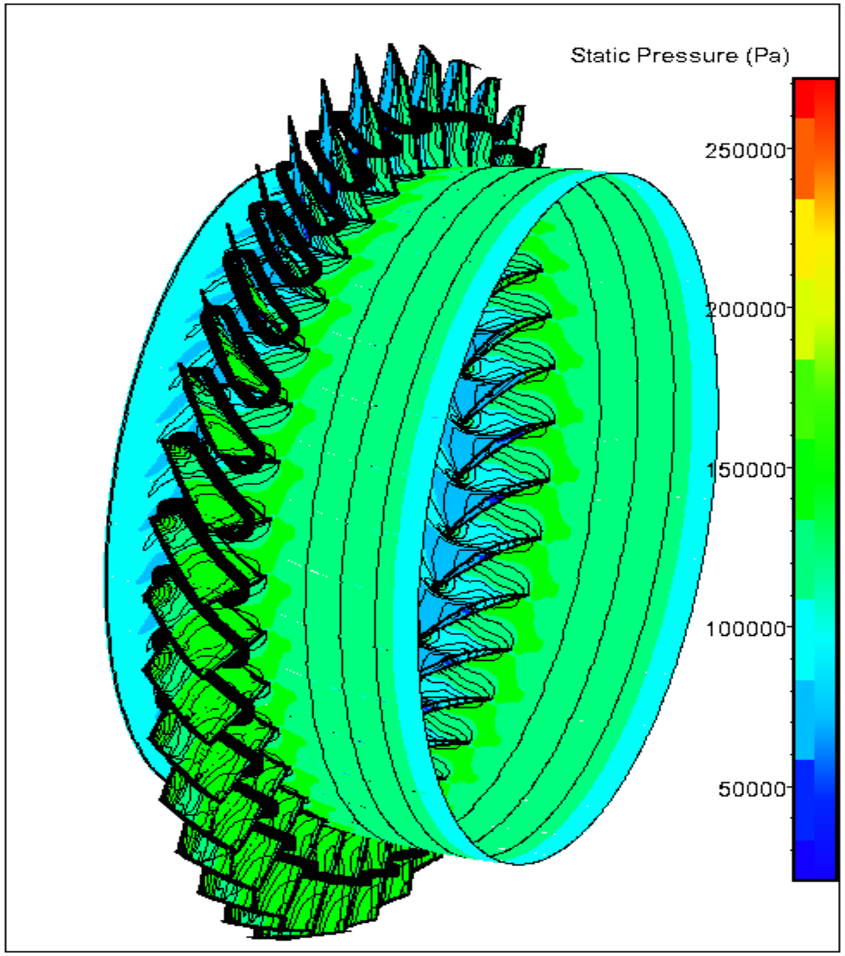
- *Polynomial Chaos Method (PCM)* –Intrusive or Non-intrusive
- *Monte-Carlo method*s--Non-intrusive
- *Sensitivity methods*, or method of moments: Intrusive

- The randomness of the flow solution is represented by pdf's of the different variables at every point and instant of time.

NASA ROTOR 37

- **NASA Rotor 37**

- Transonic compressor rotor
- Pressure ratio 2.1



Rotor 37 – computational program

- three uncertainties are considered: two of operational type and one of geometrical origin:

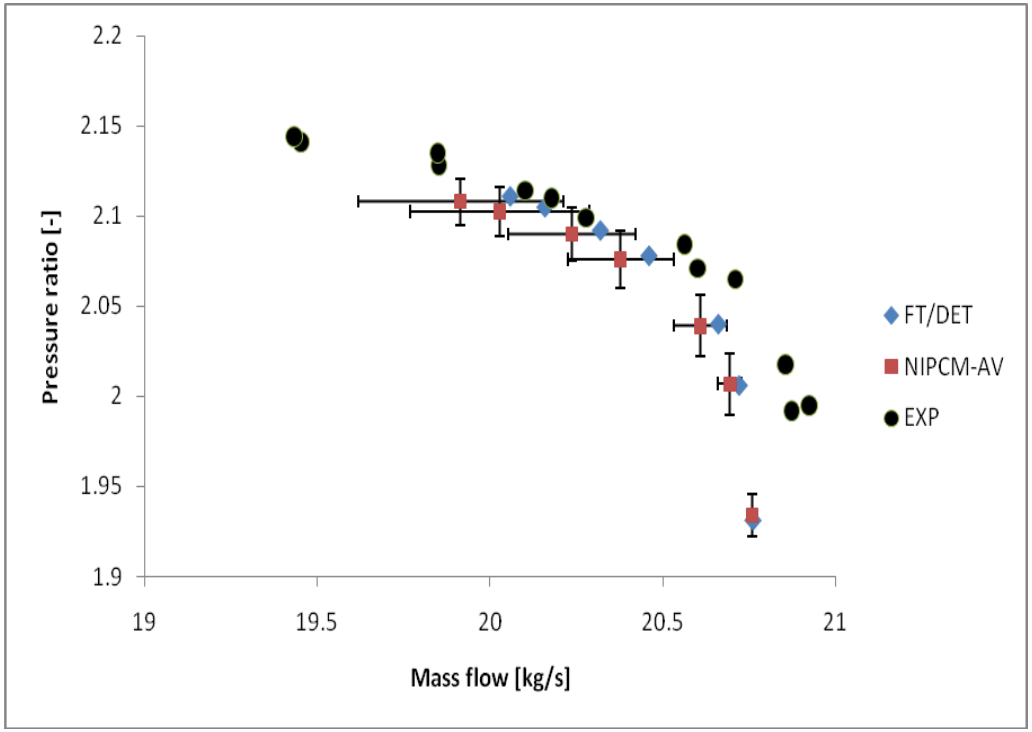
Option	Uncertainty parameter	The most likely value (m)	Minimum value (a)	Maximum value (b)	PDF-type
1	Inlet total pressure (p_t)	Standard input profiles at station 1	95% m	105% m	Symmetric beta pdf
2	Static outlet pressure	m_P=see table 1	98% m_P	102% m_P	Symmetric beta pdf
3	Tip clearance	m_H=0.356 mm	50% m_H	150% m_H	Symmetric beta pdf

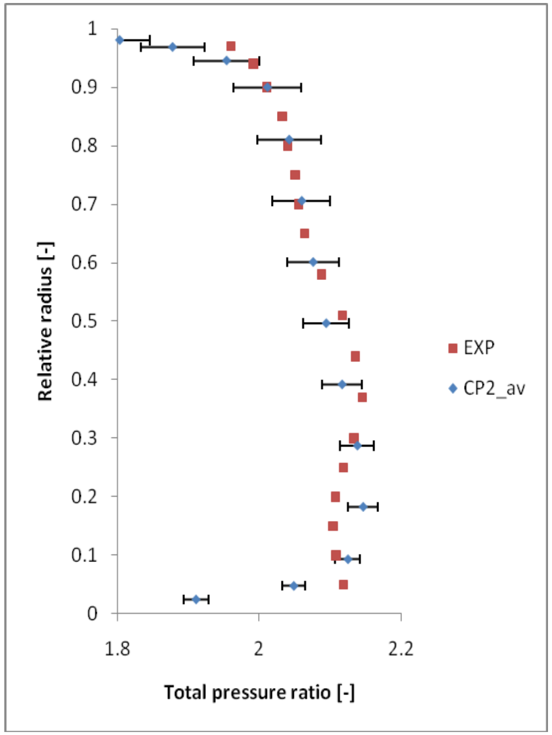
- Non-deterministic compressor maps with 7 running points have been constructed

Table 1 Running points in the compressor map

Running point	*Outlet static pressure* (Pa)
1	99215
2	110000
3	114074
4	119035
5	121033
6	123008
7	124027

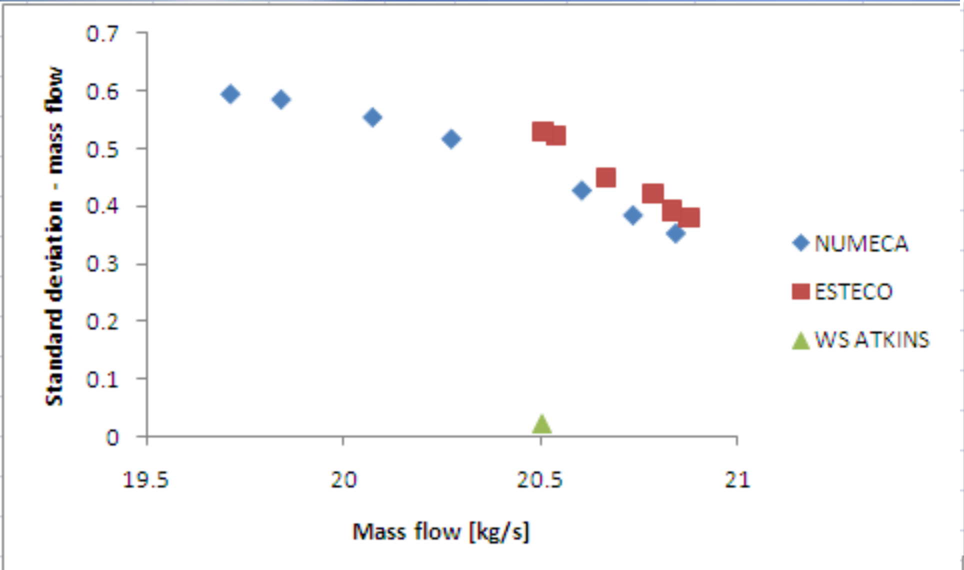
Management of uncertainties-Rotor 37

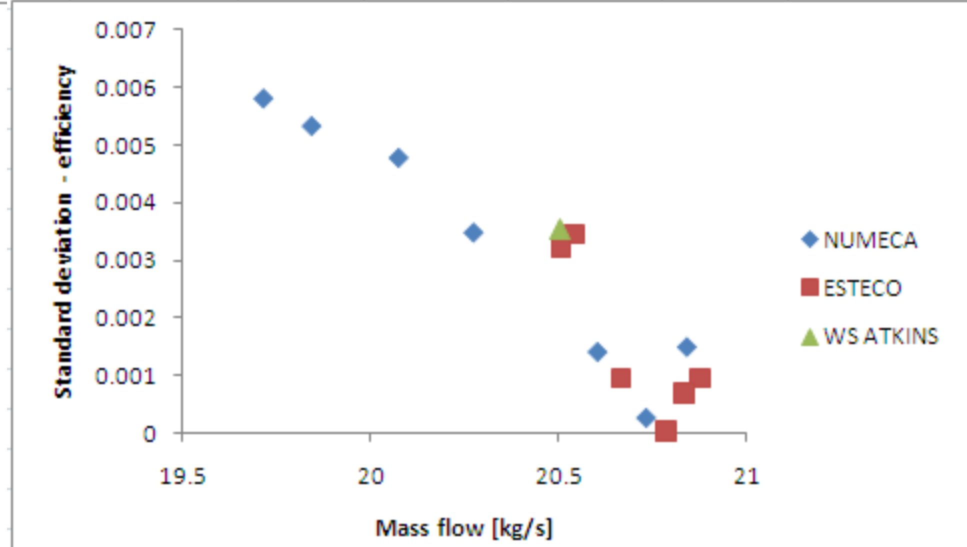




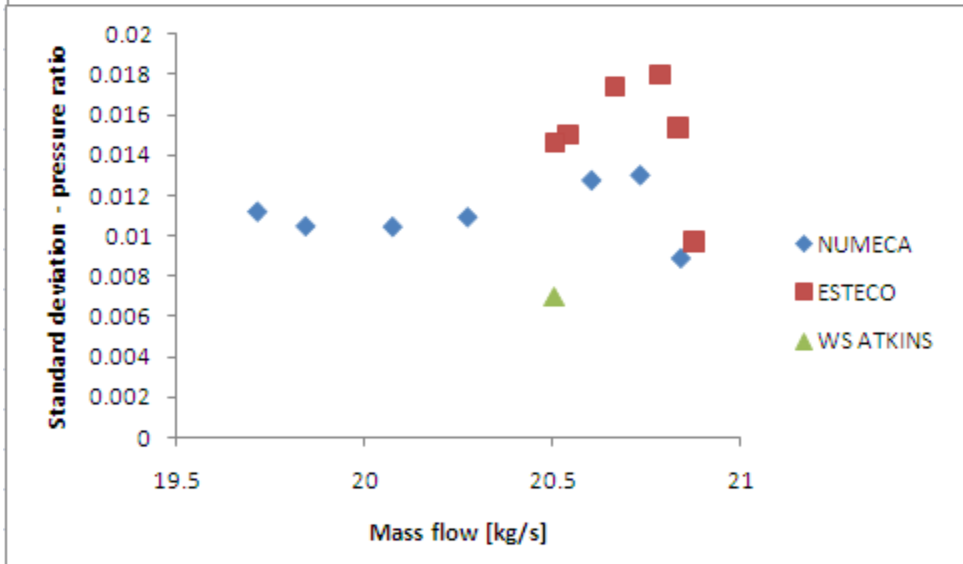
- Evaluation of Non-Intrusive Probabilistic Collocation Method of TU Delft: left – non-deterministic compressor map for the transonic NASA Rotor 37 due to imposed operational uncertainty, right – error bar plot of the radial pitch-wise averaged distribution of the total pressure ratio
- Significant differences between deterministic solutions and the average values !!!

Uncertainties for Rotor 37



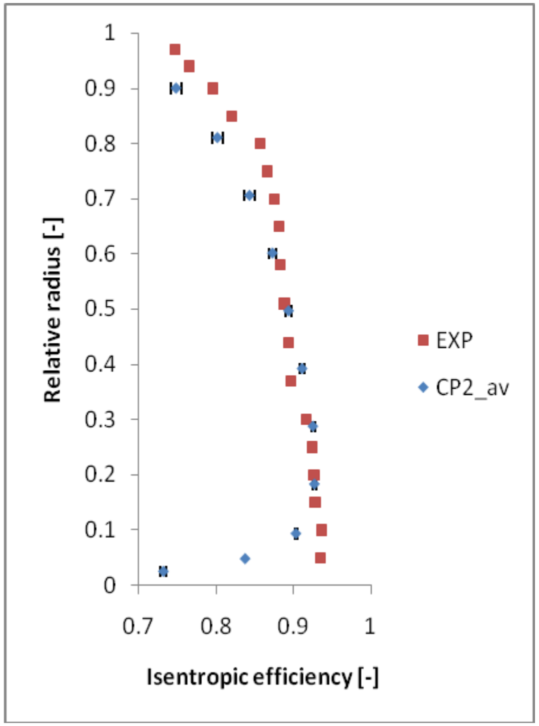


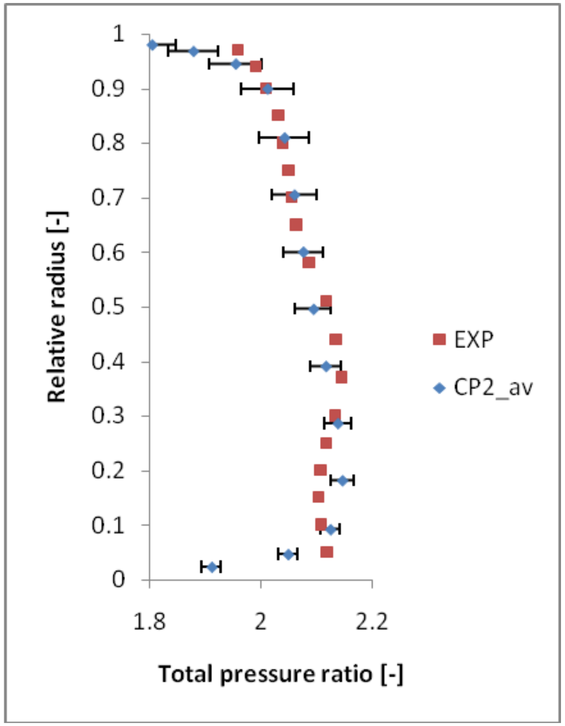
- from Dinescu and Hirsch (2009)
- Up-left figure: st.dev. mass flow rate
- Up-right figure: st.dev. efficiency
- Down-right fig.: st.dev. pres. ratio
- The scatter of the results due to:
  - type of used CFD solver,
  - convergence level,
  - mesh quality,
  - employed non-deterministic method !!!

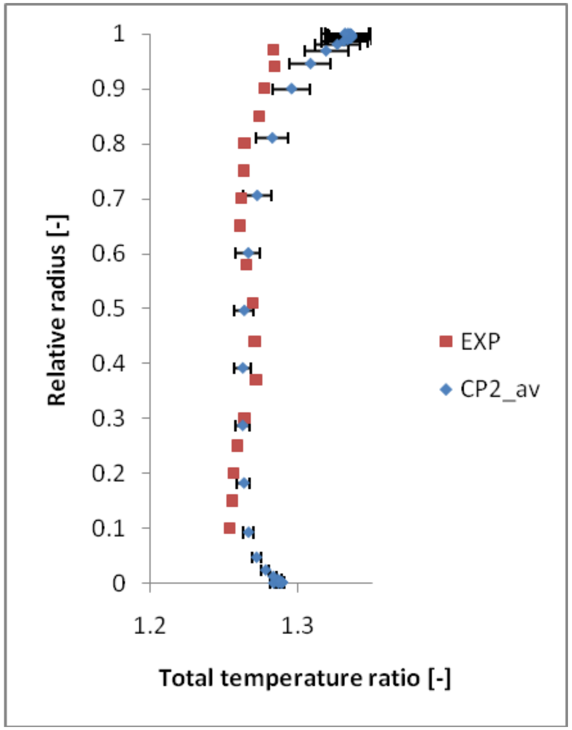


NASA Rotor 37

- Comparison with experiment for 98% chocked mass flow regime







Roads towards Industrial readiness of UQ

Large number of uncertainties:

- Methods based on sensitivity analysis with adjoint formulation and automatic differentiation have a significant potential in handling large number of uncertainties

- Monte Carlo methods (MCMs) coupled with surrogate models still need work on techniques for reducing the number of CFD computations;
  - Multilevel MCM are a highly promising approach

- Improvements of the sampling techniques in MCMs are requested or efficient meta-models (response surface methods based on radial basis functions, Kriging, etc.)

Roads towards Industrial readiness of UQ

Large number of uncertainties:

- Polynomial Chaos Methods (PCM)
  - adaptive and/or sparse grids in the same stochastic space for non-intrusive methods
  - construct surrogate models and use them instead of CFD computations in non-intrusive PCM
  - dimensional reduction: e.g., perform sensitivity analysis to identify the most relevant uncertainties and next perform UQ of the latter ones

Roads towards Industrial readiness of UQ

Geometrical uncertainties:

- Extremely challenging for intrusive PCM because the computational domain becomes random

- The random boundary is a random field which currently is decomposed in a collection of uncorrelated/independent random variables (r.v.) through:
  - Karhunen-Loeve decomposition or
  - Principal Component Analysis

- Next the uncorrelated/independent r.v. could be propagated by the chosen non-deterministic method

Roads towards Industrial readiness of UQ

Quantification of the input uncertainties:

- The precise form of the pdf of the input uncertainties has a strong, first order, effect on the non-deterministic CFD-predictions
- Quantification techniques for definition of reliable input uncertainties from scarce experimental data are necessary
- Present approaches in computational mechanics intend solving an inverse problem employing Bayesian inference approach or use Polynomial Chaos representations

Roads towards Industrial readiness of UQ

Robust design and optimization:

- robust formulations for aerodynamics shape optimization can rely on various approaches
  - multi-point optimization
  - minmax formulation (or the worst-case scenario)
  - semi-infinite formulation (or mean objective function optimization)
  - chance constraint formulation (or reliability-based design optimization)
  - robust multi-objective optimization

- the real challenge is to handle complex industrial applications where the proper mix of robust design methodology, computational efficiency of its components and accuracy of the non-deterministic simulations is considered

Roads towards Industrial readiness of UQ

Verification and validation

- It is of capital importance to develop a new generation of database with basic cases and industrial challenge cases, all containing prescribed uncertainties

- New experimental data, with controlled uncertainties of the experimental conditions, must be defined to generate outputs under the form of pdf's, to serve as validation for UQ methods.

- Establish best practice guides for UQ and RDM aeronautical applications

Conclusions

- Uncertainty Quantification is becoming a key component of industrial design process and risk management

- Moving the non-deterministic methods for UQ towards industrial readiness (TRL 5-6) asks increasing the maturity level of the present methods in order to be able reaching the objectives of industrial end-user

- R&D for UQ imposes in turn new constraints on the way the experimental test cases must be instrumented:
  - e.g., generate pdf's of the monitored uncertainties for the given experimental conditions

- Consequently, the verification and validation of UQ-methodologies needs dedicated databases with test cases complying with the new constraints