Introduction to Uncertainty Quantification

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RTO-AVT-VKI Short Course

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Objectives

- Introduce Uncertainty Quantification
  - Definitions and motivations
  - Classification of various techniques
  - Identify different types of uncertainties

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  - Autoignition: effect of reaction rate uncertainties
  - Heat transfer: material property uncertainty

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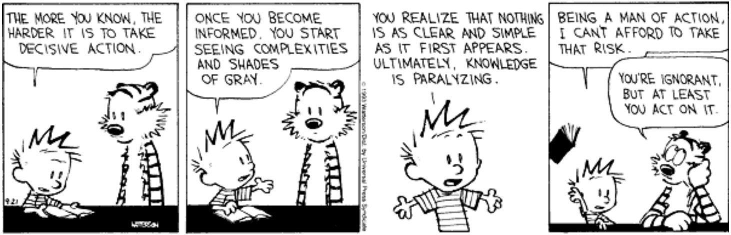
  - Heat transfer: material property uncertainty
- Convey the challenges and the opportunity in UQ Science

Outline

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

Part I

Why Uncertainty Quantification?



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...from WikiPedia

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

Why Uncertainty Quantification?

Decision Making

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

Why Uncertainty Quantification?

Validation

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

Experiments

Simulations

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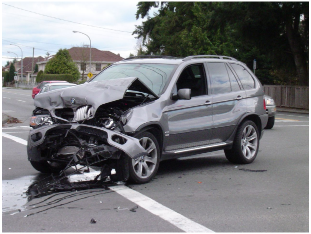

cm

Controlled tests

Real World

Why Uncertainty Quantification?

Robust Design

- System performance are unchanged (stable) when exposed to uncertainties in the operating conditions.
- **Optimization Under Uncertainty** is a powerful tool for managing the tradeoffs between optimal performance and performance stability.

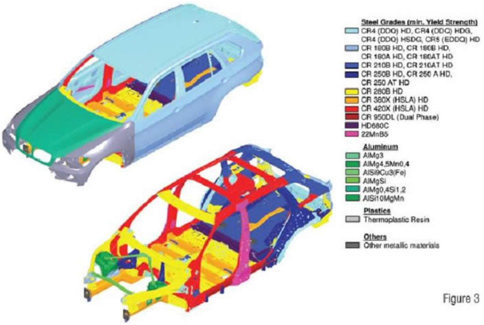

Figure 3

Why Uncertainty Quantification?

A simplistic view

- In spite of the wide spread use of Modeling and Simulation (M&S) tools it remains difficult to provide objective confidence levels in the quantitative information obtained from numerical predictions

- One of the main objective is to provide error bars on the simulations results

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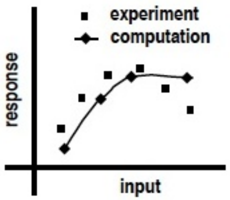

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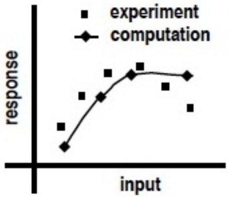
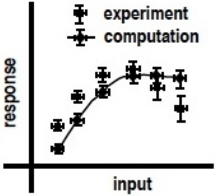


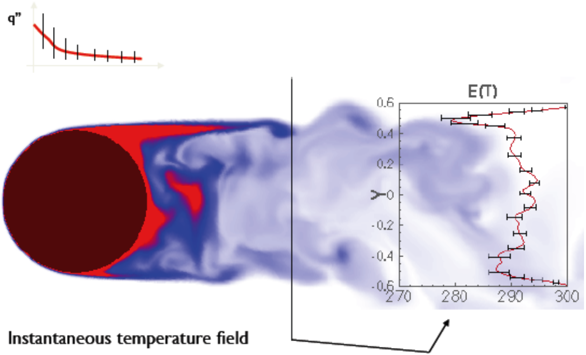


Why Uncertainty Quantification?

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



Instantaneous temperature field

Costantine & Iaccarino, AIAA-2009-0975

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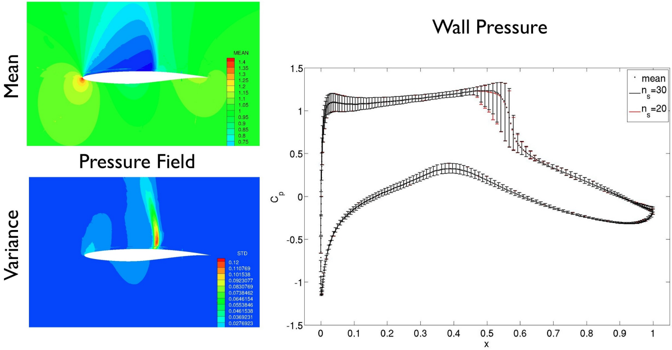
Transonic airfoil with uncertain flight conditions



Witteveen, Chantrasmi, Doostan & Iaccarino, Nodesim Workshop

Why do we care about V&V and uncertainty?

- Prefer not to be this guy
  - Expediency > intellectual integrity
  - No understanding of risks

- Natural part of scientific method
  - Observation
  - Hypothesis
  - Prediction
  - Test

V&V goes here

- Besides, we all know: $\dfrac{BEM}{VLC} \notin \mathbb{R}$

formerly a *BAC*

Slide from M. Anderson, LANL

Part II

Definitions

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

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

Verification and Validation

Definitions

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

What is V&V?

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

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

Errors vs. Uncertainties

Definitions

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

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

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Well...

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

Errors vs. Uncertainties

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- 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)
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Uncertainties

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

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

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

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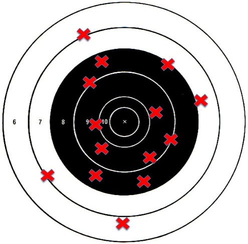
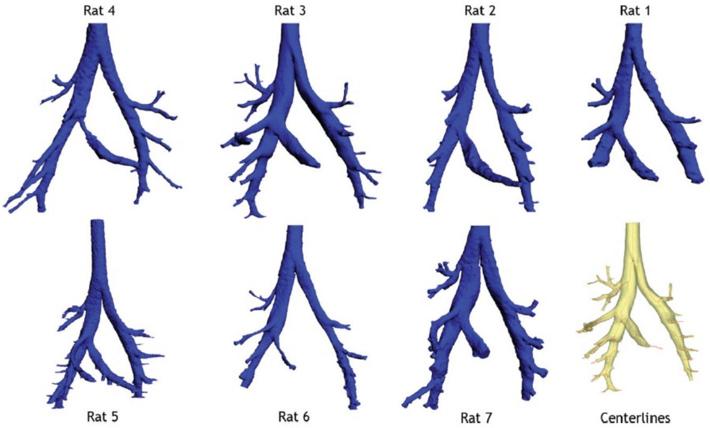
- Examples are: material properties, operating conditions manufacturing tolerances, etc.
- In mathematical modeling it is also studied as noise



Aleatory Uncertainty

Natural variance

Patient-to-patient differences



Courtesy of de Backer et al, 2009

Aleatory Uncertainty

Flight conditions

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

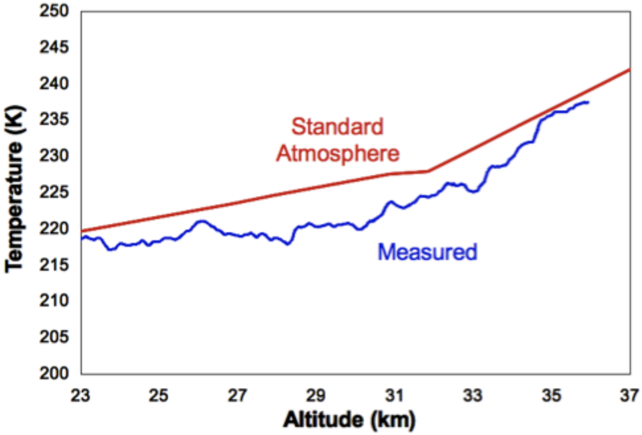


Image from Smart et al. 2003

Uncertainties

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

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

- Examples are: turbulence model assumptions or surrogate chemical models

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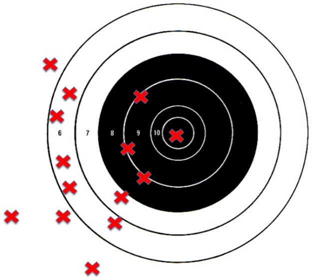
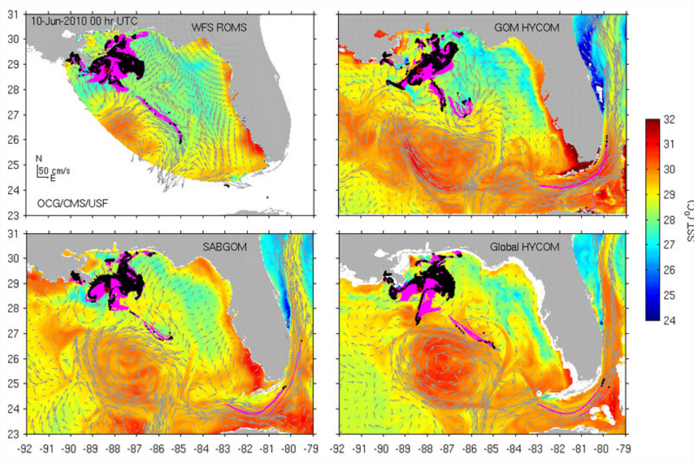
- It is NOT naturally defined in a probabilistic framework
- Can lead to strong bias of the predictions



Epistemic Uncertainty

Model uncertainty

Deepwater Horizon oil tracking forecast

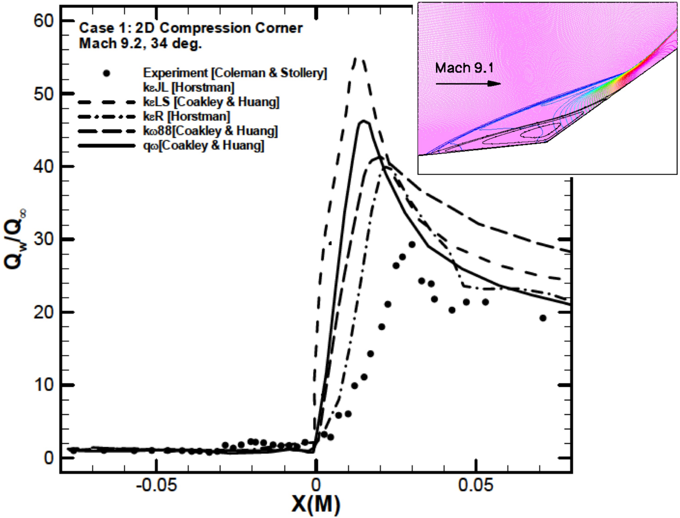


Source: University of Texas Institute of Geophysics

Epistemic Uncertainty

Model uncertainty

Predictions of heat flux over a compression ramp



Source: Roy et al, 2007

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Choose your Uncertain Battles..

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

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- 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.

Sensitivity Analysis vs. UQ

- Sensitivity analysis (SA) investigates the connection between inputs and outputs of a (computational) model
- The objective of SA is to identify how the variability in an output quantity of interest (q) is connected to an input (ξ) in the model; the result is a sensitivity derivative $\partial q / \partial \xi$

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- SA $\in$ UQ

Part III

Computations Under Uncertainty

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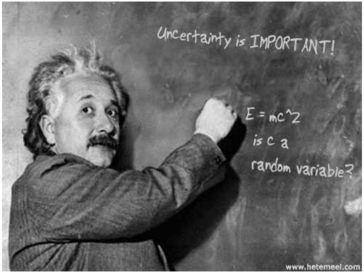
Predictive Simulations

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

A. Einstein



Uncertainty Quantification

Computational Framework

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

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

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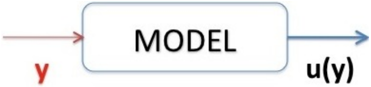

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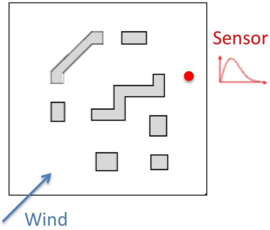

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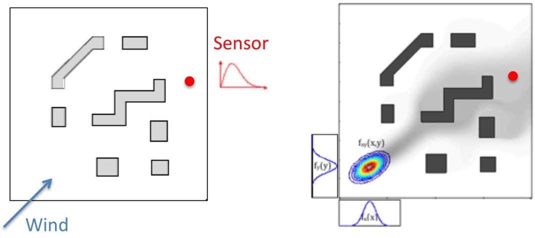

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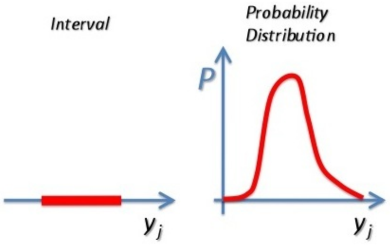

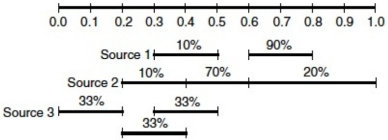

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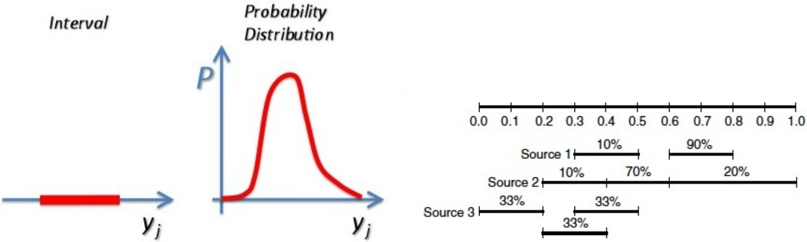

- The mathematical framework for propagating uncertainties is dependent on the data representation chosen
  - In these lecturers we focus on probabilistic methods

Uncertainty Quantification

Computational Framework

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Probabilistic Uncertainty Propagation

Perform simulations accounting for the uncertainty represented as randomness

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

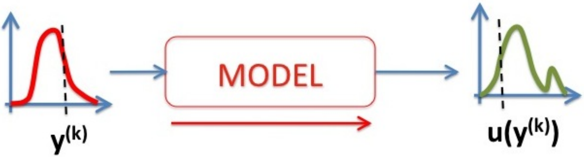
Uncertainty Propagation

Intrusive vs. Non-Intrusive Methodology

Uncertainty Propagation

Intrusive vs. Non-Intrusive Methodology

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



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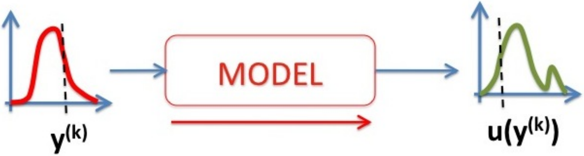
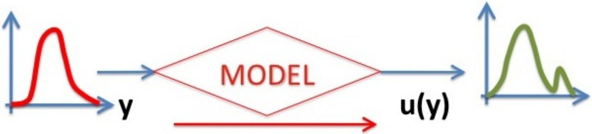


- Intrusive methods require the formulation and solution of a stochastic version of the original model



Uncertainty Propagation

Intrusive vs. Non-Intrusive Methodology

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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

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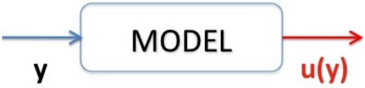
Consider a generic computational model ($\boldsymbol{y} \in \Re^{d}$ with d large)



How do we handle the uncertainties?

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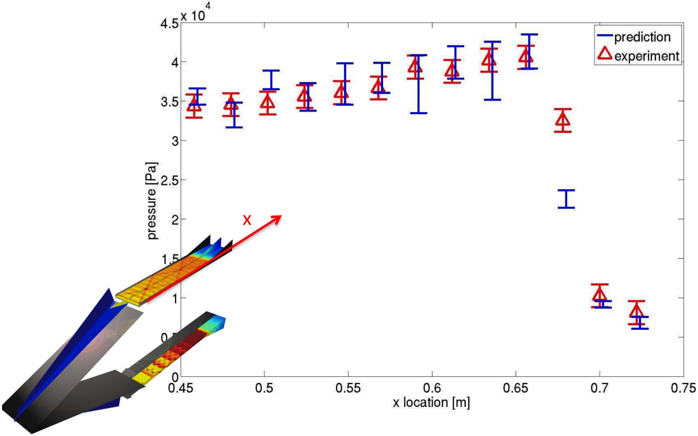
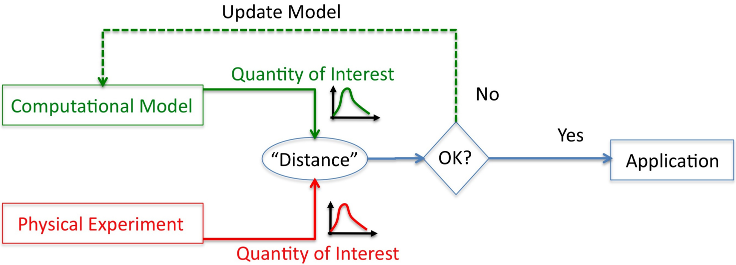
Certification

- Quantification of the confidence
- Objective validity



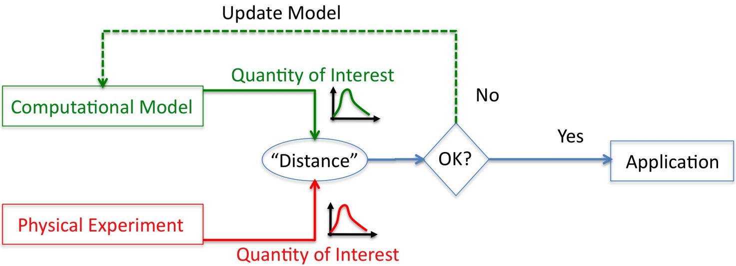
Hypersonic air-breathing vehicle - HyShot II

Validation



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

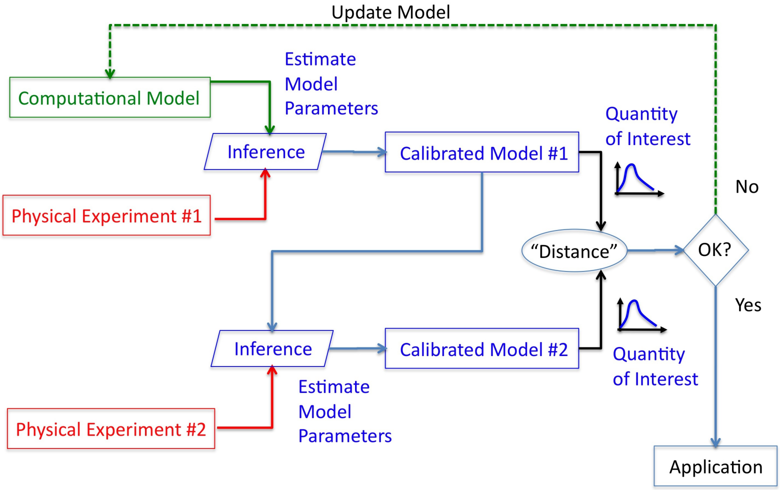
Validation



- Need to define a validation metric to compare *uncertain* quantities
- What if the measurements do not have access to the QOI?

Validation

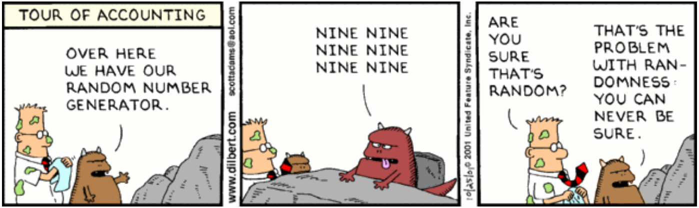
An Inference Process - PECOS @ UT Austin



- Simulations are NOT compared directly to data!

Part IV

Probabilistic Uncertainty Propagation



Uncertainty = Randomness

- Straightforward Monte Carlo sampling

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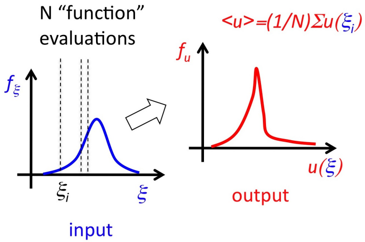

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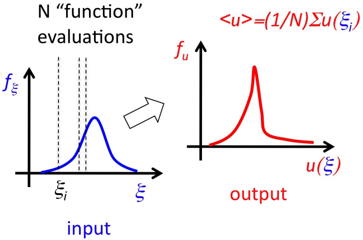

- ...not feasible with computationally-expensive function evaluations!

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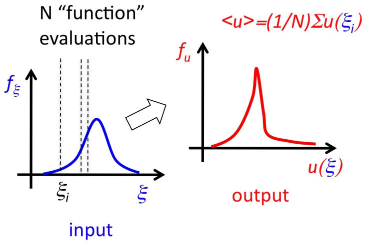

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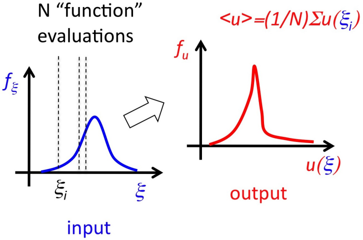

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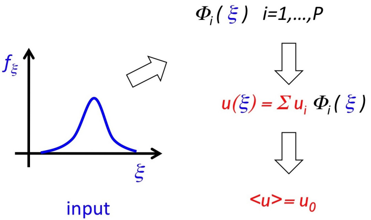
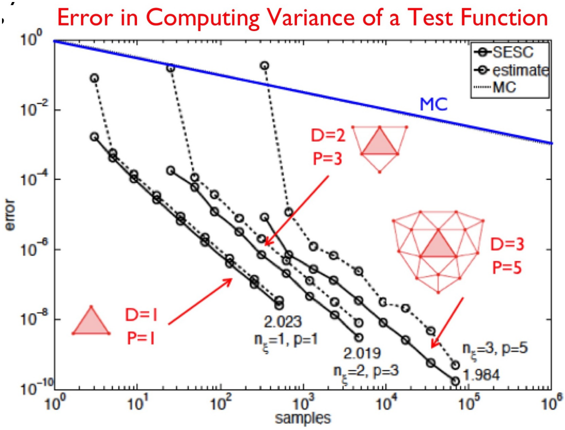


Uncertainty = Randomness

- Beyond Monte Carlo
  - Advanced Sampling: LHS, importance-sampling, quasi-random sequence, ...
  - Intrusive methods: Polynomial chaos
  - Non-intrusive approaches: Stochastic collocation

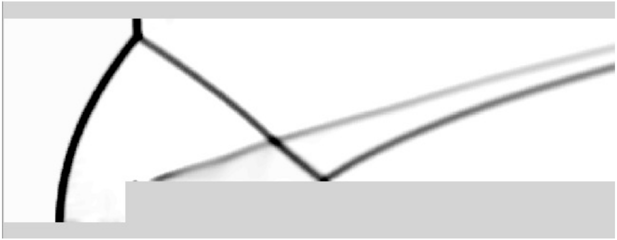


Part V

Examples

Fluid Dynamics of High Speed Flows

Known Inflow Mach Number (deterministic simulation)



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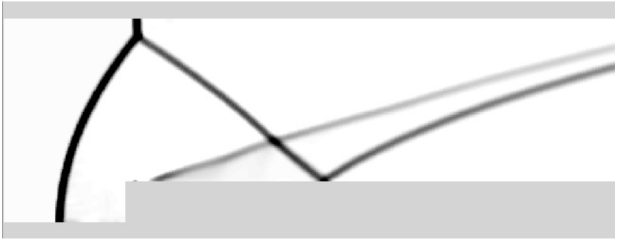

Uncertain Inflow Mach Number (average of stochastic simulations)

Uncertainty in Ignition Delay Time

Michael Mueller - ME470 Final Project

- Determination of Ignition Delay Time is an important design consideration
- Accumulation of radicals starts chain reaction causing sudden ignition of mixture
- What is the effect of uncertainties in reaction rates?

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  - Hydrogen chemistry (9 species, 25 elementary reactions)
  - What is the uncertainty?

Hydrogen Chemistry

Reaction Rate Uncertainties

- Rate (and their uncertainties) are available in the literature
- Modified Arrhenius form $k = AT^n exp(-E/RT)$
- The uncertainty factor *UF* is such that $[k \times UF, k/UF]$ provide *probable* bounds!
- *Assume* that the reaction rate are independent, lognormally distributed r.v.

Reaction	A	n	E	UF
$H + O_2 \leftrightarrow O + OH$	2.64e16	−0.67	71.30	1.5
$O + H_2 \leftrightarrow H + OH$	4.59e4	2.70	26.19	1.3
$OH + H_2 \leftrightarrow H + H_2O$	1.73e8	1.51	14.35	2.0
$OH + OH \leftrightarrow O + H_2O$	3.97e4	2.40	−8.83	1.5
$H + H + M \leftrightarrow H_2 + M$	1.78e18	−1.00	0.00	2.0
$H + H + H_2 \leftrightarrow H_2 + H_2$	9.00e16	−0.60	0.00	2.5
$H + H + H_2O \leftrightarrow H_2 + H_2O$	5.62e19	−1.25	0.00	2.0
$H + OH + M \leftrightarrow H_2O + M$	4.40e22	−2.00	0.00	2.0
$H + O + M \leftrightarrow OH + M$	9.43e18	−1.00	0.00	3.0
$O + O + M \leftrightarrow O_2 + M$	1.20e17	−1.00	0.00	2.0
$H + O_2 + M \leftrightarrow HO_2 + M$	6.33e19	−1.40	0.00	1.2
$H_2 + O_2 \leftrightarrow HO_2 + H$	5.92e5	2.43	223.85	2.0
$OH + OH + M \leftrightarrow H_2O_2 + M$	2.01e17	−0.58	−9.59	2.5
$HO_2 + H \leftrightarrow O + H_2O$	3.97e12	0.00	2.81	3.0
$HO_2 + H \leftrightarrow OH + OH$	7.49e13	0.00	2.66	2.0
$HO_2 + O \leftrightarrow OH + O_2$	4.00e13	0.00	0.00	1.2
$HO_2 + OH \leftrightarrow H_2O + O_2$	2.38e13	0.00	−2.09	3.0
	1.00e16	0.00	72.51	3.0
$HO_2 + HO_2 \leftrightarrow O_2 + H_2O_2$	1.30e11	0.00	−6.82	1.4
	3.66e14	0.00	50.21	2.5
$H_2O_2 + H \leftrightarrow HO_2 + H_2$	6.05e6	2.00	21.76	3.0
$H_2O_2 + H \leftrightarrow H_2O + OH$	2.41e13	0.00	16.61	2.0
$H_2O_2 + O \leftrightarrow HO_2 + OH$	9.63e6	2.00	16.61	3.0
$H_2O_2 + OH \leftrightarrow HO_2 + H_2O$	2.00e12	0.00	1.79	2.0
	2.67e41	−7.00	157.32	2.0

Davis, Joshi, Wang, Egolfopoulos, Proc. Combust. Inst. 30, 2005

Ignition Delay Time

Uncertainty Propagation

- Conditions: Stoichiometric Hydrogen-Air Mixture (29.6% H_2; 14.8% O_2); Temperature: 1000 K; Pressure: 1 atm;
- Non-intrusive LHS Sampling (25 uncertain variables)

Ignition Delay Time

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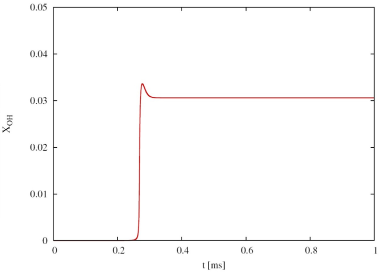
Number of Samples	Mean [ms]	UF
100	0.202060	1.7362
1000	0.201304	1.7054
10000	0.201256	1.7039
100000	0.201263	1.7075

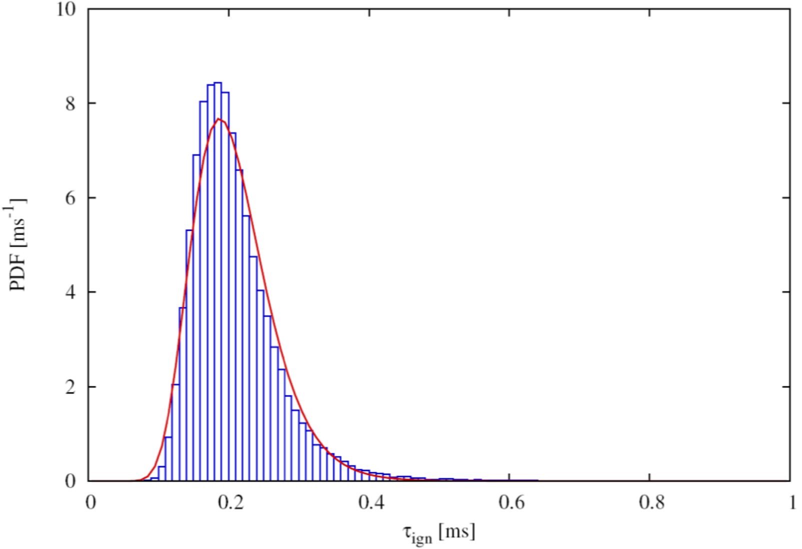
One Sample Showing Ignition at ~0.25 ms



DAKOTA UQ Suite from Sandia National Lab. used for this example

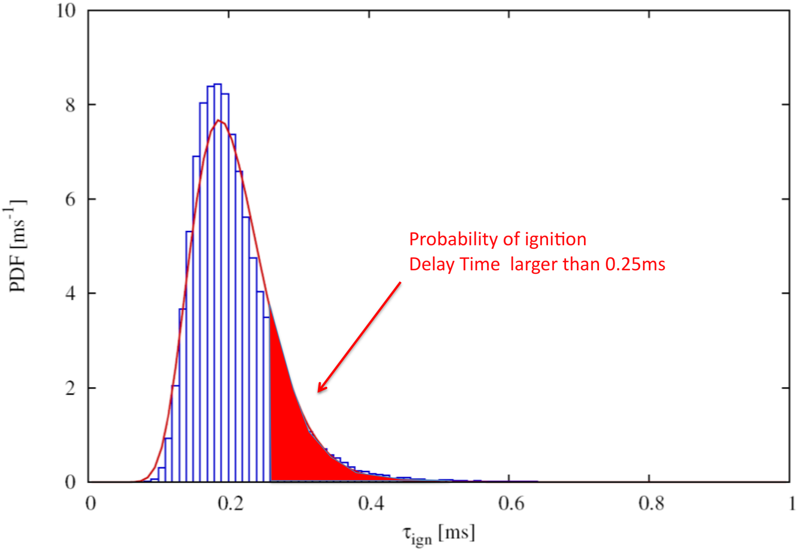
Ignition Delay Time

Uncertainty Propagation



Ignition Delay Time

Uncertainty Propagation



Ignition Delay Time

Inverse Problem

- What uncertainty in the reaction rates can we tolerate to ensure that the probability of ignition delay time exceeding 0.25 ms is less than 10%?

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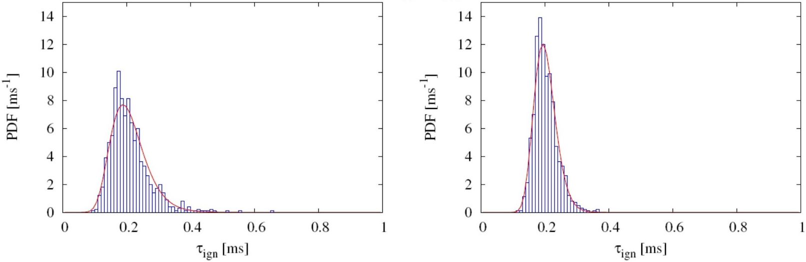
Quantity	Nominal	Optimal
UF Branching Reaction	1.5	1.29
Mean τ_{ign} [ms]	0.201304	0.198947
UF τ_{ign}	1.7054	1.4023
Probability of Failure	0.191	0.100

Ignition Delay Time

Uncertainty Propagation

Nominal | Optimal

N = 1k

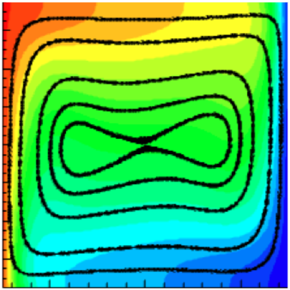


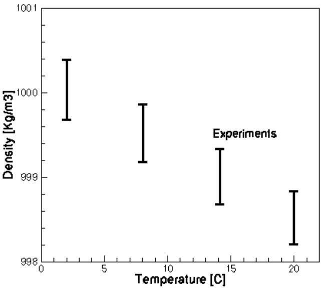
- Overall uncertainty in the IDT is reduced
- Failure probability below critical requirement

Uncertainty in Buoyancy-Driven Convection

Gary Tang - ME470 Final Project

- Fluid driven by the temperature gradient induced by hot/cold wall.
- Assume that there is uncertainty in the relationship between temperature and density, with density measured at various temperatures..
- What is the average temperature on the bottom wall?

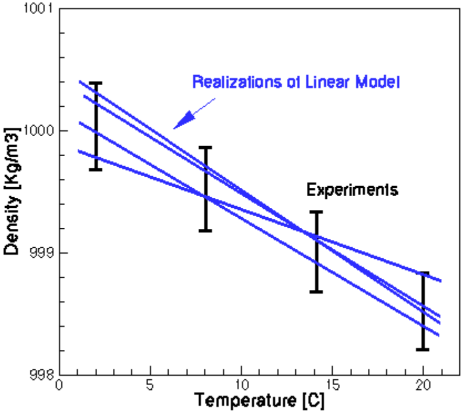




Density/Temperature Relationship

Interpreting the measurements

- A linear model appears to be appropriate to capture the experimental scatter!
- Can build an *uncertain* model with two random variables, constra



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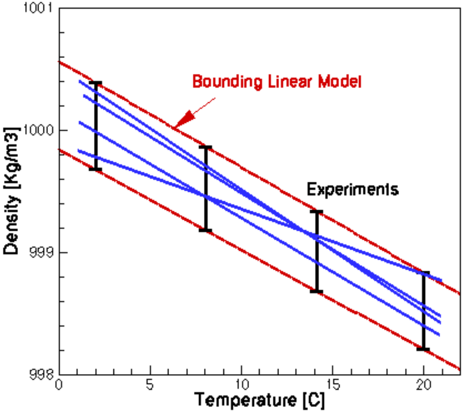
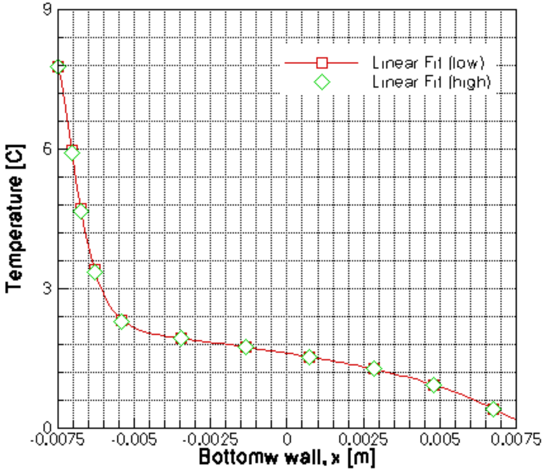


Driven Cavity

Uncertainty Quantification

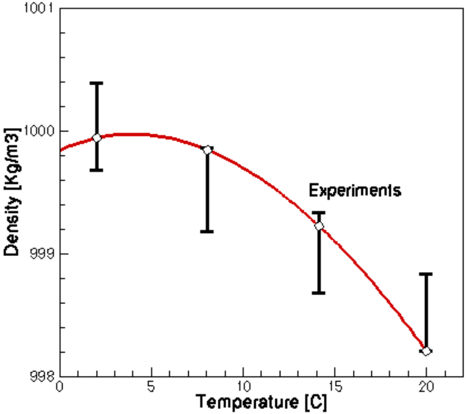
- Variability is limited! No sensitivity!



Density/Temperature Relationship

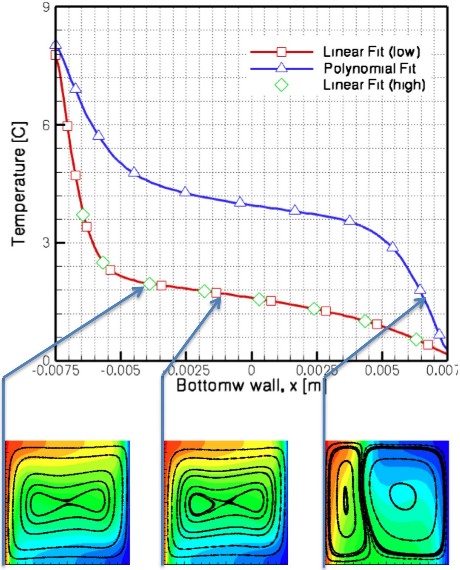
Interpreting the measurements

- *Perfect* experiments would have allowed a precise determination of the density/temperature relationship...

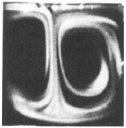


Driven Cavity

Uncertainty Quantification



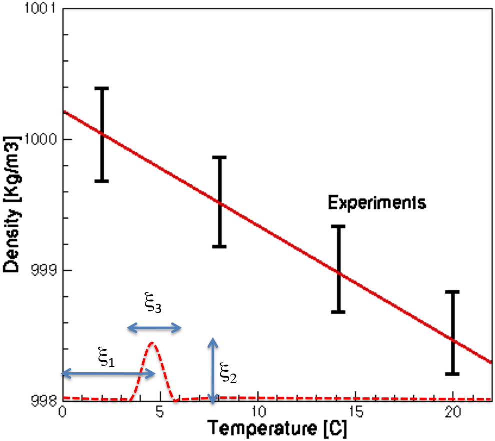
Experiment



Density/Temperature Relationship

Interpreting the measurements

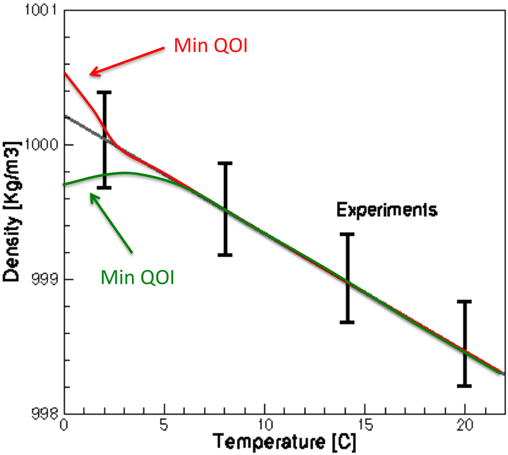
- Alternative approach (in the absence of perfect experiments) is NOT to rely on the linear model...



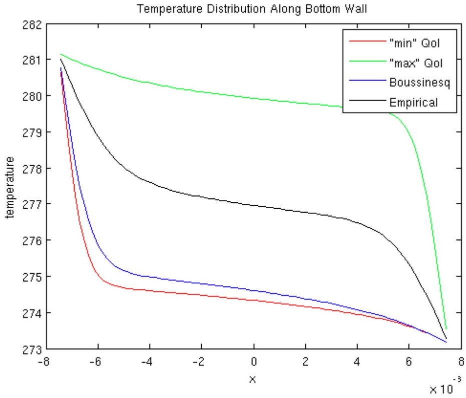
Density/Temperature Relationship

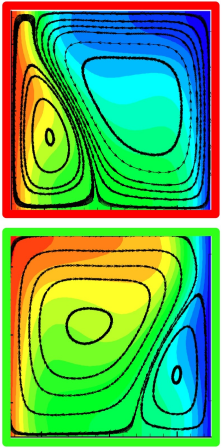
Interpreting the measurements

- Perform an optimization under uncertainty to find the MIN and MAX average temperature on the bottom wall!



Driven Cavity
Uncertainty Quantification





- The optimization procedure *finds* the density/temperature relationships that lead to MIN and MAX of the average temperature on the bottom wall!

Concluding

- Uncertainty Quantification plays a critical role in Validation!

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  ...but there are a lot of other exciting applications of the same methodologies, especially in combination with optimization tools.

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  - Interpretation and representation of the uncertainties

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- Uncertainty Quantification plays a critical role in Validation!

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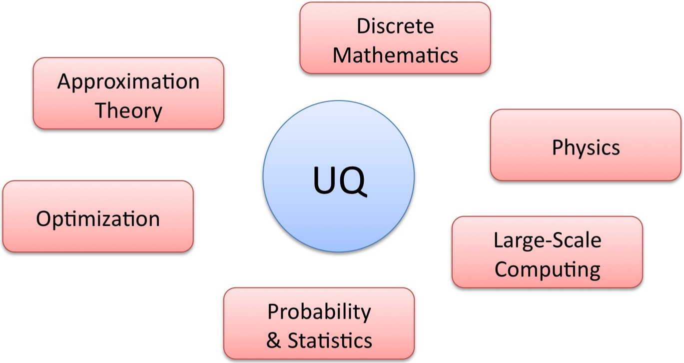
- Applications of UQ to realistic problems remains challenging:
  - Interpretation and representation of the uncertainties
  - Algorithmic advances are still required for costly computations, large number of uncertain inputs, discontinuous responses

Concluding

an ICME recruiting slide



UQ requires a broad range of skills...

Thank You

http://uq.stanford.edu

RTO-AVT-VKI Short Course

April 15-16, 2011

Stanford CA, USA