ME270 – Fall 2021

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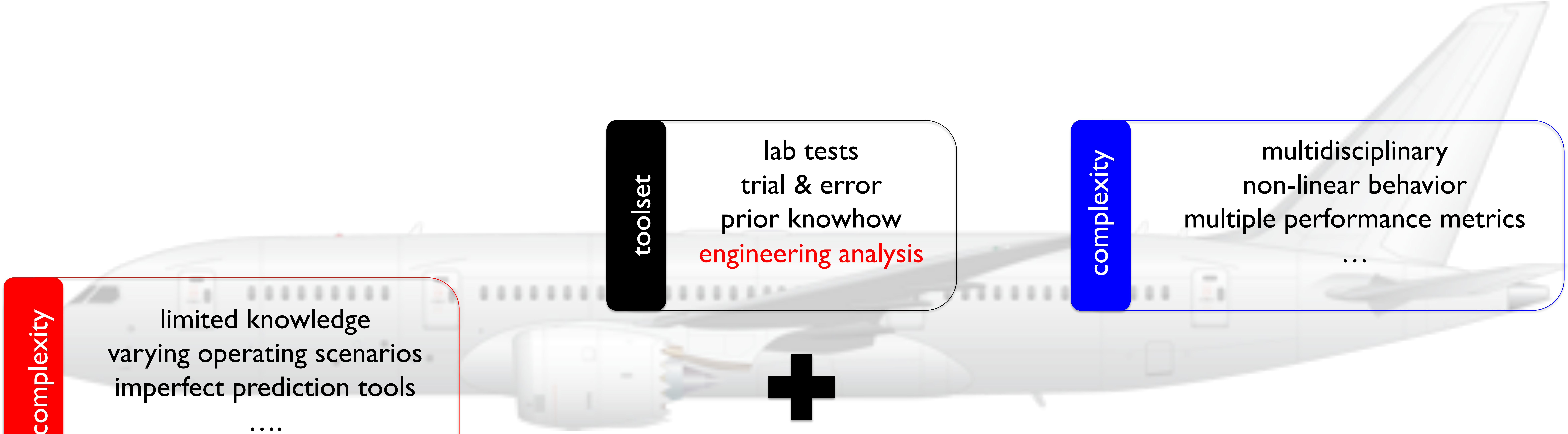
computational design of complex engineering systems

computational design of complex engineering systems



toolset

lab tests
trial & error
prior knowhow
engineering analysis

complexity

multidisciplinary
non-linear behavior
multiple performance metrics
...

complexity

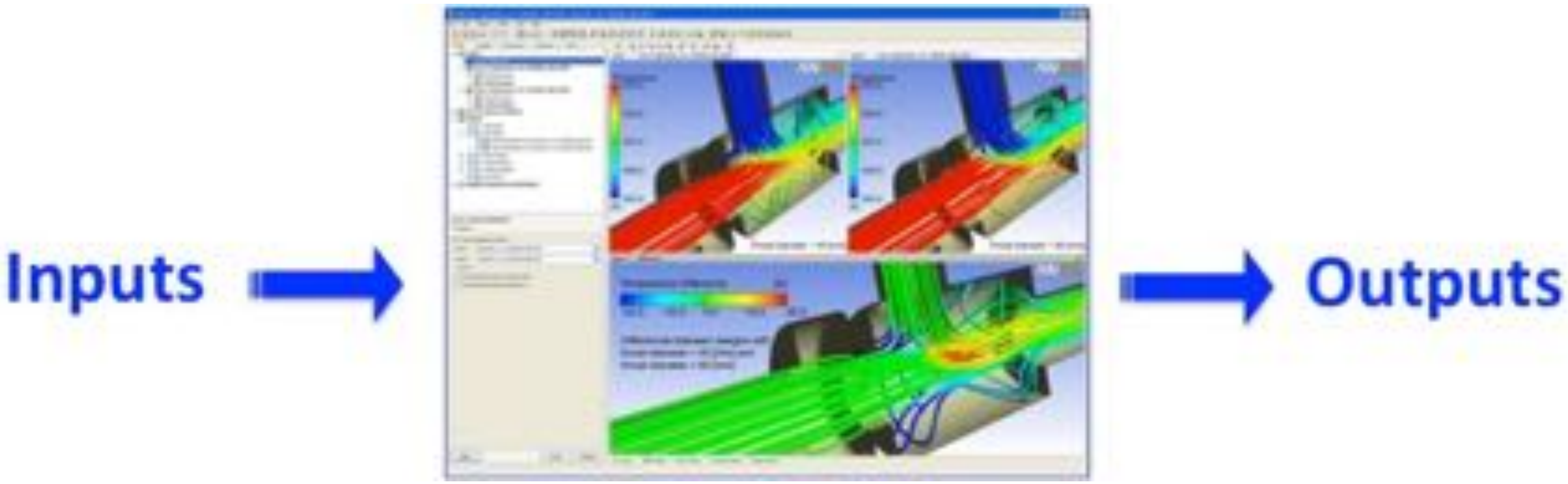
limited knowledge
varying operating scenarios
imperfect prediction tools
....

+

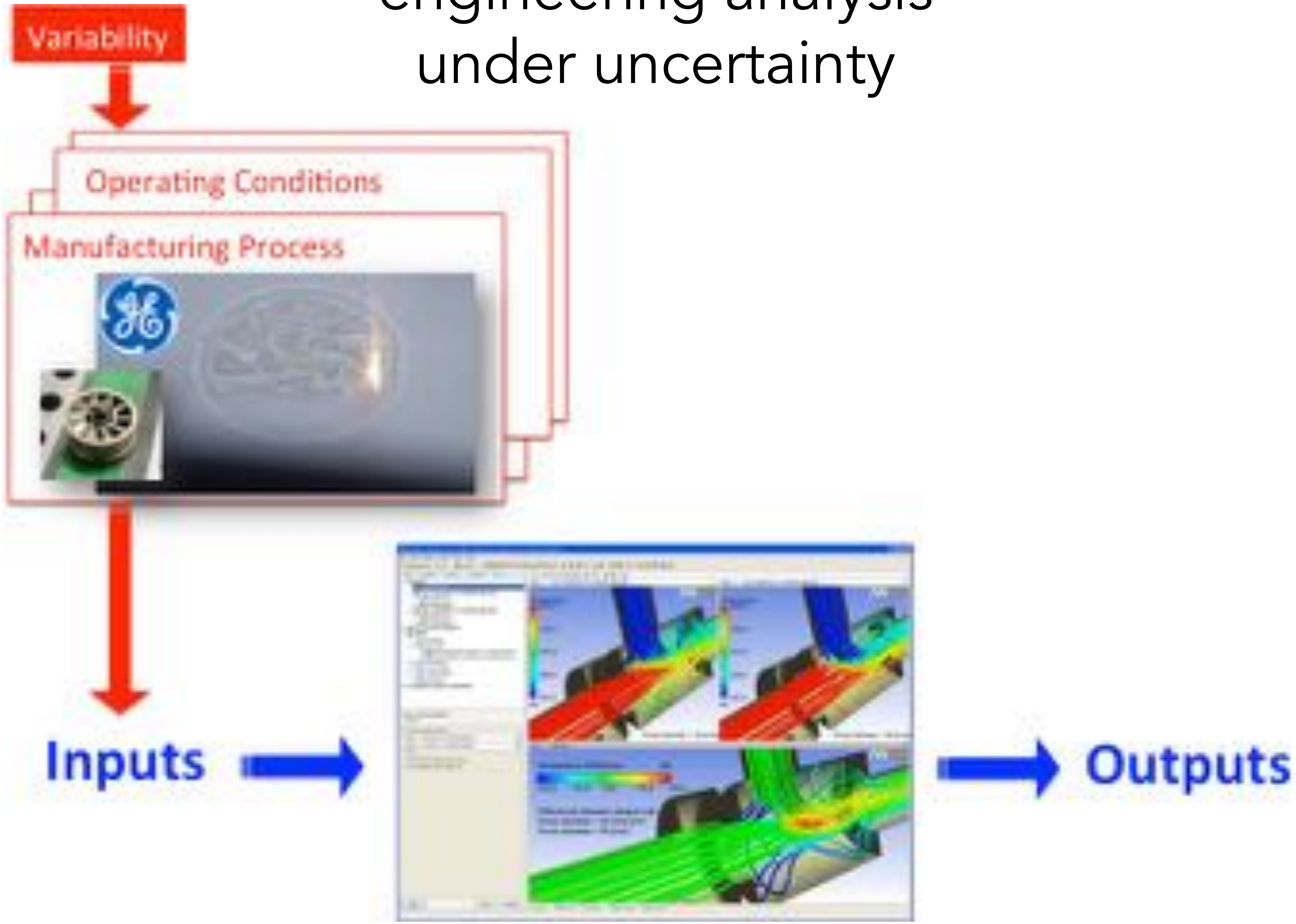
toolset++

optimization
sensors/data
explicit uncertainty estimates
....

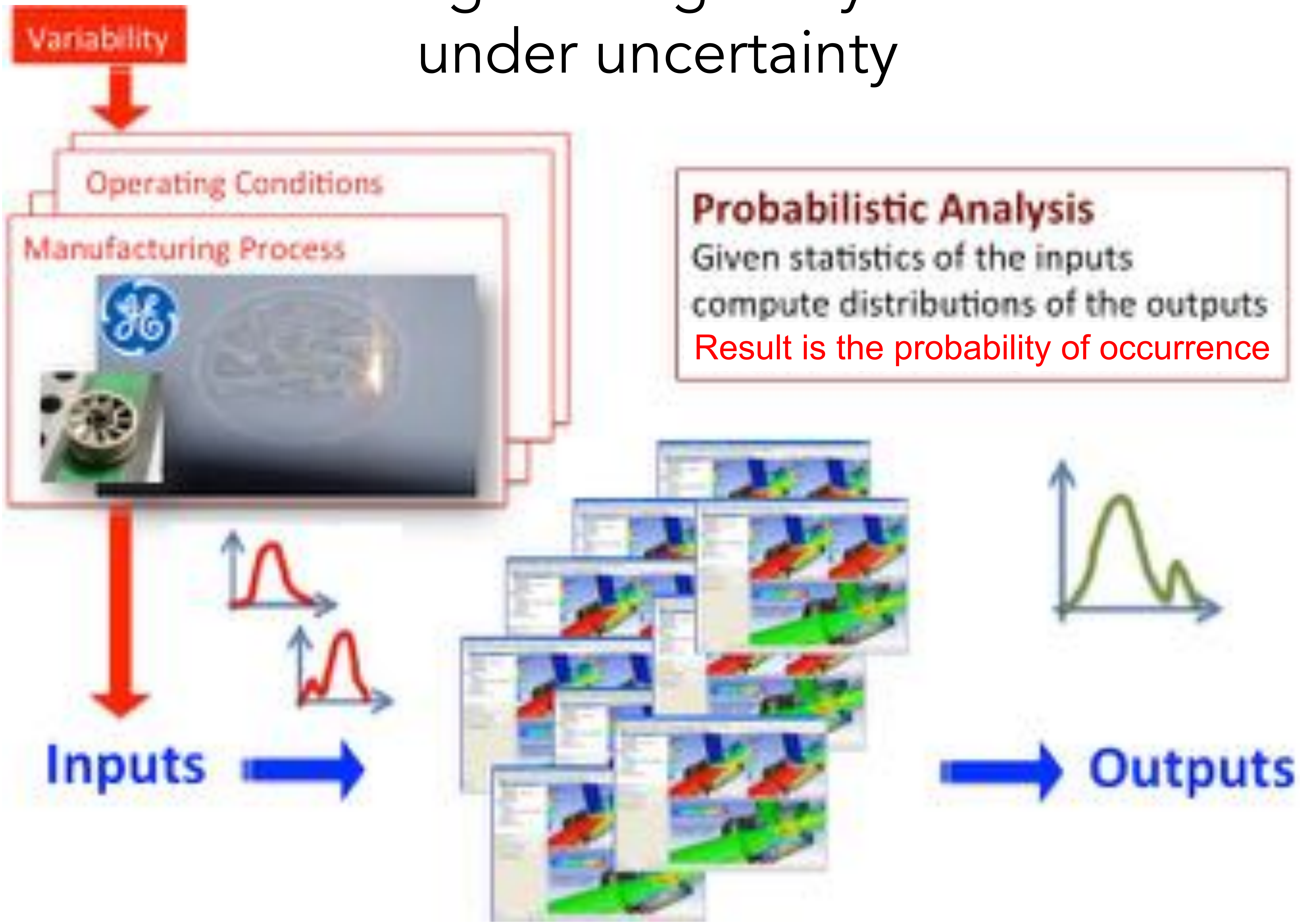
engineering analysis



engineering analysis under uncertainty



engineering analysis under uncertainty

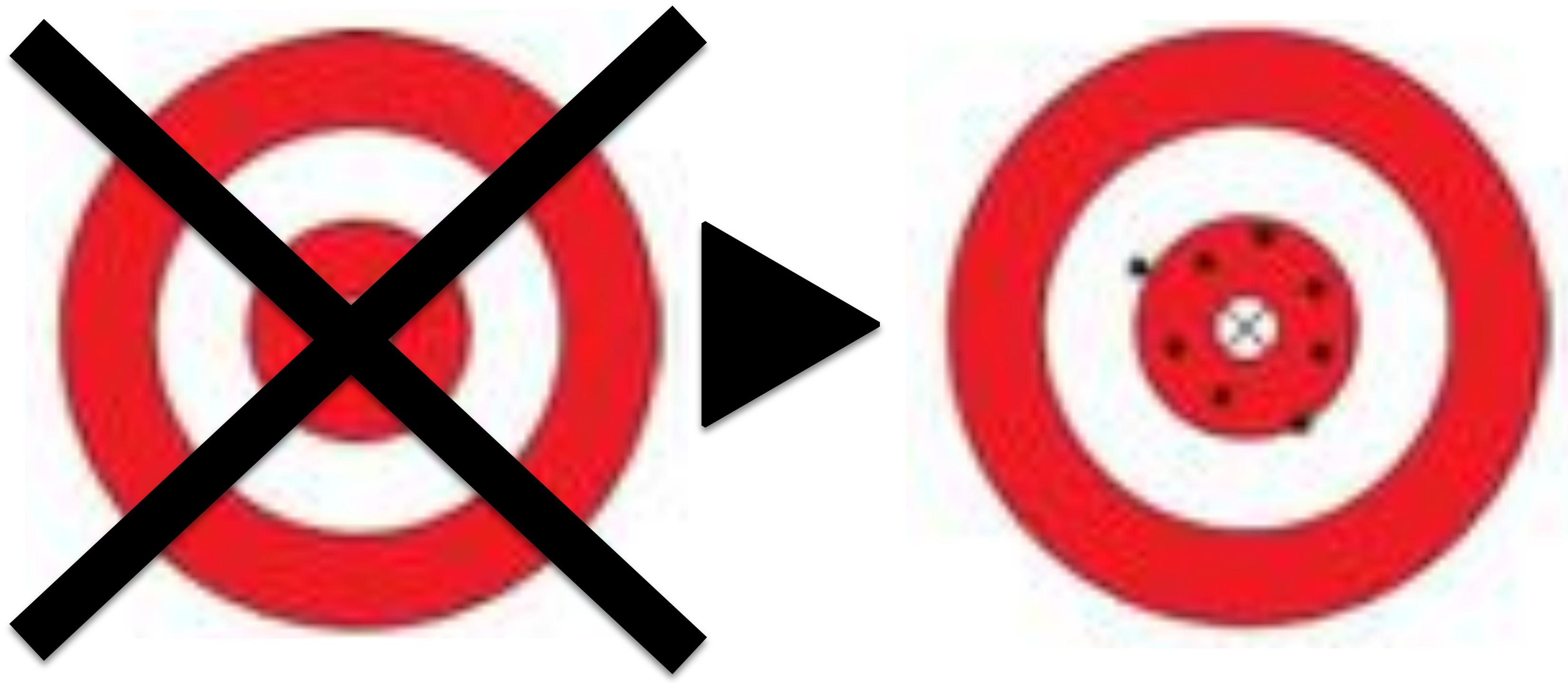


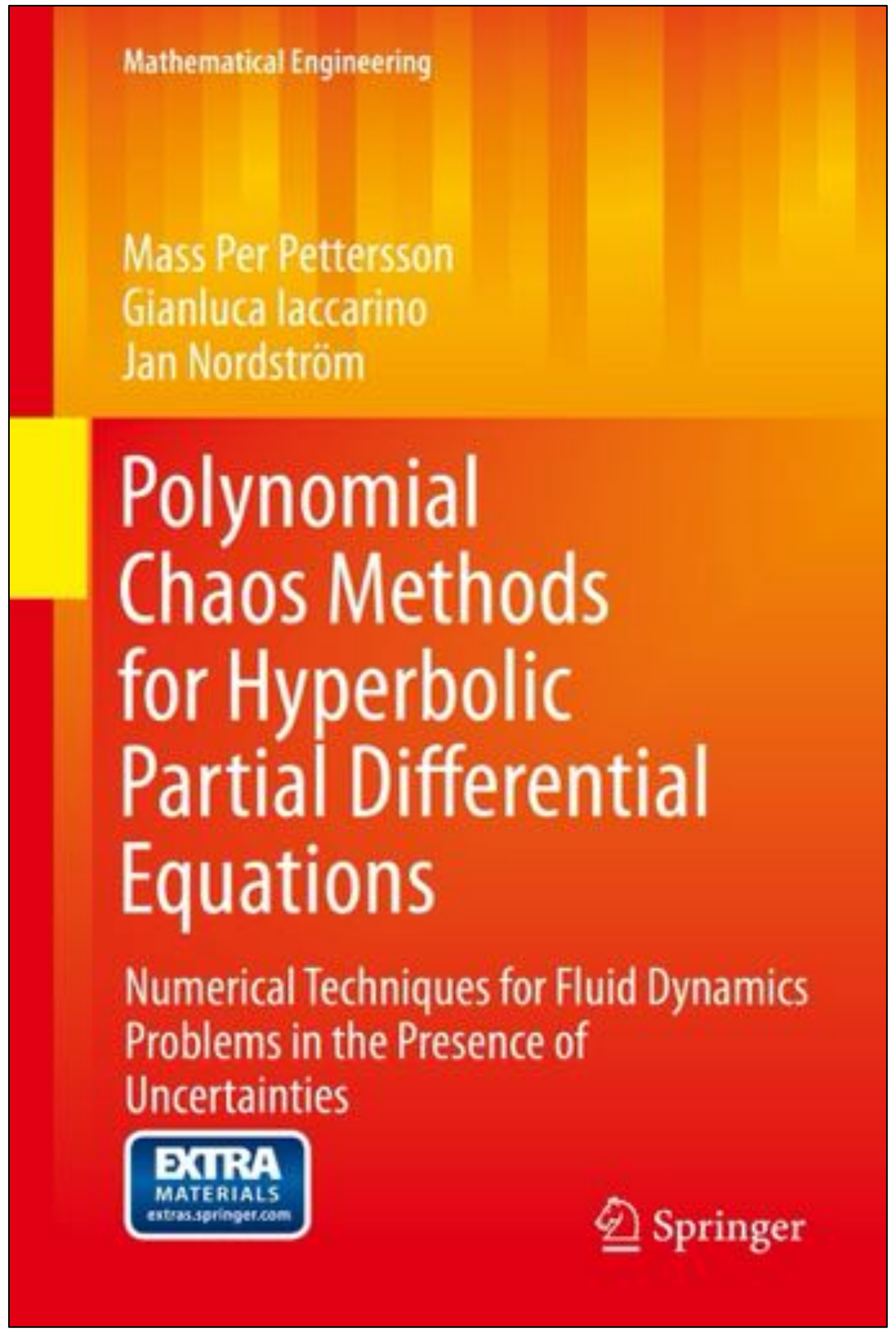
engineering analysis
under uncertainty

Uncertainty = Variability ▶ **Probabilistic analysis**

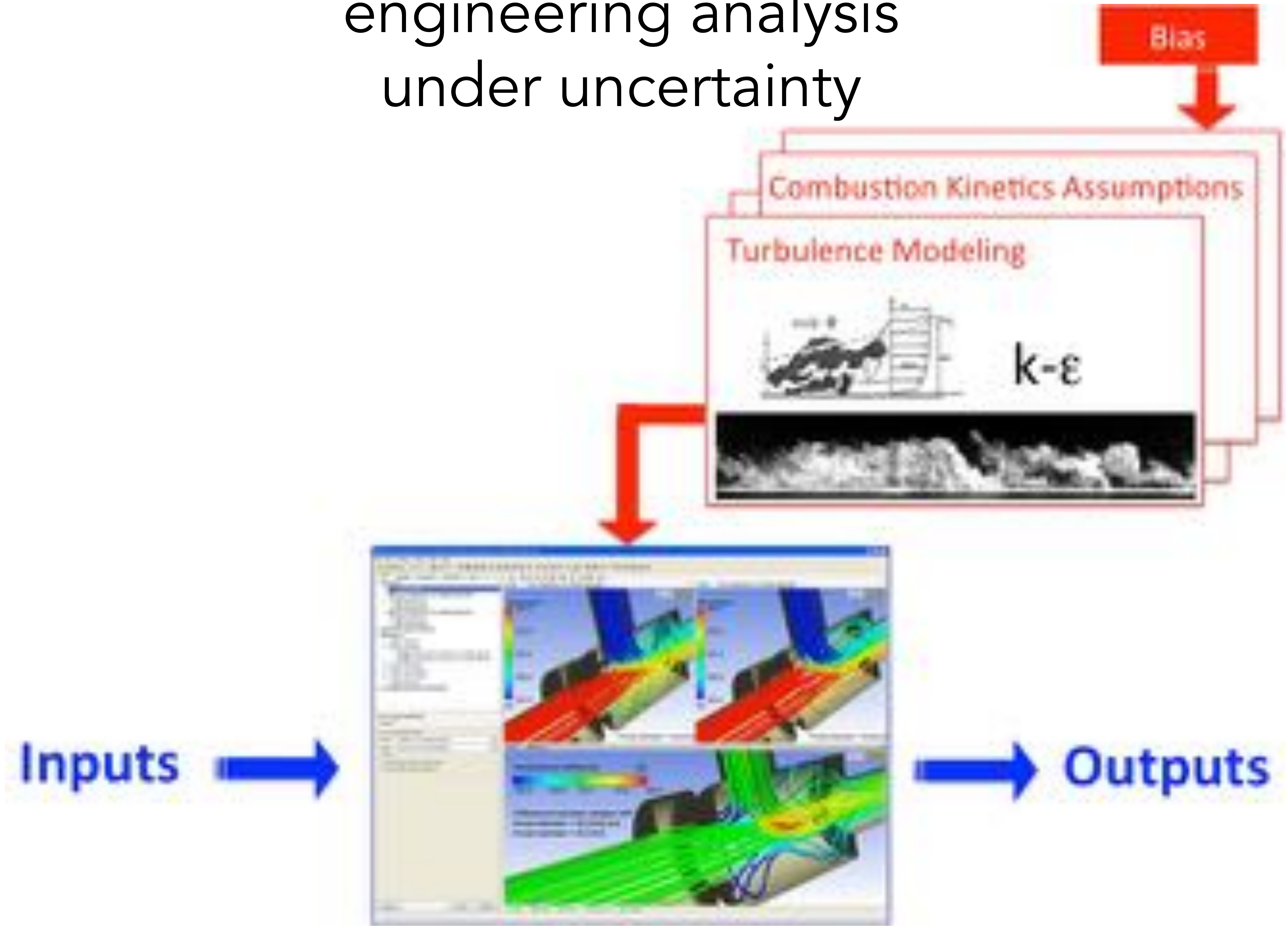
sampling strategies
- Monte Carlo
- quasi random sequences
- Latin Hypercube
- …

approximation strategies
- stochastic collocation
- polynomial chaos
- …

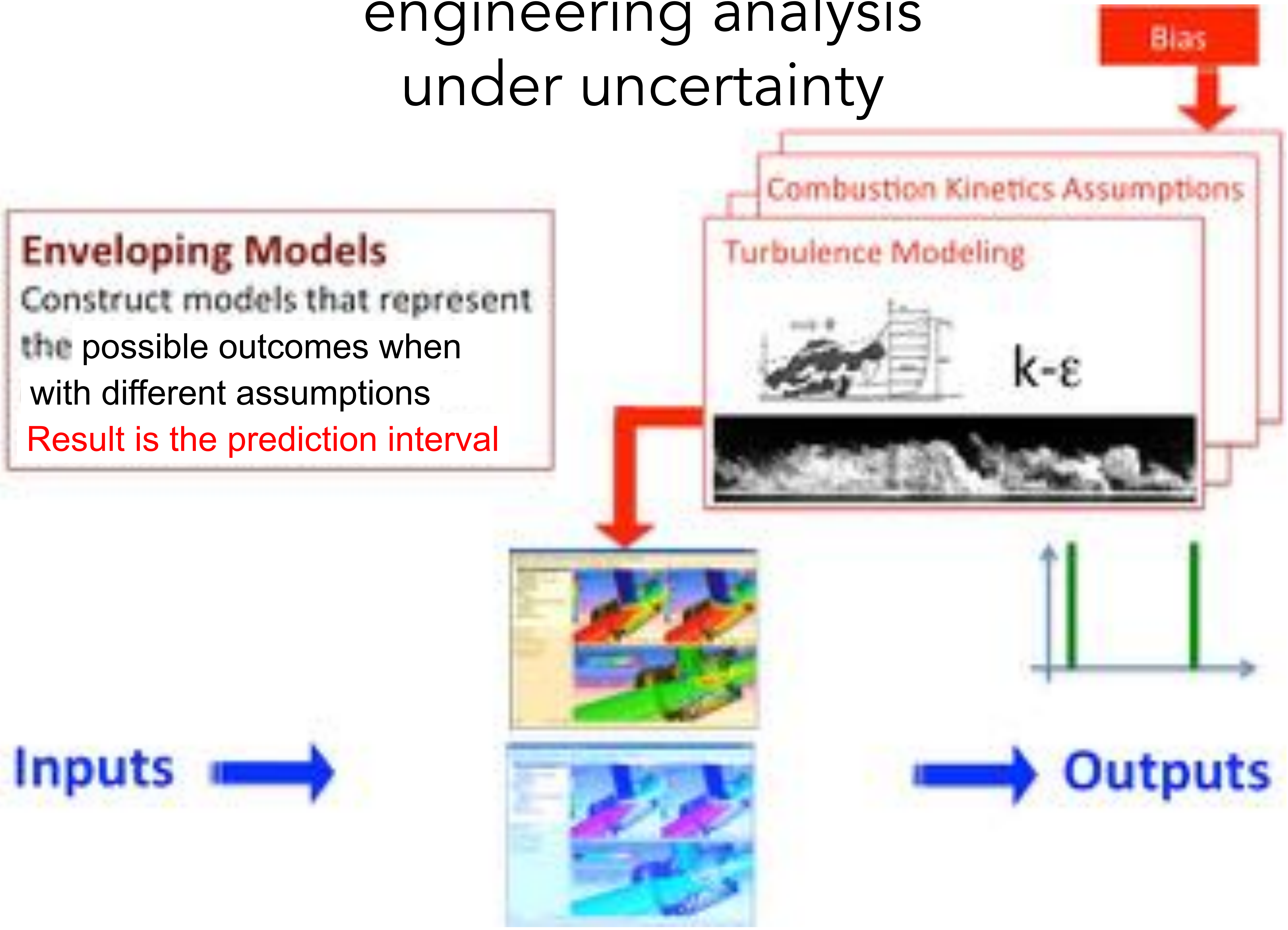




engineering analysis under uncertainty



engineering analysis under uncertainty



engineering analysis under uncertainty

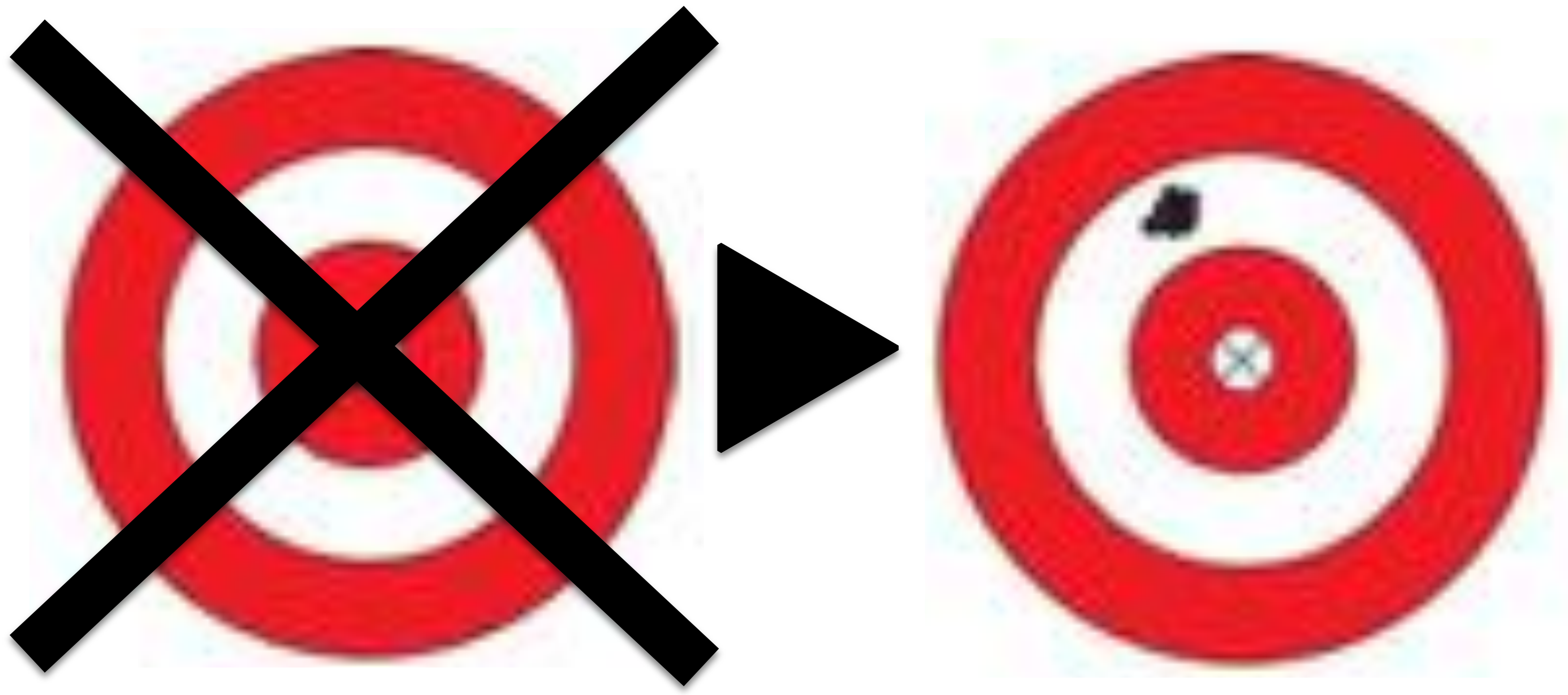
Uncertainty = Bias ▶ non probabilistic methods

Physics based

- Enveloping methods for turbulence

Formal bounds

- best/worst case analysis
- interval analysis
- …



PHYSICAL REVIEW FLUIDS 2, 024605 (2017)

Eigenspace perturbations for uncertainty estimation of single-point turbulence closures

Gianluca Iaccarino, Aashwin Ananda Mishra,* and Saman Ghili
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(Received 12 September 2016; published 27 February 2017)

Reynolds-averaged Navier-Stokes (RANS) models represent the workhorse for predicting turbulent flows in complex industrial applications. However, RANS closures introduce a significant degree of epistemic uncertainty in predictions due to the potential lack of validity of the assumptions utilized in model formulation. Estimating this uncertainty is a fundamental requirement for building confidence in such predictions. We outline a methodology to estimate this structural uncertainty, incorporating perturbations to the eigenvalues and the eigenvectors of the modeled Reynolds stress tensor. The mathematical foundations of this framework are derived and explicated. Thence, this framework is applied to a set of separated turbulent flows, while compared to numerical and experimental data and contrasted against the predictions of the eigenvalue-only perturbation methodology. It is exhibited that for separated flows, this framework is able to yield significant enhancement over the established eigenvalue perturbation methodology in explaining the discrepancy against experimental observations and high-fidelity simulations. Furthermore, uncertainty bounds of potential engineering utility can be estimated by performing five specific RANS simulations, reducing the computational expenditure on such an exercise.

DOI: 10.1103/PhysRevFluids.2.024605

I. INTRODUCTION

In spite of over a century of research, no analytical solutions for the equations governing turbulent flows are available. With the present state of computational resources, a purely numerical resolution of turbulent time and length scales encountered in engineering problems is not viable in industrial design practice. Consequently, almost all investigations have to resort to some degree of modeling. Turbulence models are constitutive relations attempting to relate quantities of interest to flow parameters using assumptions and simplifications derived from physical intuition and observations. Reynolds-averaged Navier-Stokes (RANS) -based models represent the pragmatic recourse for complex engineering flows, with a vast majority of simulations, in both academia and industry, resorting to this avenue. Despite their widespread use, RANS-based models suffer from an inherent structural inability to replicate fundamental turbulence processes and specific flow phenomena, as they introduce a high degree of epistemic uncertainty into the simulations arising due to the model form.

Uncertainty quantification for RANS-based closures attempts to assess the trustworthiness of model predictions of quantities of interest and is thus of considerable utility in establishing RANS models as tools for engineering applications. To address structural uncertainties, Singh and Duraisamy [1] and Parish and Duraisamy [2] utilize a data-driven approach wherein full-field data sets are utilized to infer and calibrate the functional form of model discrepancies. This is augmented by machine learning algorithms to reconstruct model corrections. Ling and Templeton [3] employ a data-driven approach along with a variety of machine learning algorithms to identify regions in the flow where high degrees of model-form uncertainty are extant. Recently, a physics-based nonparametric approach to estimate the model-form uncertainties has been developed by Emory *et al.* [4]. This framework approximates structural variability via sequential perturbations injected

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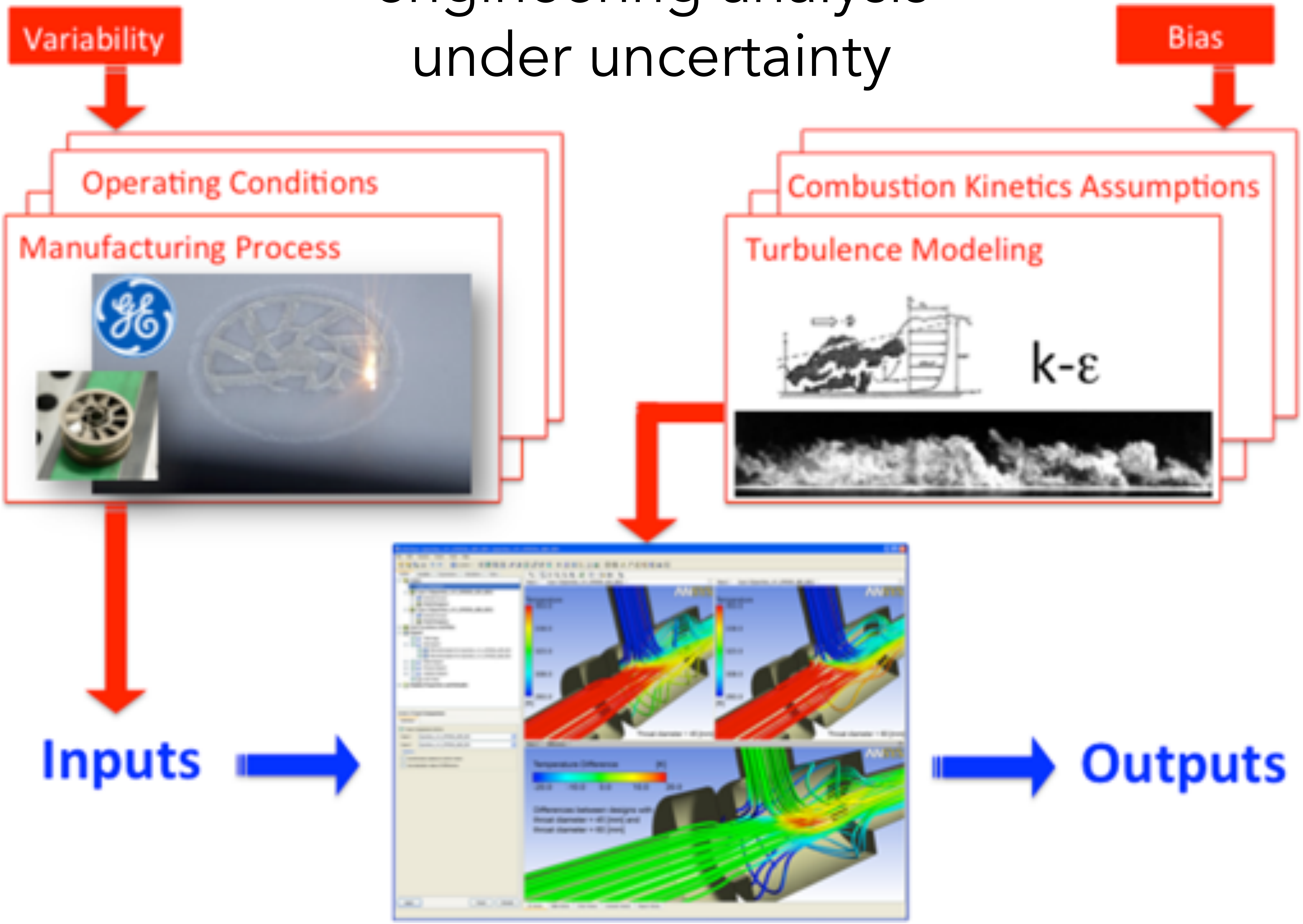
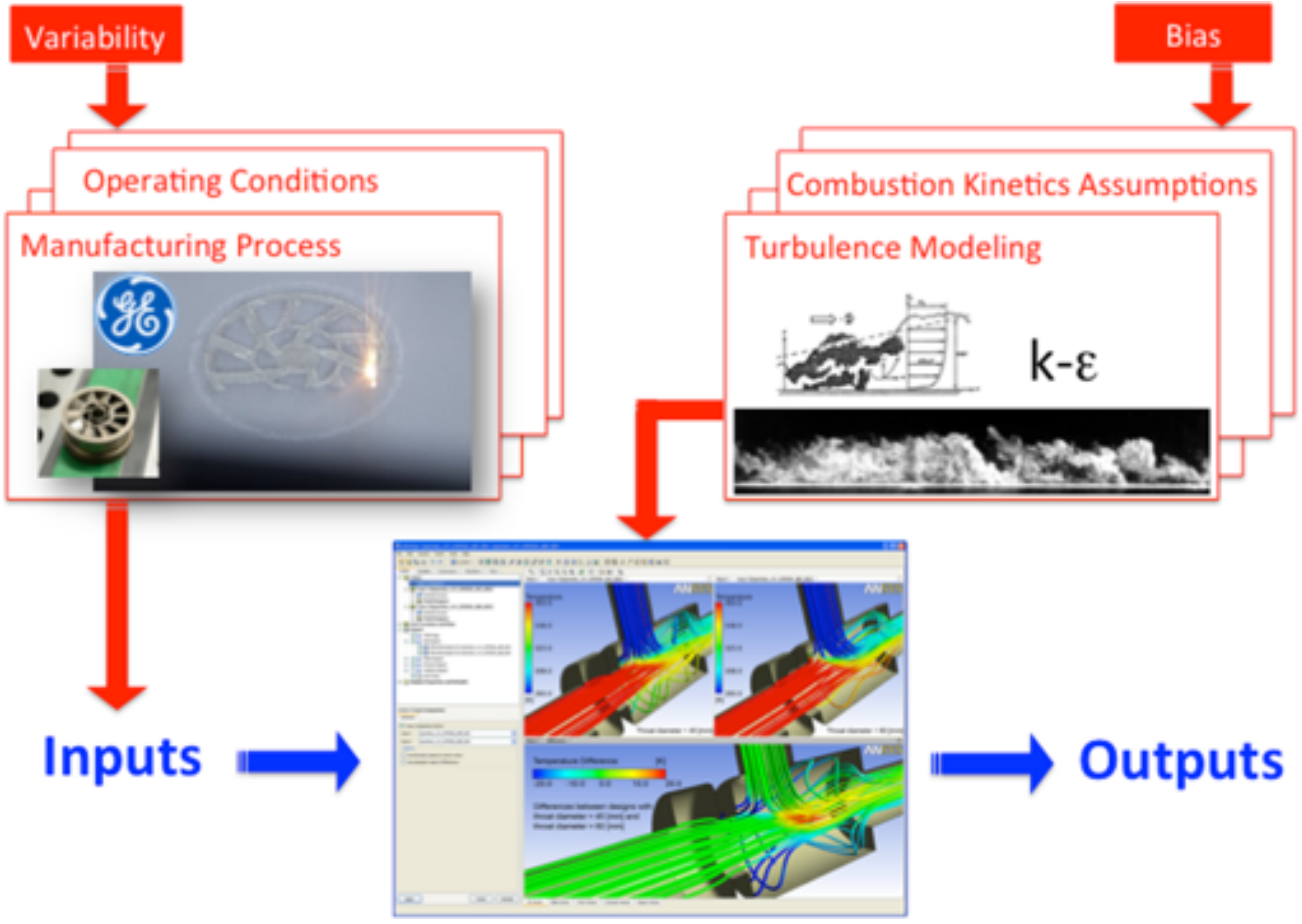
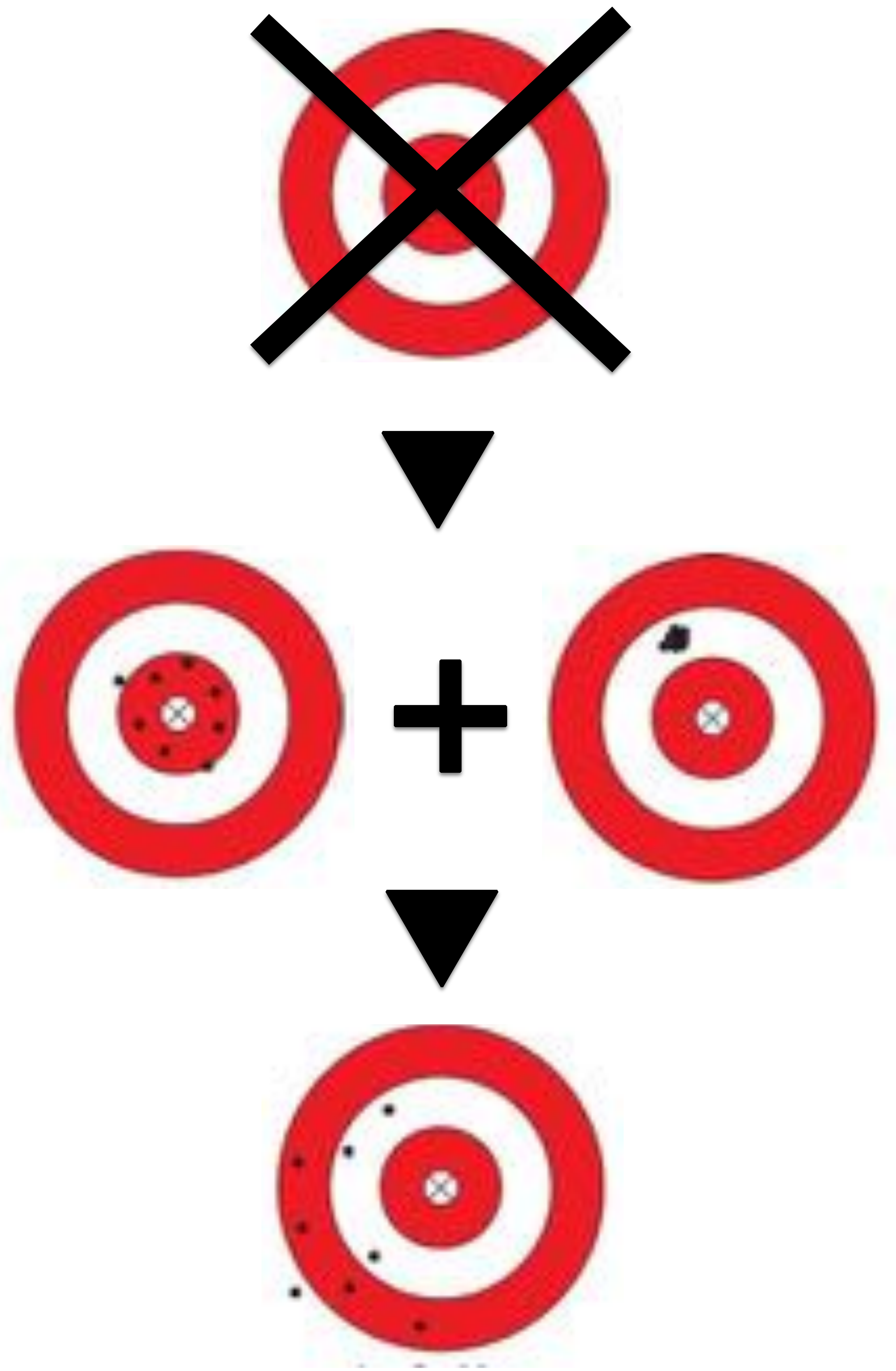
engineering analysis under uncertainty



engineering analysis under uncertainty





ME270

advances in computing
with uncertainties

topics for today

communicating uncertainties

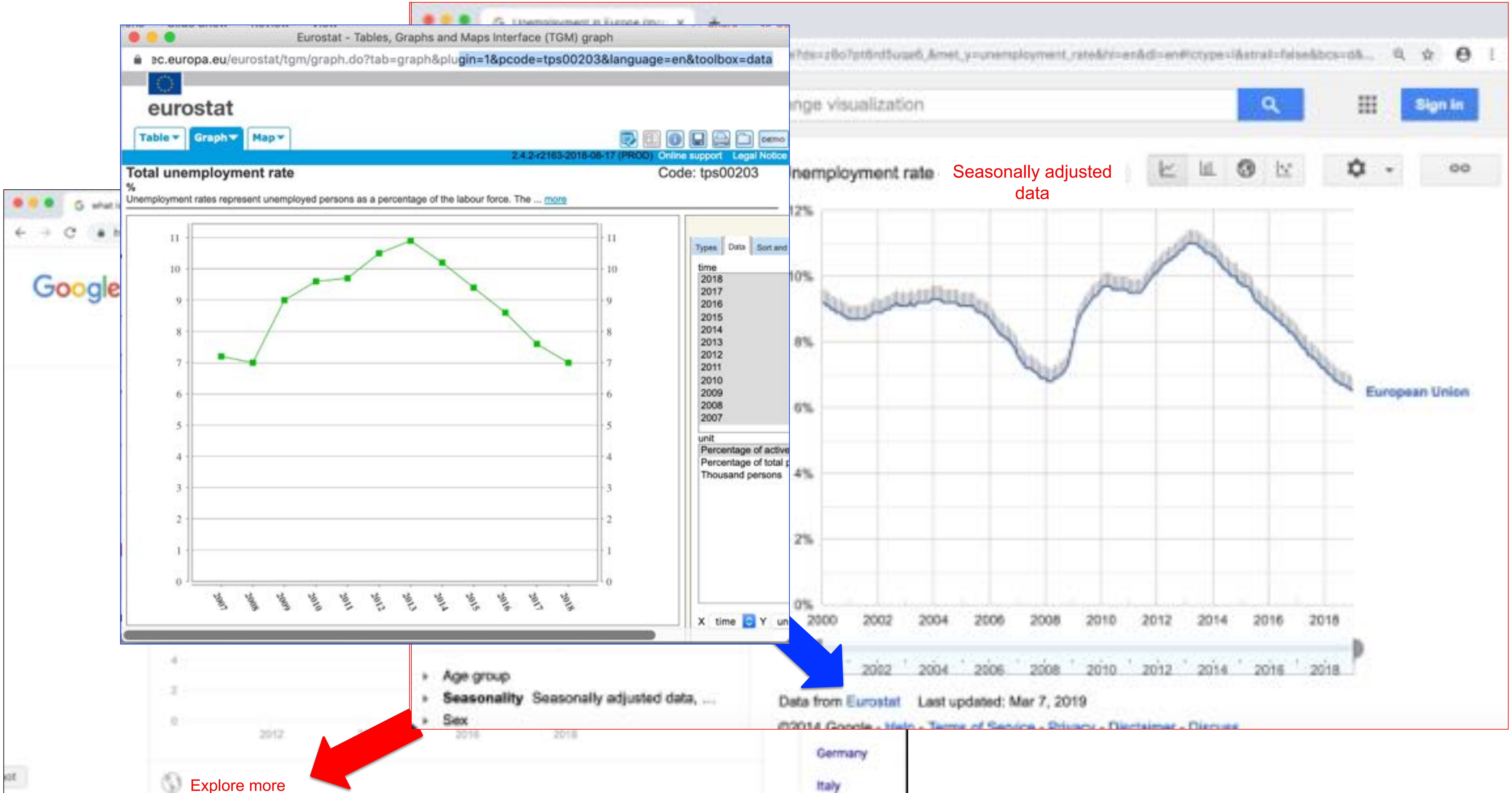
optimization with uncertainties

uncertainties without probabilities

communicating uncertainties

official economic statistics

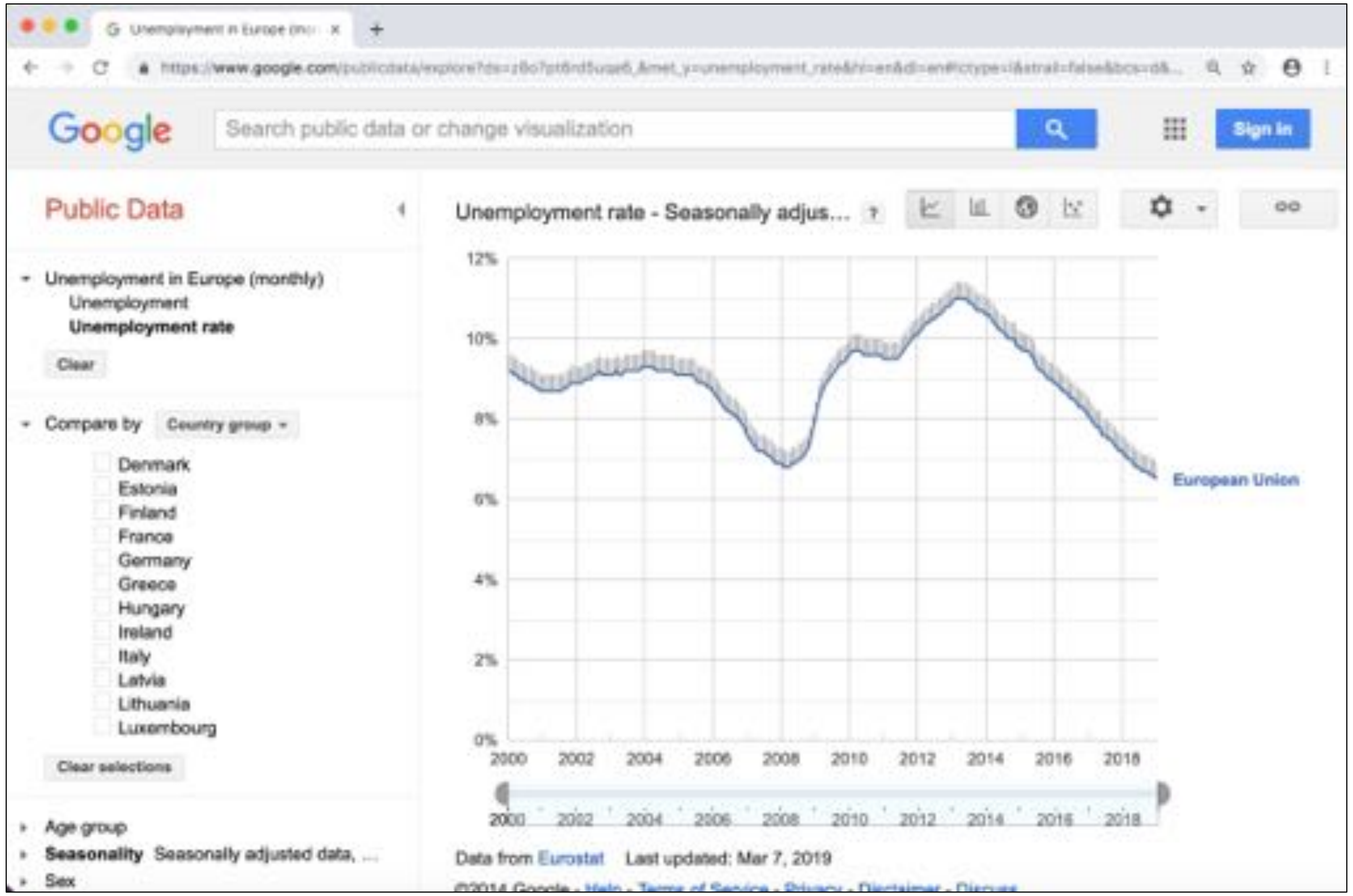
official economic statistics



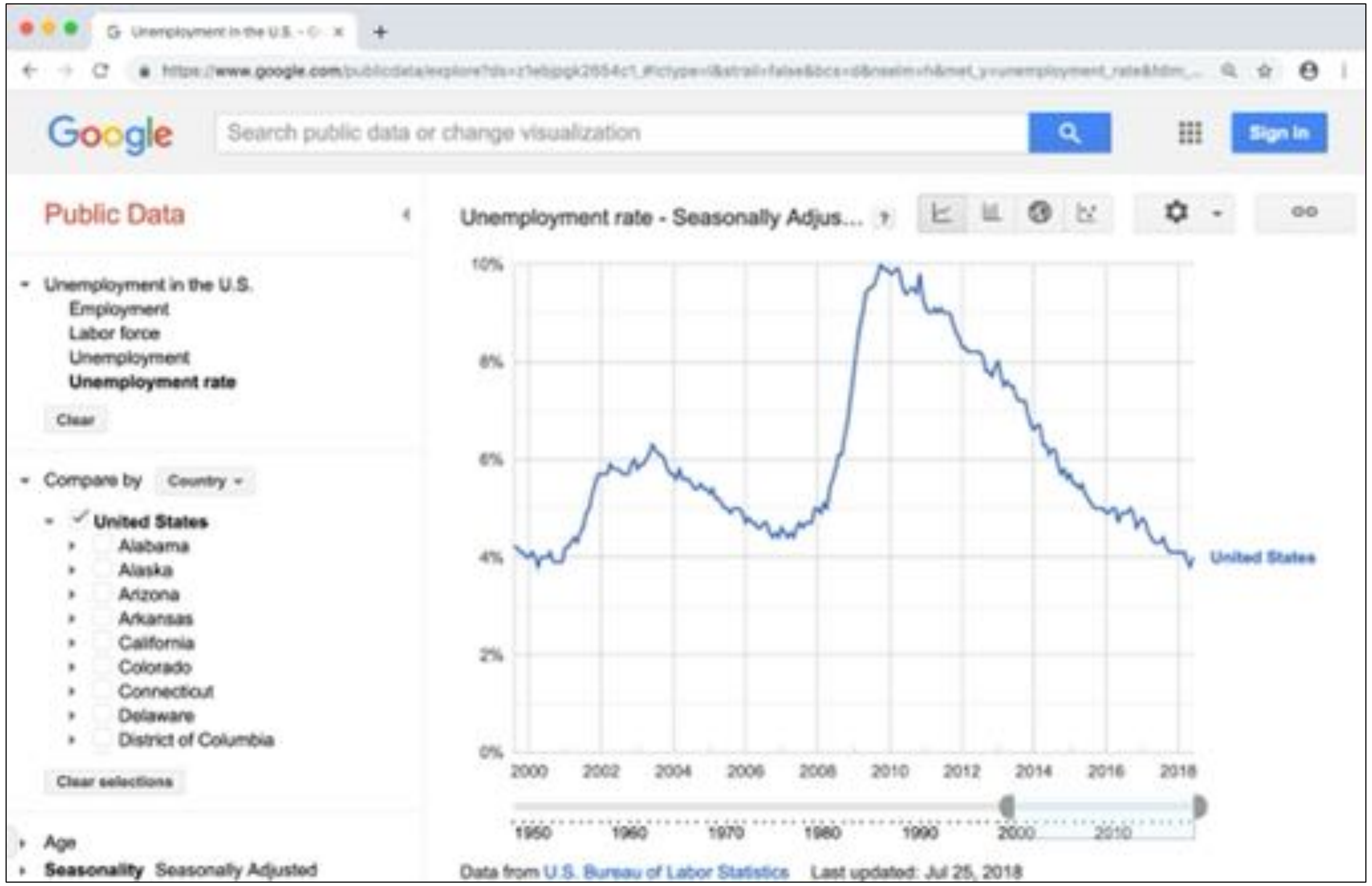
the unemployment rate is 6.8%!

official economic statistics

What is the unemployment rate in Europe? *What is the unemployment rate in US?*

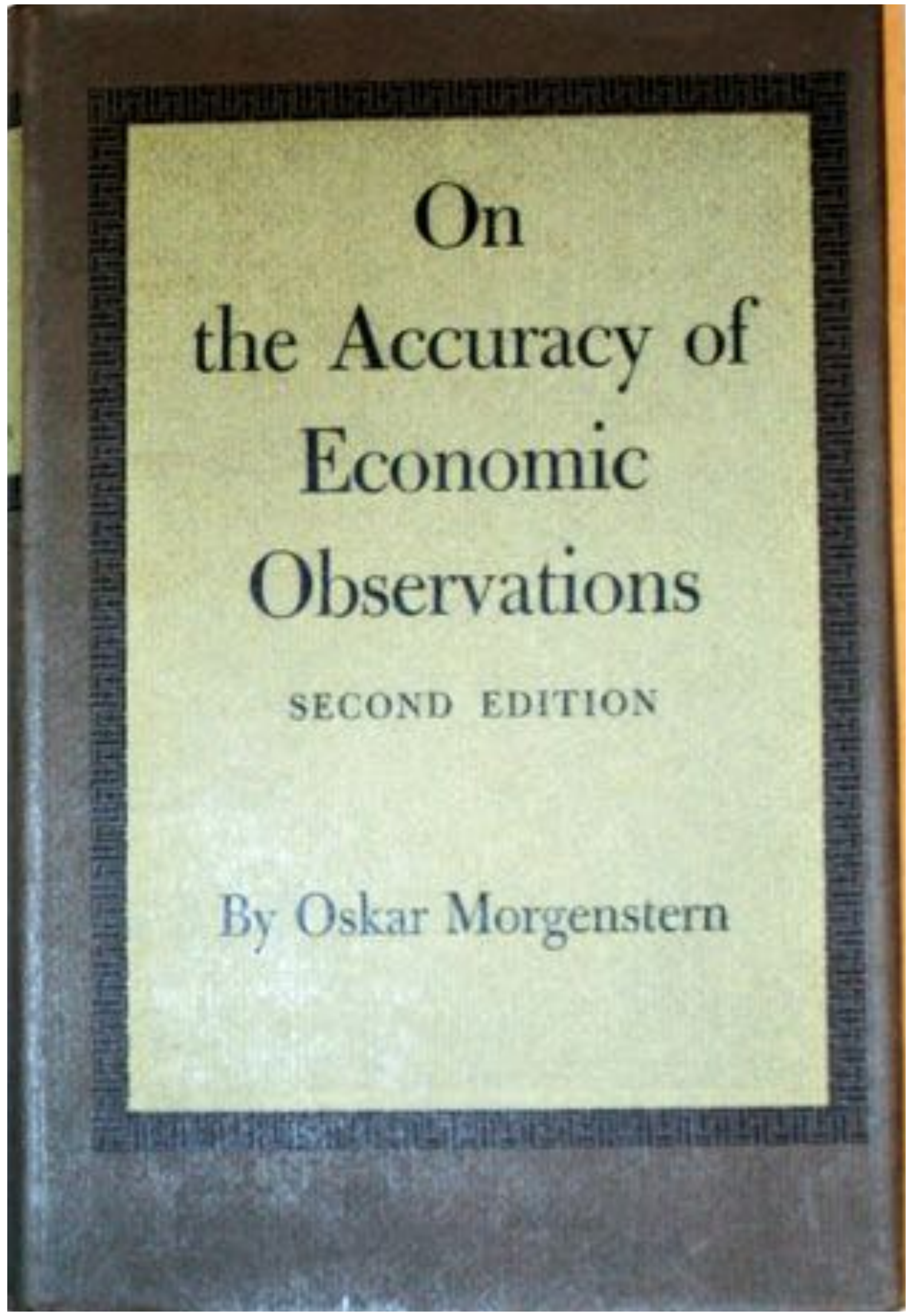


Data from Eurostat

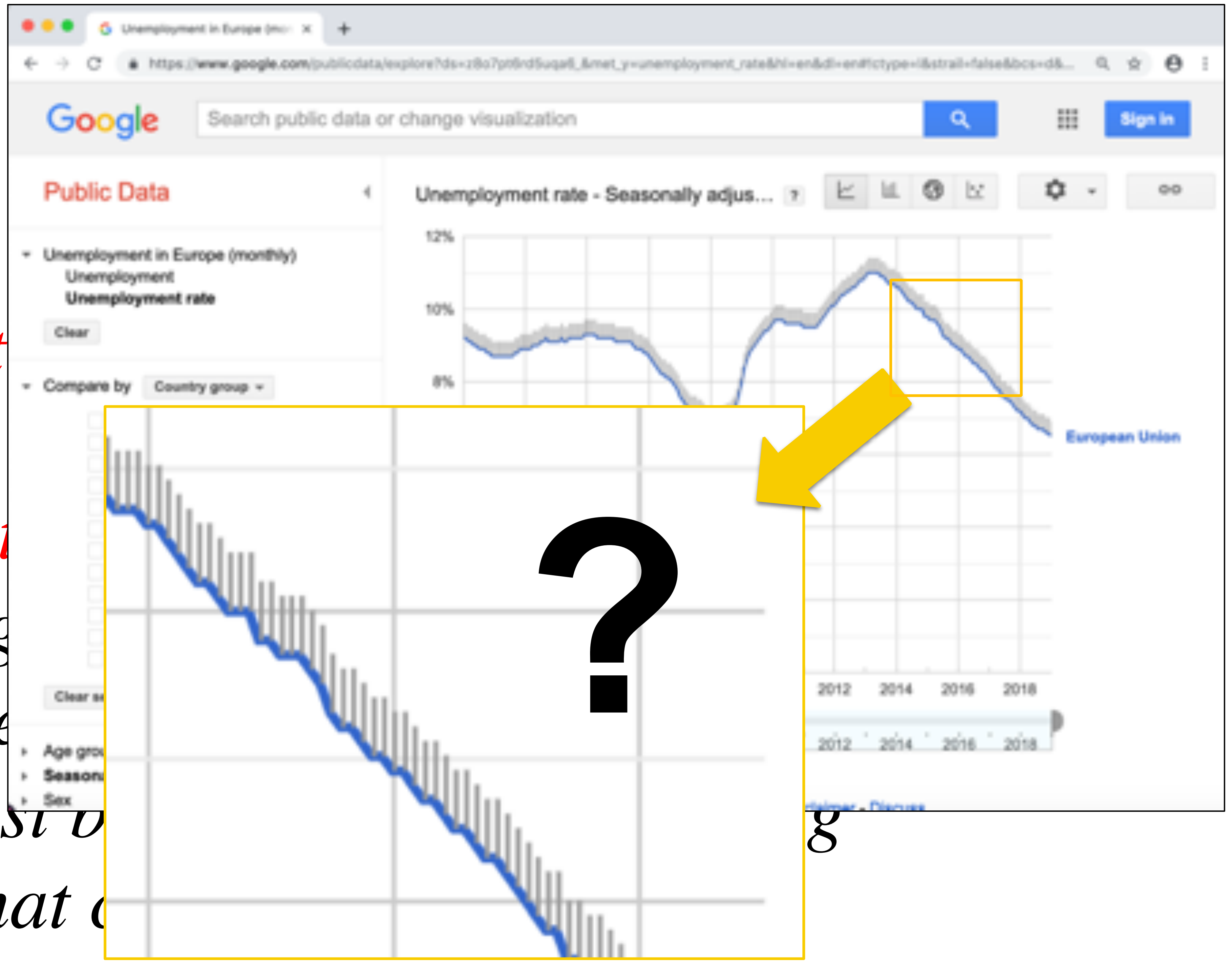


Data from US Bureau of Labor Statistics

errors in official economic statistics



Perhaps the greatest st
even at short notice, is
be only published toget
error. Even if only roug
produce a wholesome e
economic statistics must b
claims and demands that c
scientifically. The publication of error estimates would have a profound influence on the whole situation.



Morgenstern (1963a, pp. 304–05)

are there errors?

the unemployment rate is "about" 6.8%!

Sampling Errors & Non-Sampling Errors

- limited number of respondents

probabilistic methods

- delays in data collection
- inability to obtain information from a group or a region
- temporal/seasonal factors
- mistakes made by respondents
- data collection and processing errors
- …

non probabilistic methods

errors or uncertainties?

"Errors in scientific results due to *software bugs* are not limited to a few high-profile cases that lead to retractions and are widely reported. Here I estimate that in fact most scientific results are probably wrong if data have passed through a computer, and that these errors may remain largely undetected. The opportunities for both subtle and profound errors in software and data management are boundless, yet they remain surprisingly underappreciated."
Soergel, 2015

"Any computer code longer than 600 lines has a *bug*!"
Jameson, 2007

verification is for errors....
not the topic of this class

uncertainties...

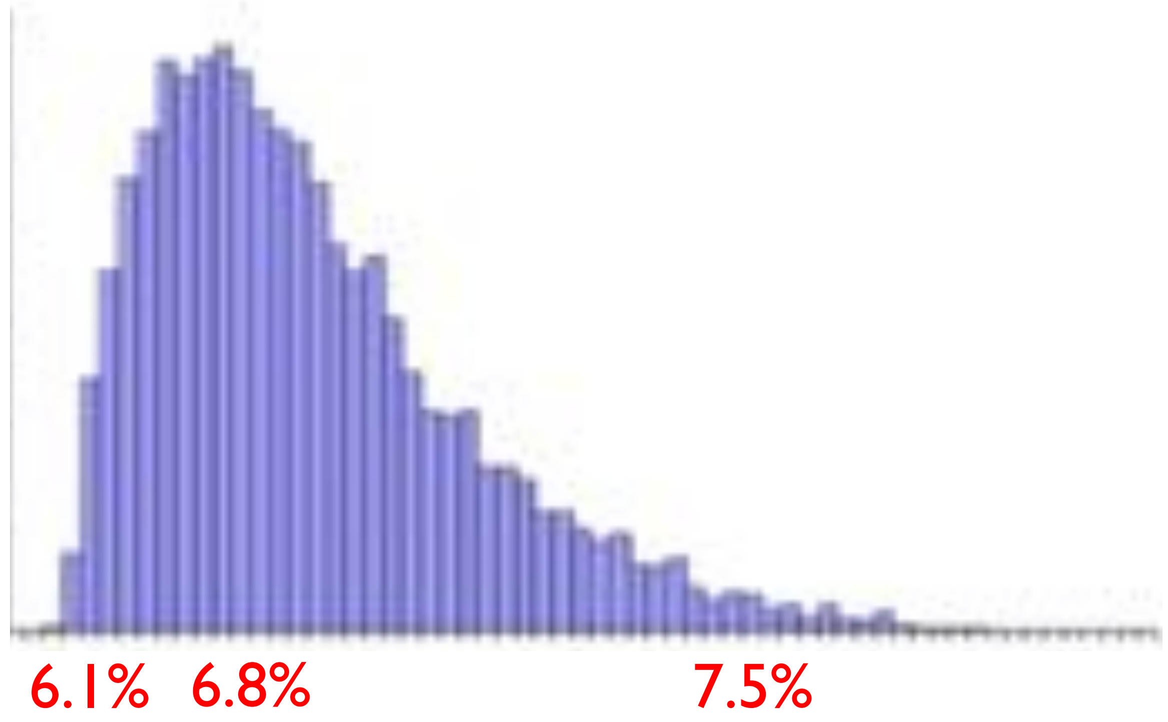
probabilistic vs non-probabilistic
aleatory vs epistemic
stochastic vs deterministic
irreducible vs reducible
….

the unemployment rate is 6.8%!

▼

"uncertainty quantification"

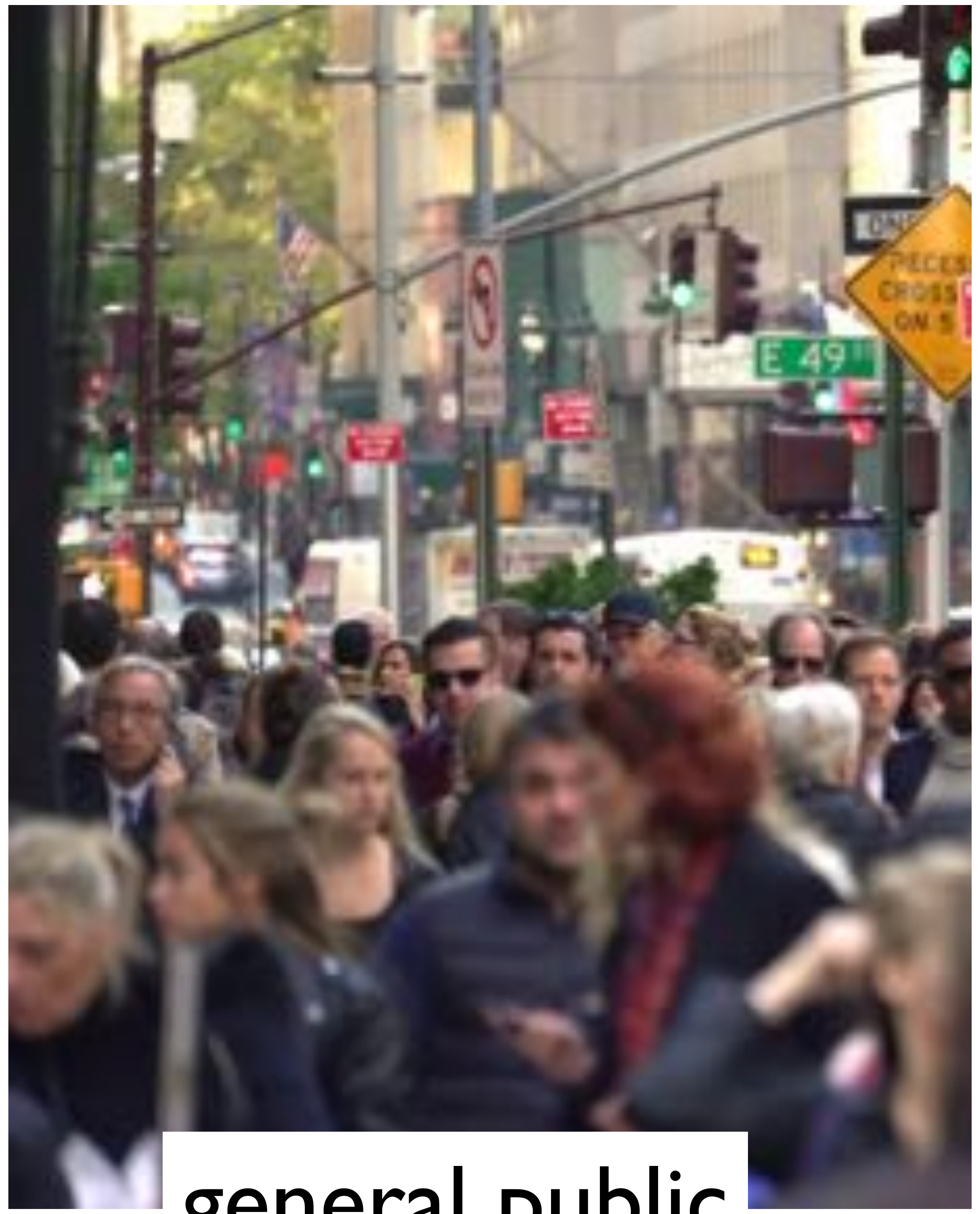
▼

the unemployment rate is 

communicating uncertainties: audience

Perhaps not
- can be cumbersome and confusing
- erodes confidence in the message
- …

Certainly yes
- increases understanding
- might lead to future improvements
- fosters collaboration and transparency
- …



general public


domain experts

communicating uncertainties: audience

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?

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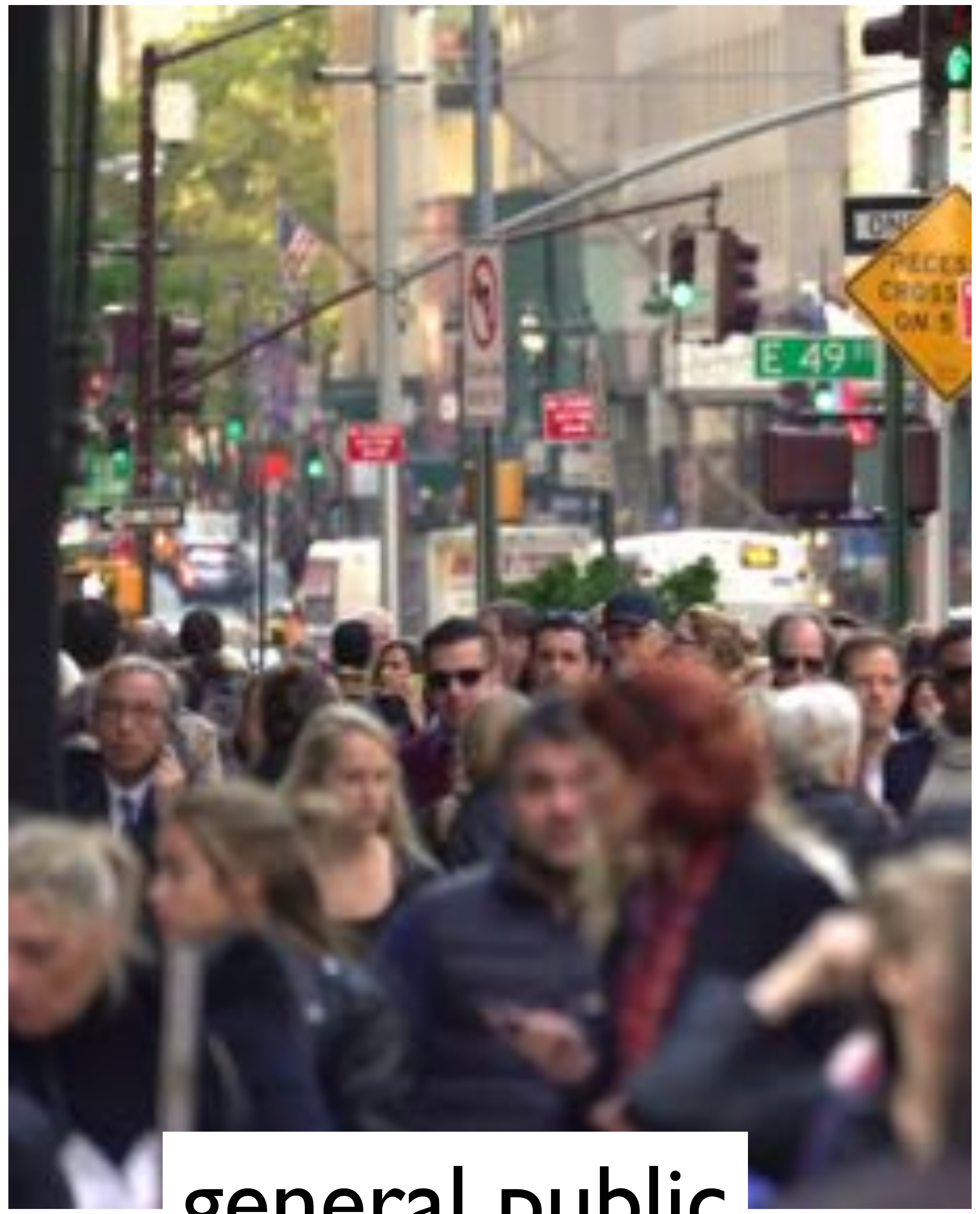


general public

decision makers

domain experts

communicating uncertainties: metrics

Qualitative vs Quantitative

Level	Legal standard
11	virtually certain
10	‘beyond a reasonable doubt’
9	‘clear and convincing evidence’
8	‘clear showing’
7	‘substantial and credible evidence’
6	‘preponderance of the evidence’
5	‘clear indication’
4	‘probable cause’/’reasonable belief’
3	‘reasonable indication’
2	‘reasonable, articulable grounds for suspicion’
1	‘no reasonable grounds for suspicion’/’inchoate hunch’/’fanciful conjecture’
0	Insufficient even to support a hunch or conjecture

intuitive, descriptive

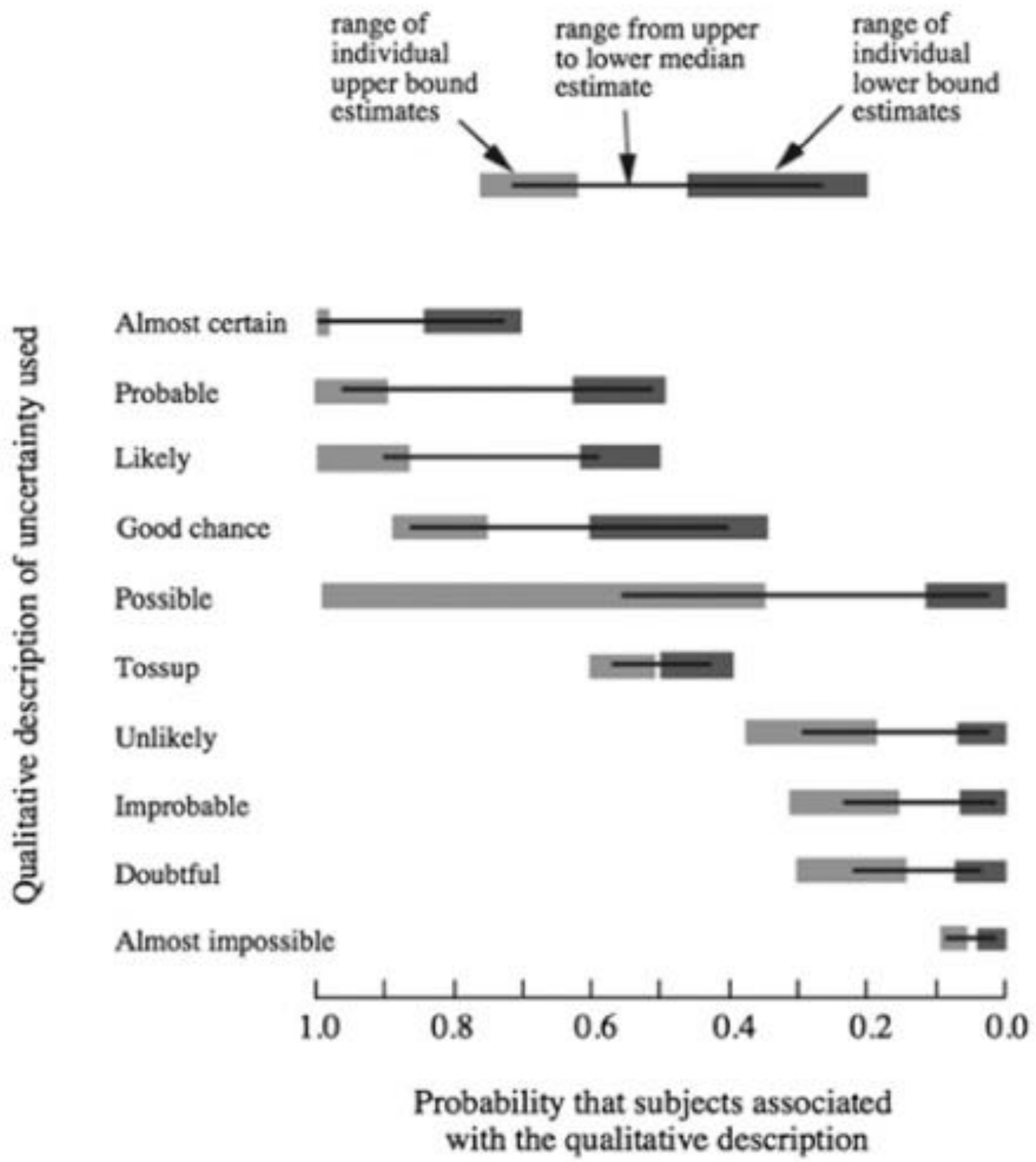
- Count
- Missing Count
- Sum
- Mean
- Standard Deviation (Std Dev)
- Standard Error (Std Error)
- Lower 95% Confidence Limit for the Mean (95% LCL)
- Upper 95% Confidence Limit for the Mean (95% UCL)
- Median
- Minimum
- Maximum
- Range
- Interquartile Range (IQR)
- 90th Percentile (90th Pctile)
- Variance
- Mean Absolute Deviation (MAD)
- Mean Absolute Deviation from the Median (MADM)
- Coefficient of Variation (COV)
- Coefficient of Dispersion (COD)
- Skewness
- Kurtosis

technical, objective

communicating uncertainties: metrics

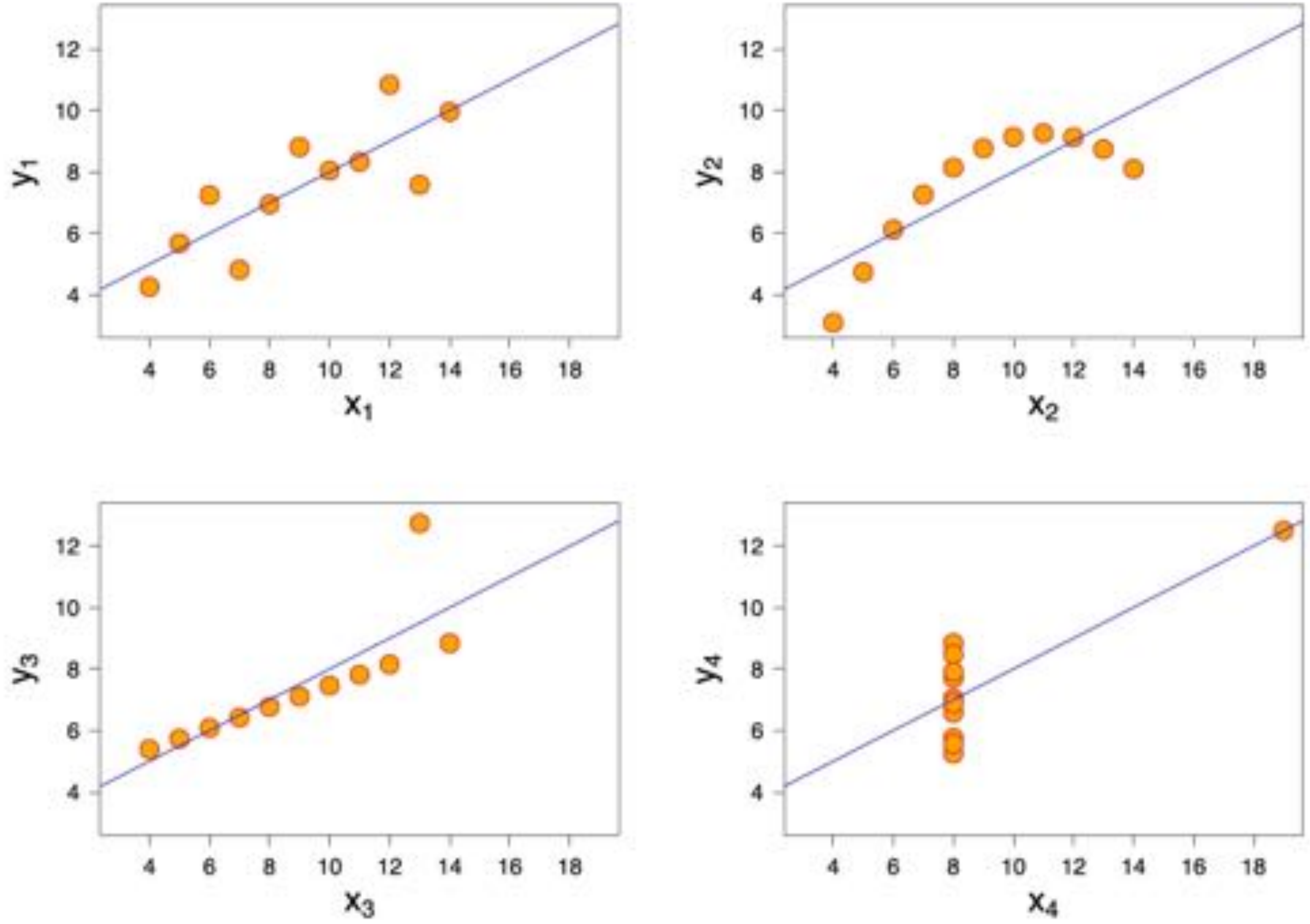
Qualitative vs Quantitative

M. Granger Morgan, www.pnas.org/cgi/doi/10.1073/pnas.1319946111



intuitive, descriptive

Anscombe, F.J. (1973). Graphs in Statistical Analysis. - The American Statistician 27, 1, 17–21.



technical, objective

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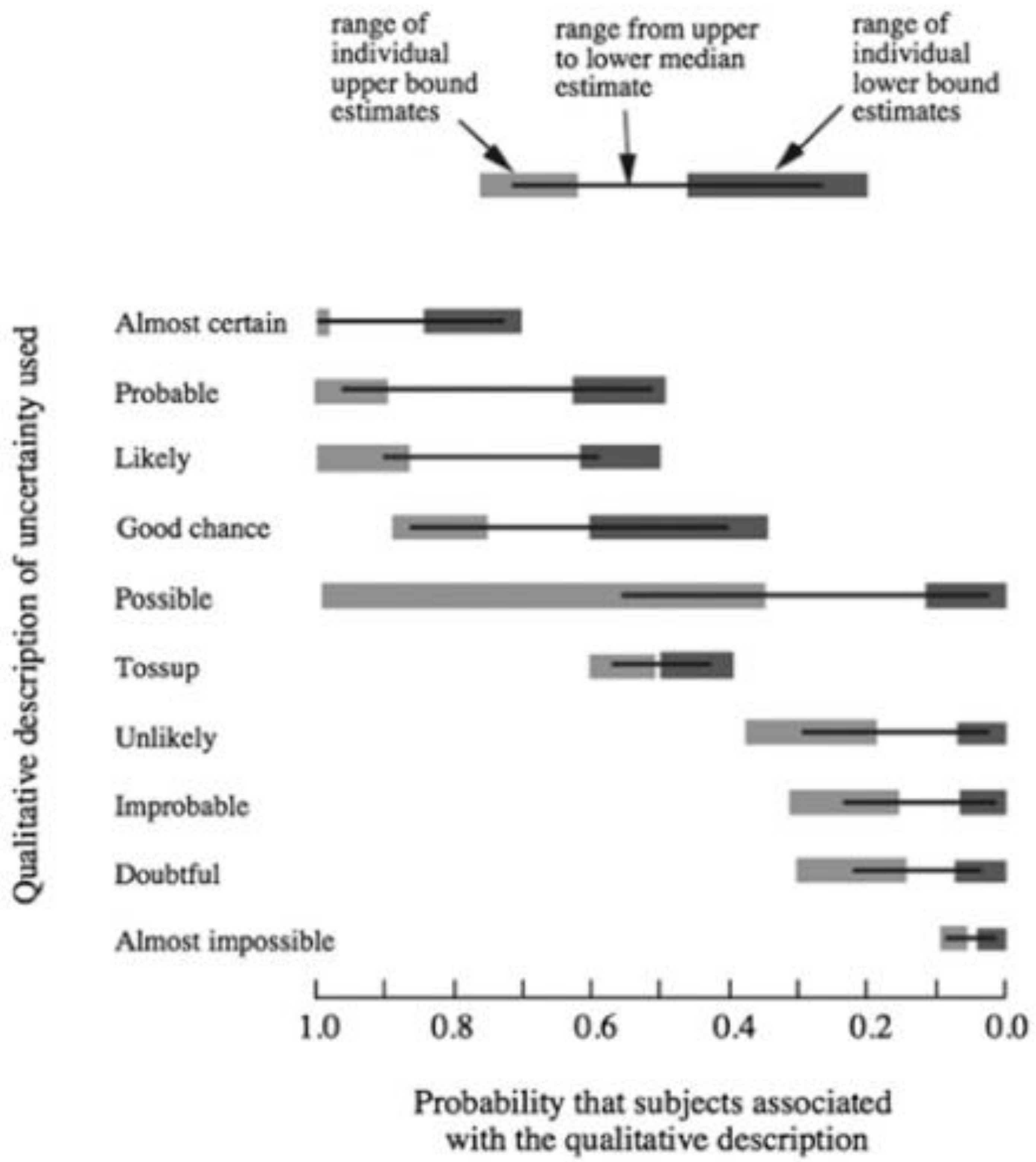
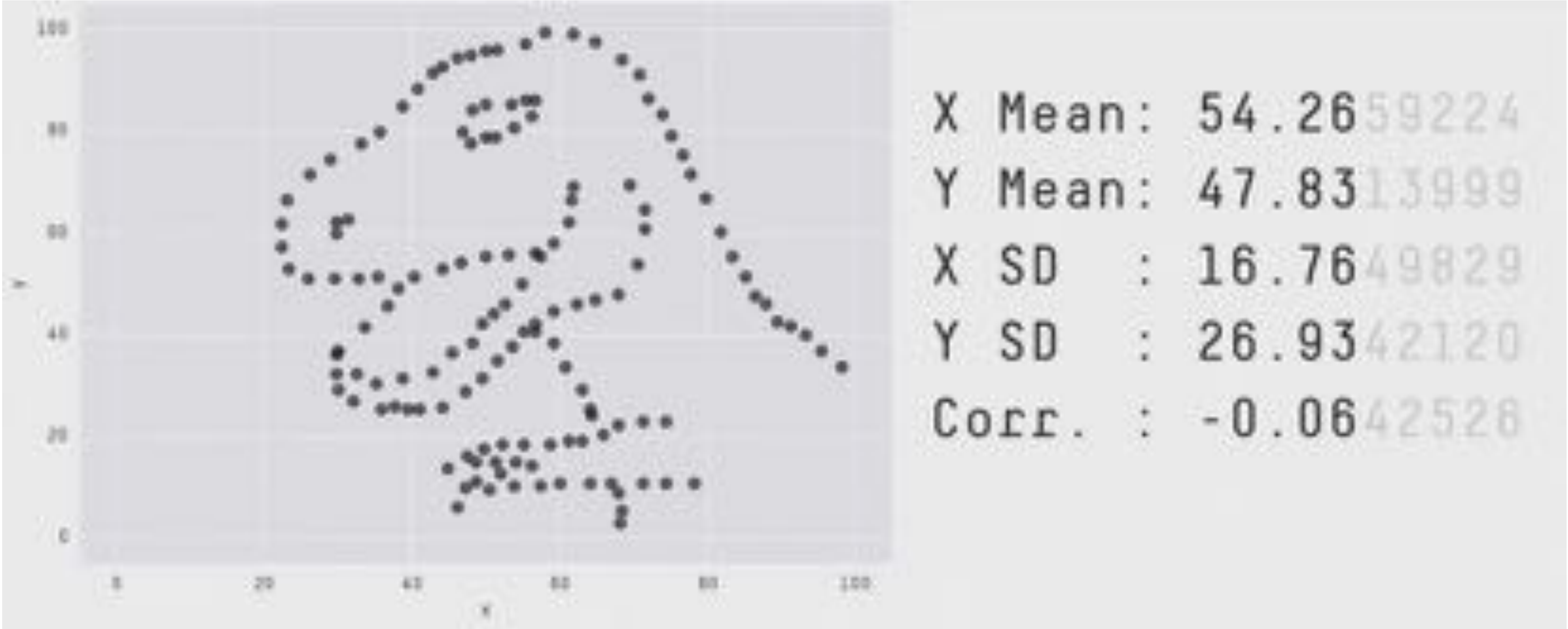


intuitive, descriptive

F. Matejka, G. Fitzmaurice, Autodesk



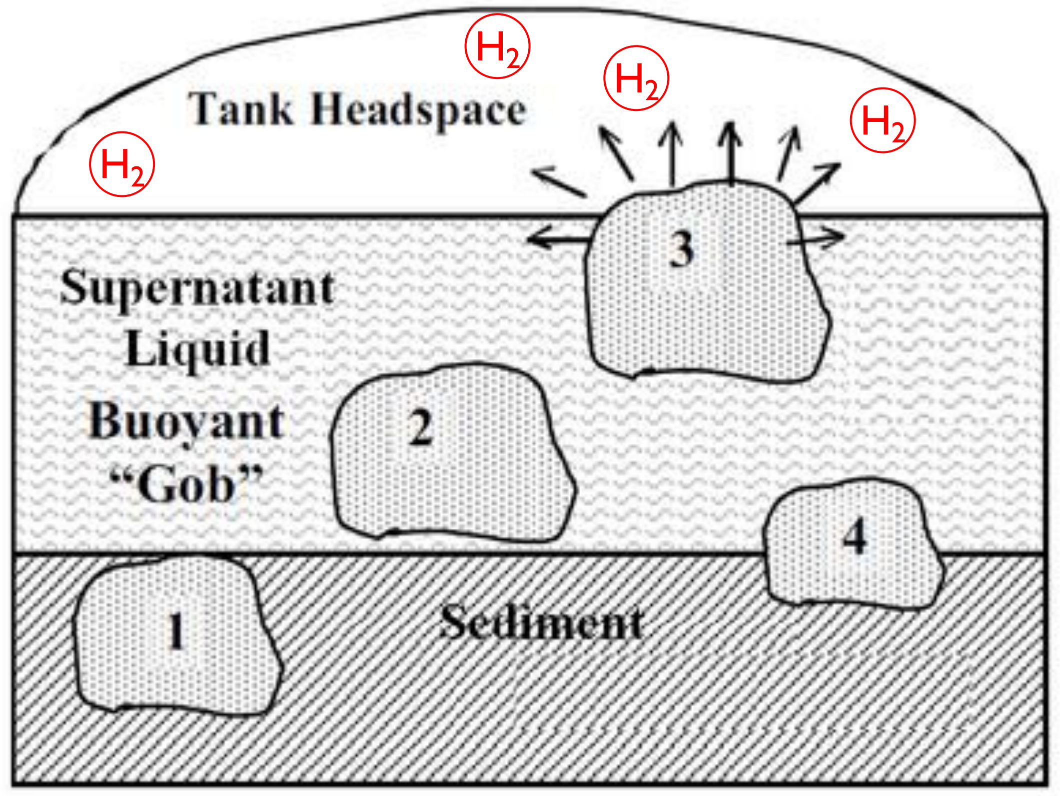
technical, objective

a case study
QMU in high-consequence decisions

QMU in high-consequence decisions

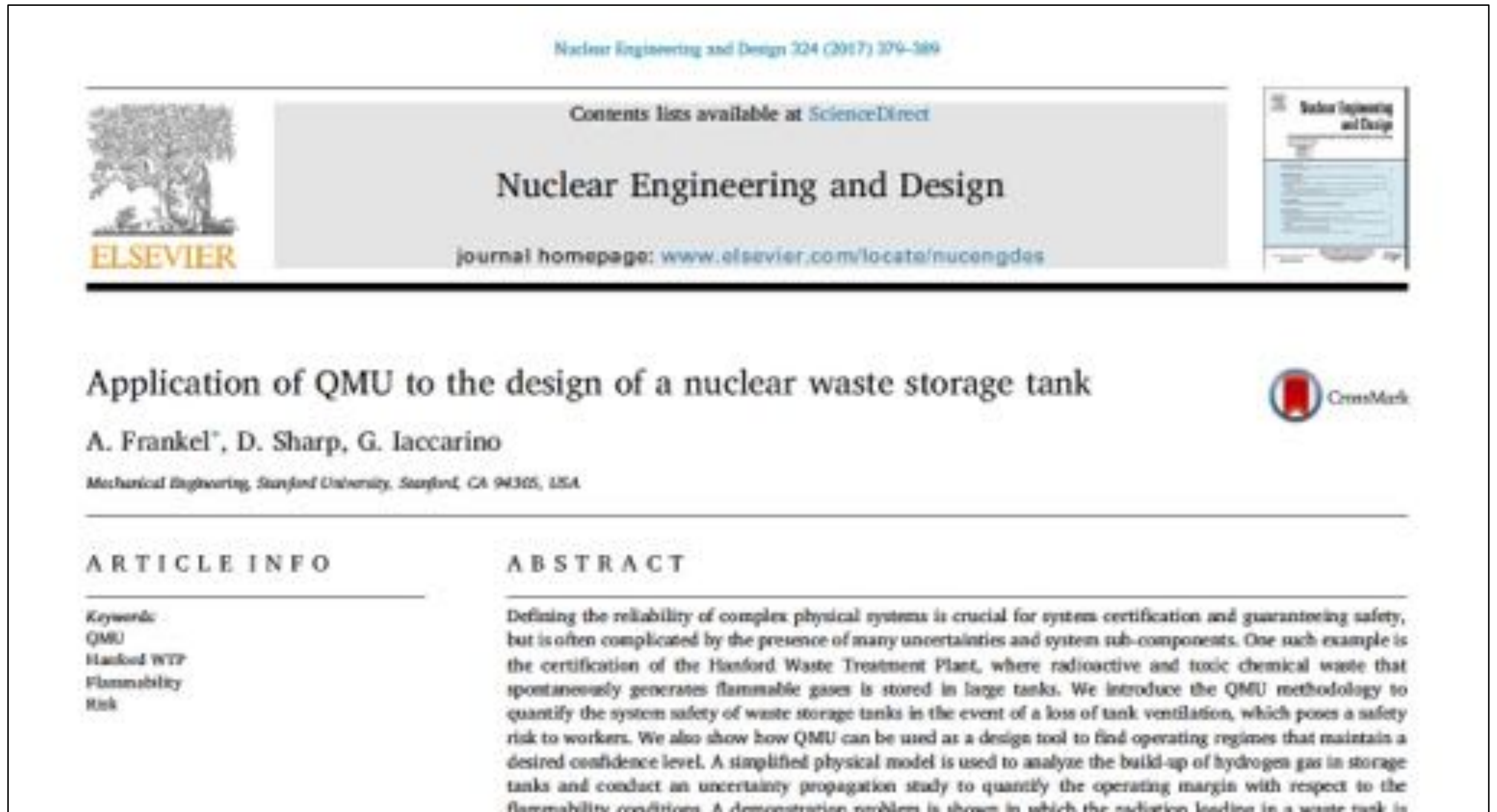
The Hanford site is a repository of leftover waste from nuclear reactors & medical devices

- Safety concern: hydrogen buildup in tanks and explosion risk



Risk assessment involves:

- Complex physical analysis and forecasting
- Careful characterization of the uncertainties
- Identification of remedial actions
- Communication of the outcomes to decision makers



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Application of QMU to the design of a nuclear waste storage tank

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ARTICLE INFO

Keywords:
QMU
Hanford WTP
Flammability
Risk

ABSTRACT

Defining the reliability of complex physical systems is crucial for system certification and guaranteeing safety, but is often complicated by the presence of many uncertainties and system sub-components. One such example is the certification of the Hanford Waste Treatment Plant, where radioactive and toxic chemical waste that spontaneously generates flammable gases is stored in large tanks. We introduce the QMU methodology to quantify the system safety of waste storage tanks in the event of a loss of tank ventilation, which poses a safety risk to workers. We also show how QMU can be used as a design tool to find operating regimes that maintain a desired confidence level. A simplified physical model is used to analyze the build-up of hydrogen gas in storage tanks and conduct an uncertainty propagation study to quantify the operating margin with respect to the flammability conditions. A demonstration problem is shown in which the radiation loading in a waste tank is

QMU in high-consequence decisions

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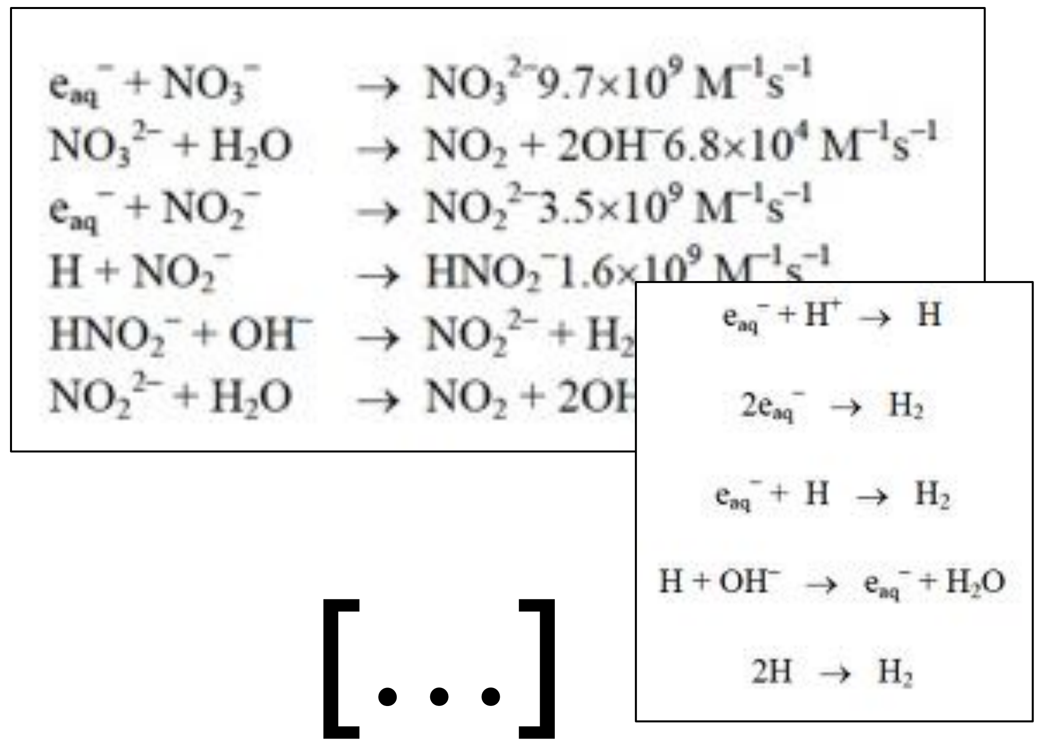
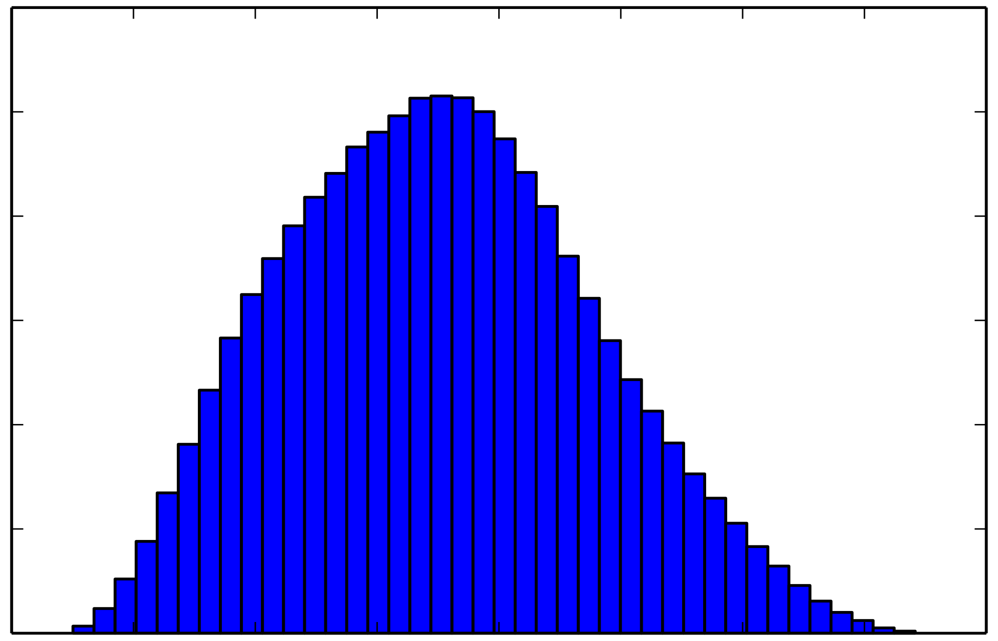


1) Identification of the Uncertainties

- Composition of the tank content: radioactive compounds, organic solvents and water
- Physical processes in the tank: chemical pathways, molecular aggregation and mixing, tank corrosion, etc…

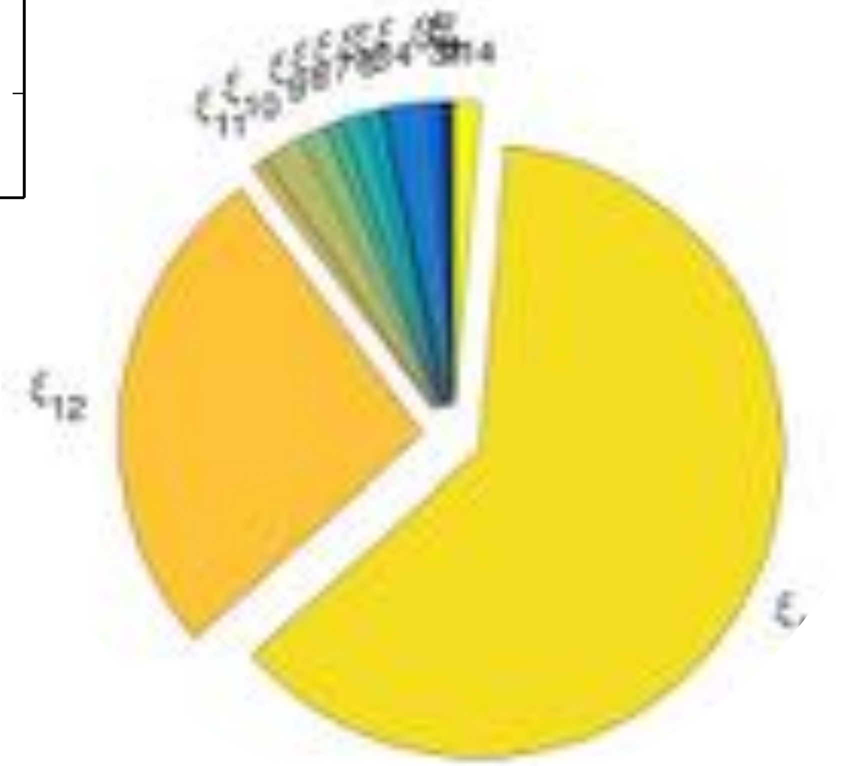
2) Uncertainty Quantification

- Forecasting: probabilistic physics-based thermo-chemical simulations
- Statistical analysis: Best estimate of the H_2 concentration


H_2 concentration

3) Communication of the outcomes

- Best estimate: $E[H_2]$ +/- STDEV
- Expert analysis: ranking of the sources of uncertainty (ANOVA)



QMU in high-consequence decisions

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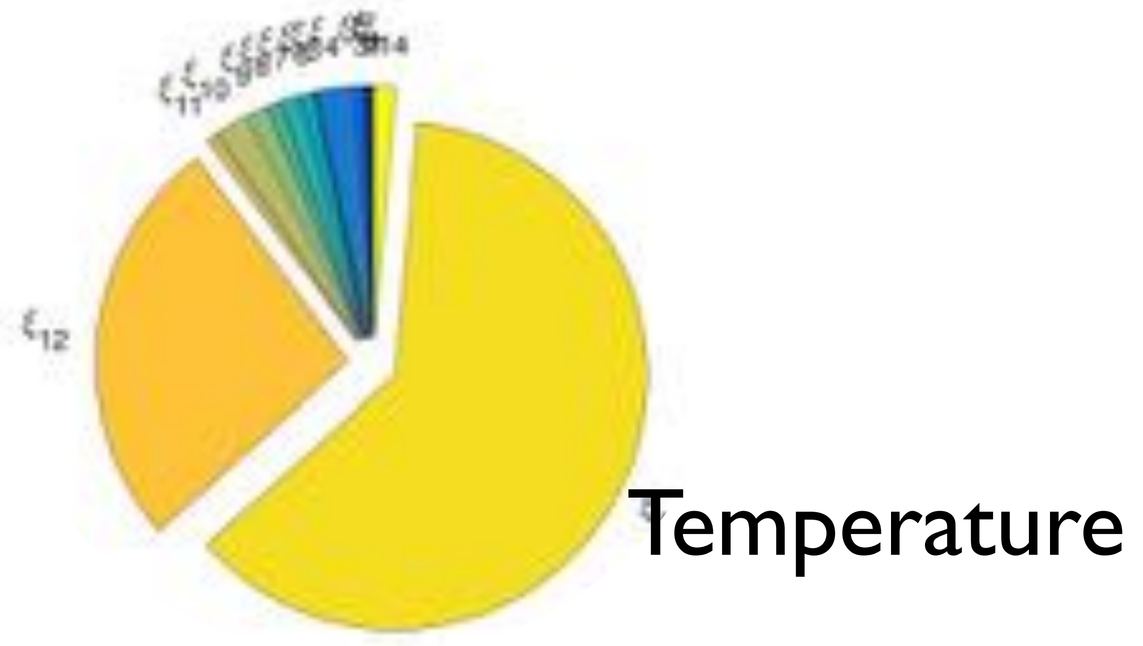


Surprise

most important uncertainty factor is the temperature in the tank, NOT the composition

Rather than H_2 concentration focus on the **decision**

- Temperature increase can lead to much faster build up of hydrogen
- How much time it takes for concentration to exceed critical value?
- Estimate the Time To Lower Flammability Level (TTLFL)

Decision: Is the time-to-flammability more than 14 days? first responders can then ventilate the tank and avoid explosions

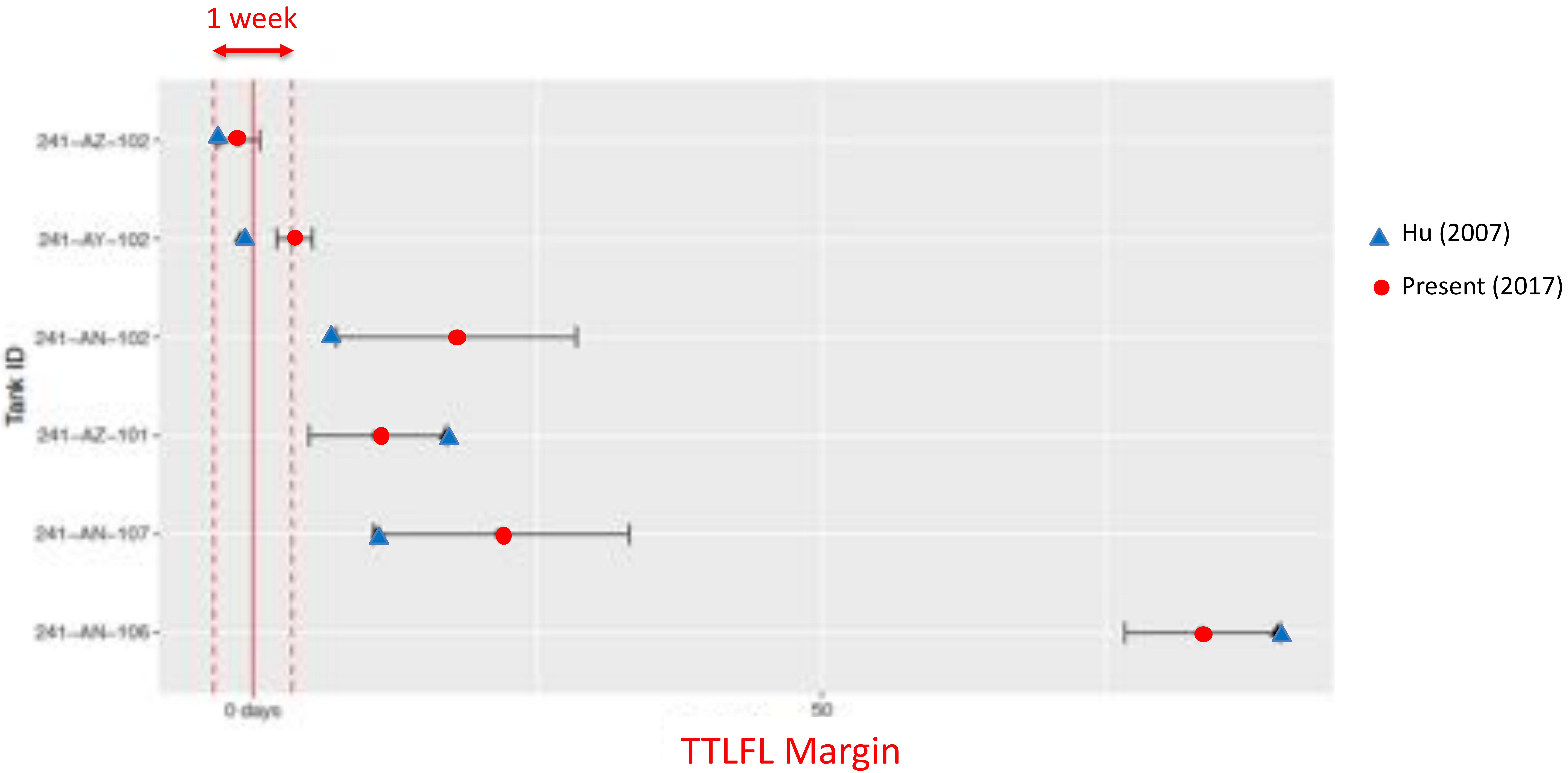
$$Q = \frac{\textbf{TTLFL Margin}}{\textbf{TTLFL Uncertainty}}$$

Q ↑ confidence/slack ↑

QMU: Quantification of Margins and Uncertainties

Tank	M (days)	U (days)	Q = M/U
241-AZ-102	-1.37	0.523	-2.63
241-AY-102	3.60	0.45	8.08
241-AZ-101	10.8	2.03	5.33
241-AN-102	18.2	5.02	3.63
241-AN-107	21.9	4.78	4.57
241-AN-106	83.3	2.52	33.0
241-SX-103	60.8	28.2	2.16
241-AY-101	324	18.6	17.4
241-SX-105	137	67.7	2.03

QMU in high-consequence decisions



summary

errors are uncertainties are NOT the same

- errors are avoidable and should/will be corrected
- uncertainties are unavoidable and must be acknowledged

uncertainties come in multiple forms

communicating uncertainties is an important element

- must depend on the audience
- must depend on the context/use case

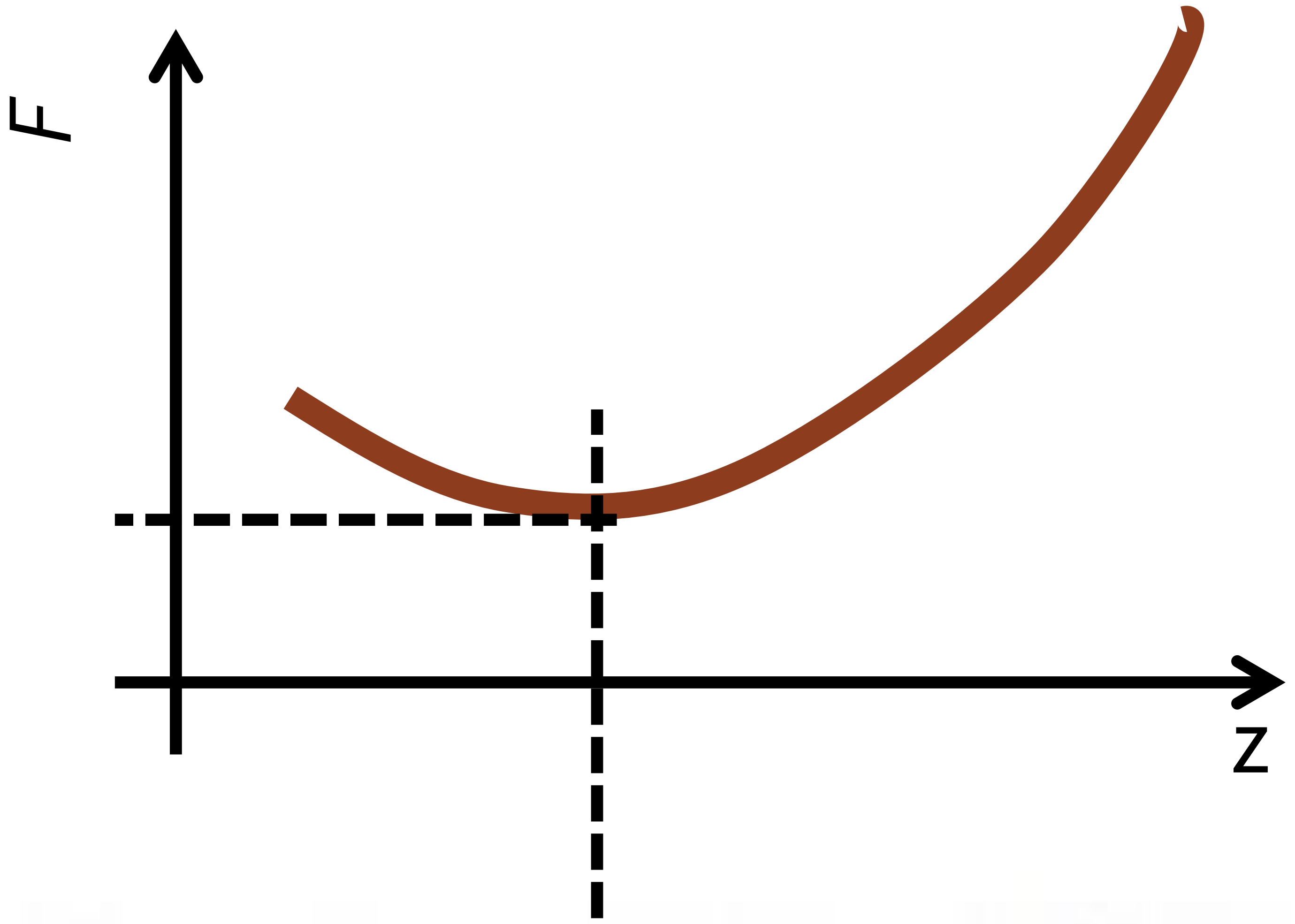
optimization under uncertainty

optimization

in its simplest form, optimization refers to the selection of the best among various options based on a specific criterion (goal a.k.a. objective)

given a "design parameter", ie an input that can vary in a range, an optimization algorithms searches in the space of the possible solutions to find the "best"

$$\min_{z \in [z_A, z_B]} F(z)$$



$$z^* = \arg \min_{z \in [z_A, z_B]} F(z)$$

many specific formulations (linear programming, constrained, etc.) and many strategies to solve the problem…

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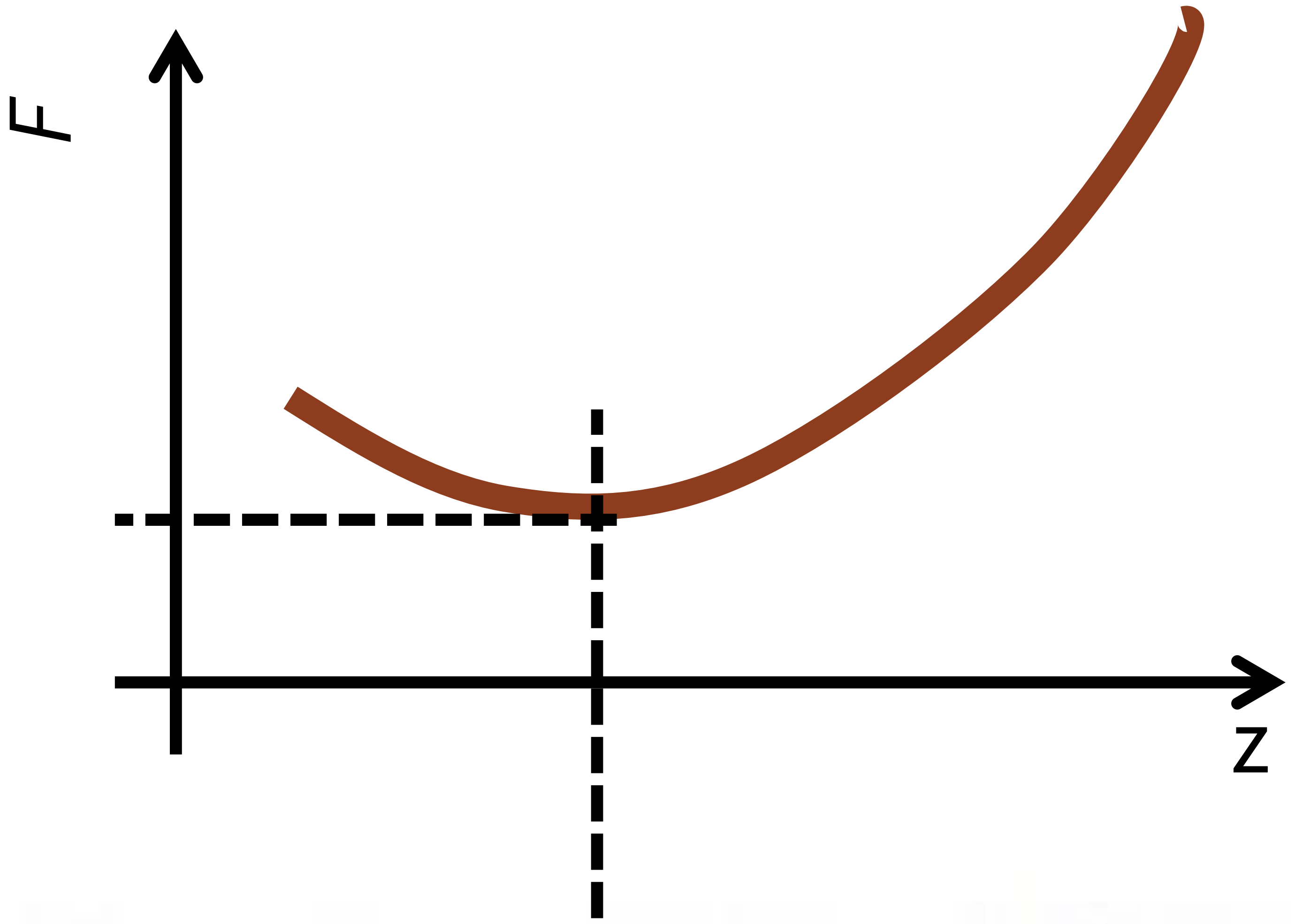

$$z^* = \arg \min_{z \in [z_A, z_B]} F(z)$$

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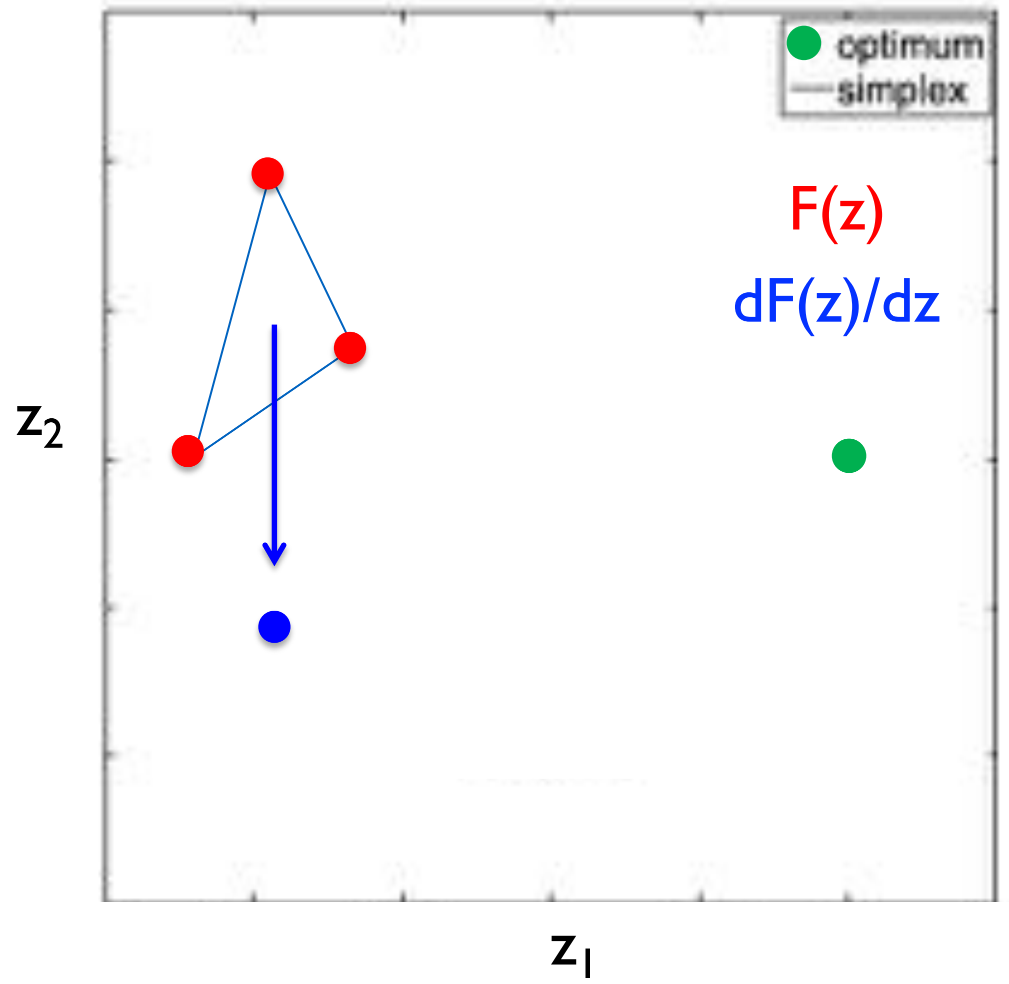
Nelder-Mead Algorithm

- Gradient-descend optimizer
- Simple & Fast



optimization under uncertainty

…as you know uncertainties are always present in applications.

How do we account for uncertainties in an optimization problem?

first step is to recognize the "design" variables and the uncertainties in the system – assume they are distinct:

$$\underset{\text{objective}}{f} = f(\underbrace{s}_{\text{design variables}}, \underbrace{\omega}_{\text{uncertain variables}})$$

If we treat the uncertainties as probabilistic variables, then

$$\underset{s}{\text{minimize}}\ f(s, \omega)$$

the objective is itself random

optimization under uncertainty

$$\underset{s}{\text{minimize}} \; f(s, \omega)$$

minimizing the random objective is possible but not typically the preferred approach

$$\underset{s}{\text{minimize}} \quad \mathbb{E}\{f(\omega, s)\}$$

consider the expectation (the mean) of the objective! optimizing the system so that the mean response is minimized has lots of practical applications

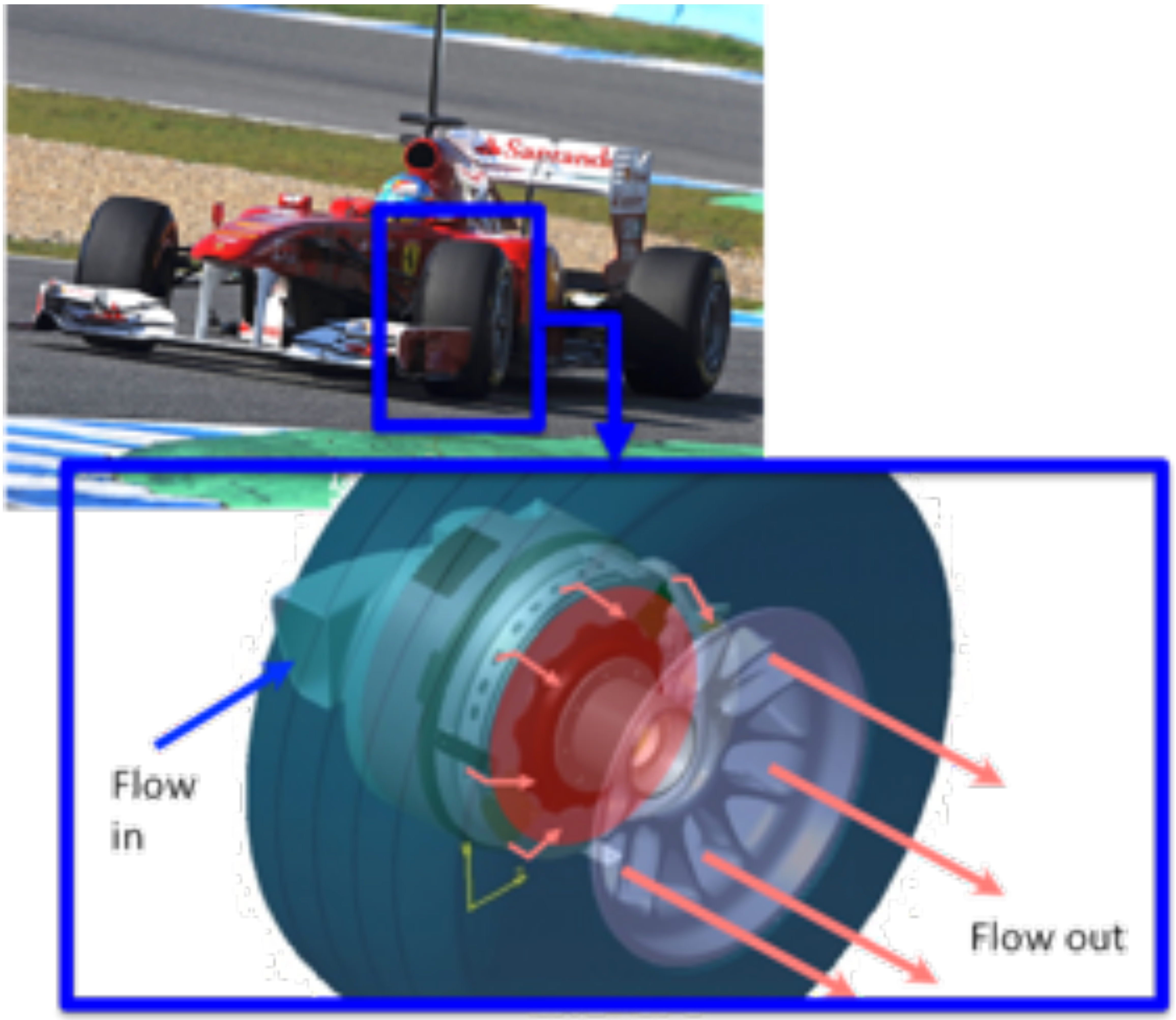
$$\underset{s}{\text{minimize}} \quad \begin{matrix} \mathbb{E}\{f(\omega, s)\} \\ \sigma^2\{f(\omega, s)\} \end{matrix}$$

consider the expectation (the mean) and the variance simultaneously leads to a multiobjective optimization; this is referred to as robust optimization.

$$\underset{s}{\text{minimize}} \quad \mathrm{P}\{f < f_{\text{crit}}\}$$

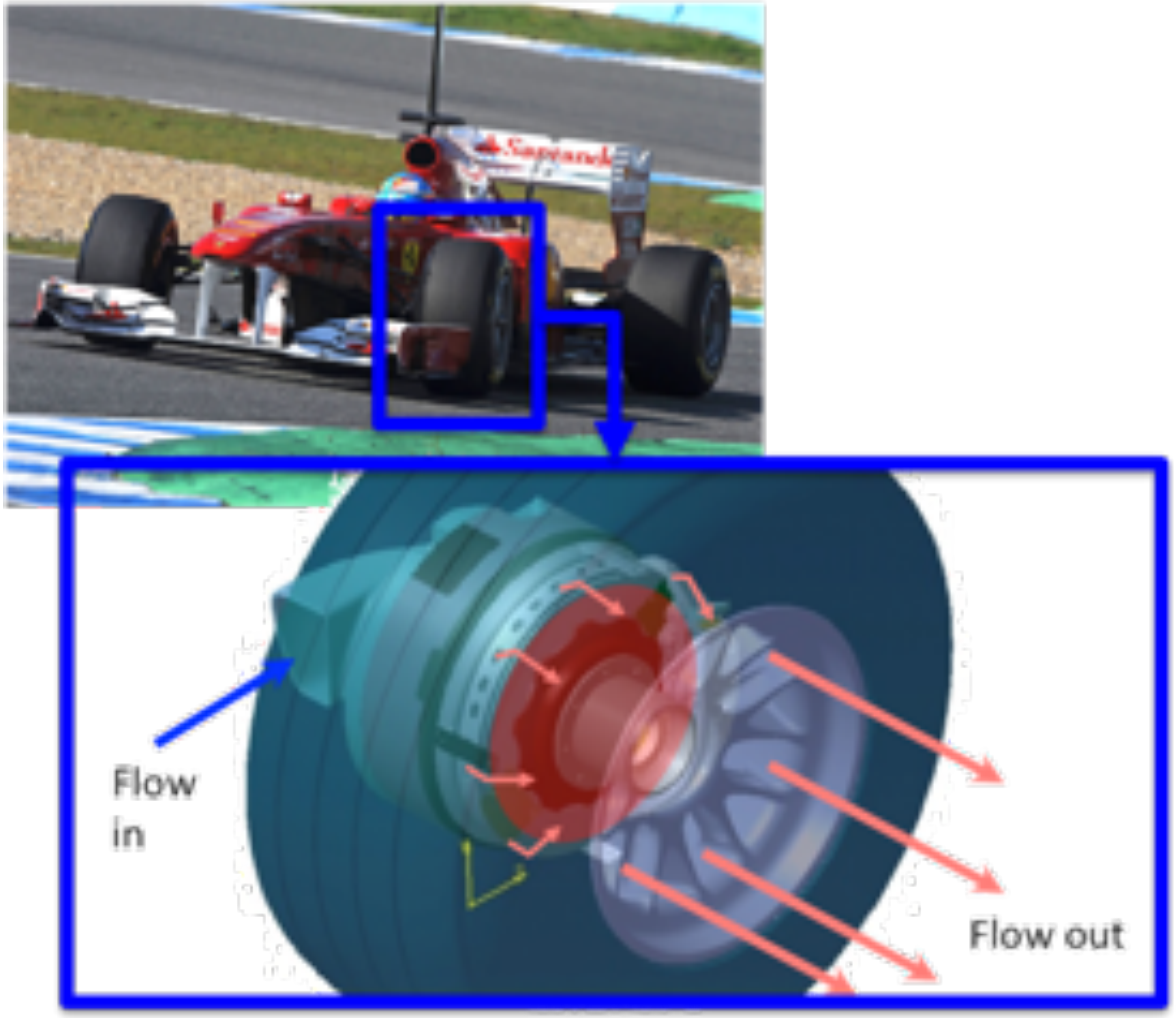
consider the probability of your objective exceeding a critical value; this is referred as reliability-based optimization.

optimization under uncertainty – an example

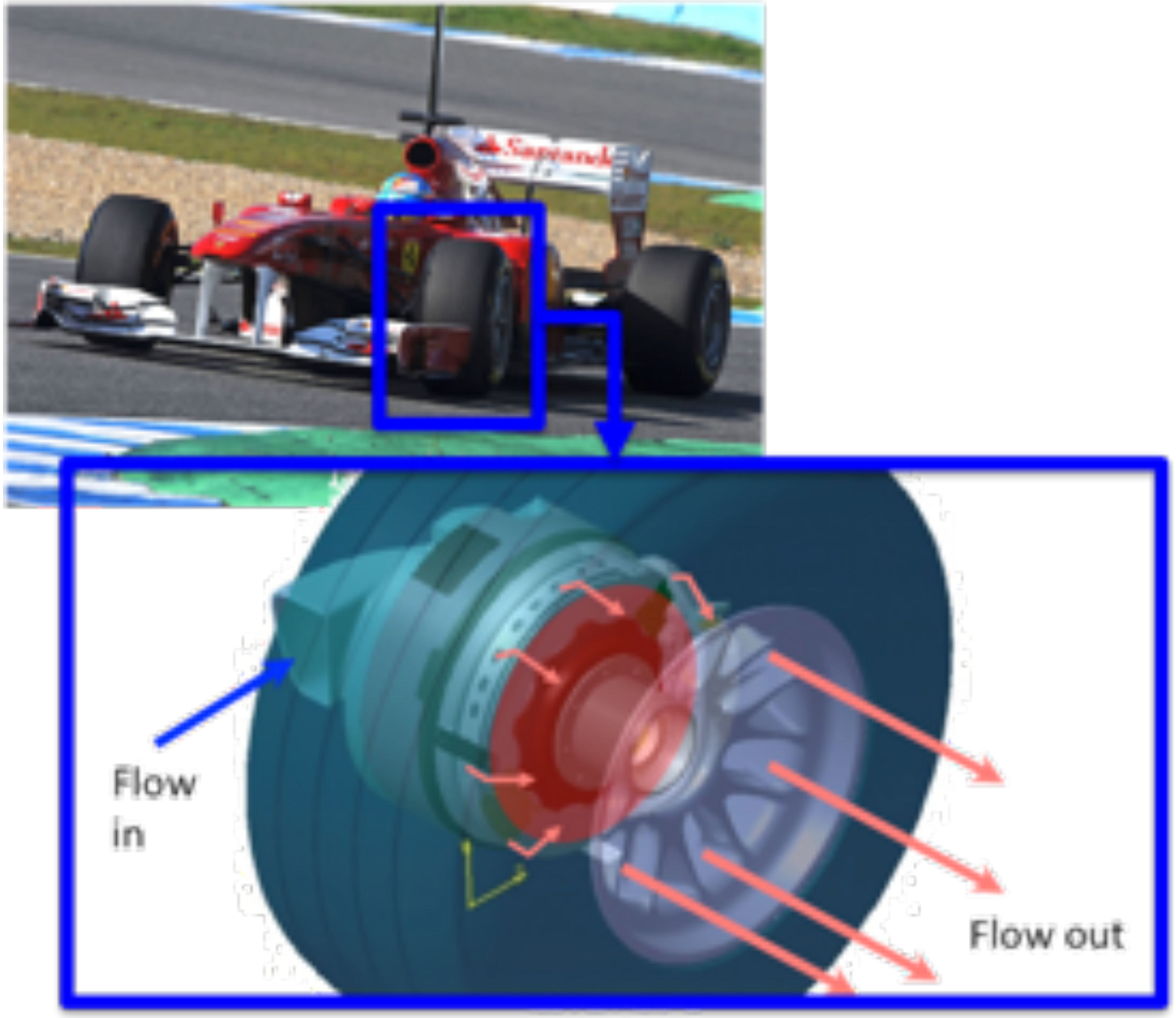


Optimize the shape of the brake duct to maximize cooling and minimize drag

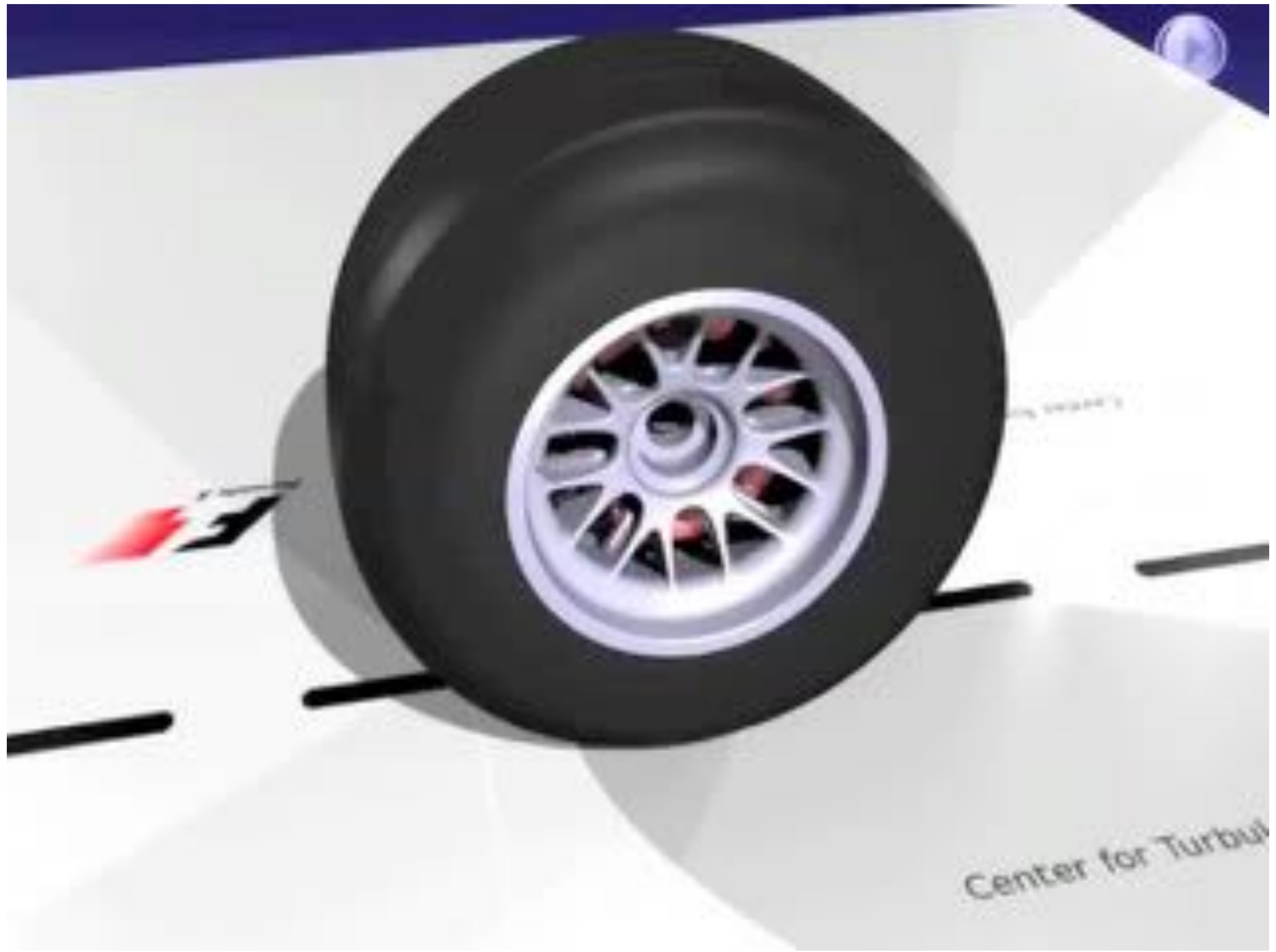
optimization under uncertainty – an example



optimization under uncertainty – an example

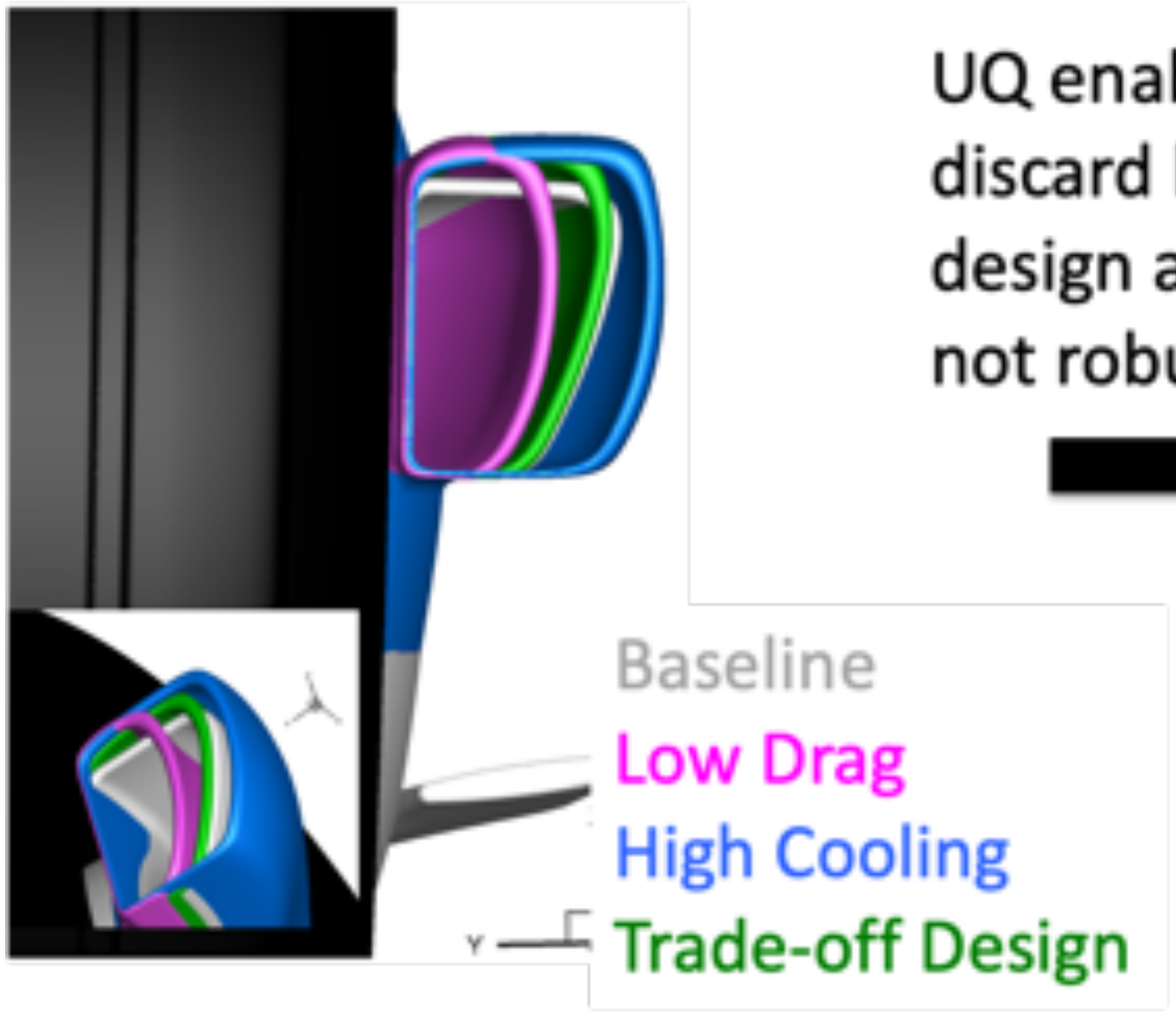


…no uncertainties so far.
But what is the effect of tire deformation?



optimization under uncertainty – an example

optimization under uncertainty – an example

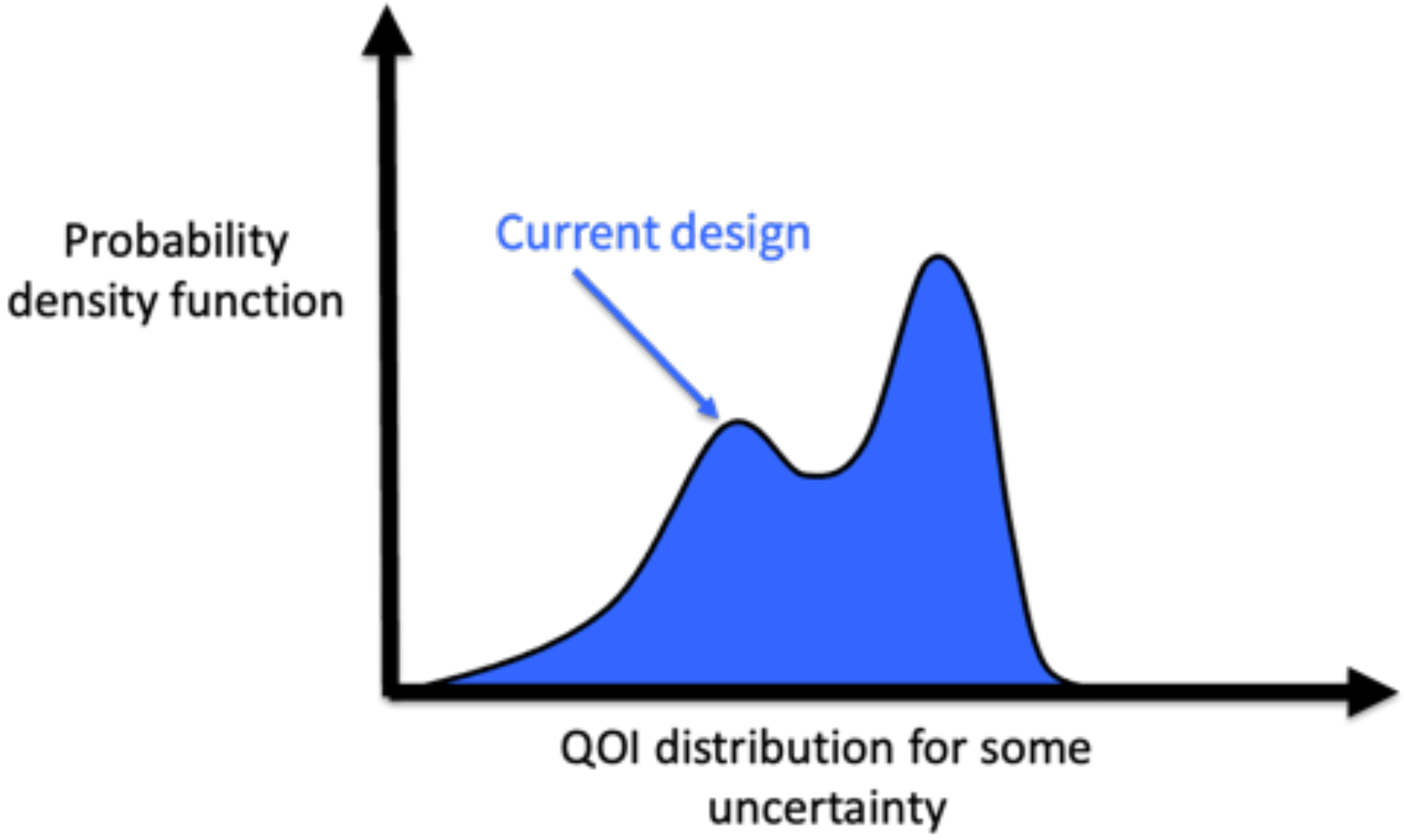


UQ enables to discard low-drag design as being not robust

a case study
density-matching optimization

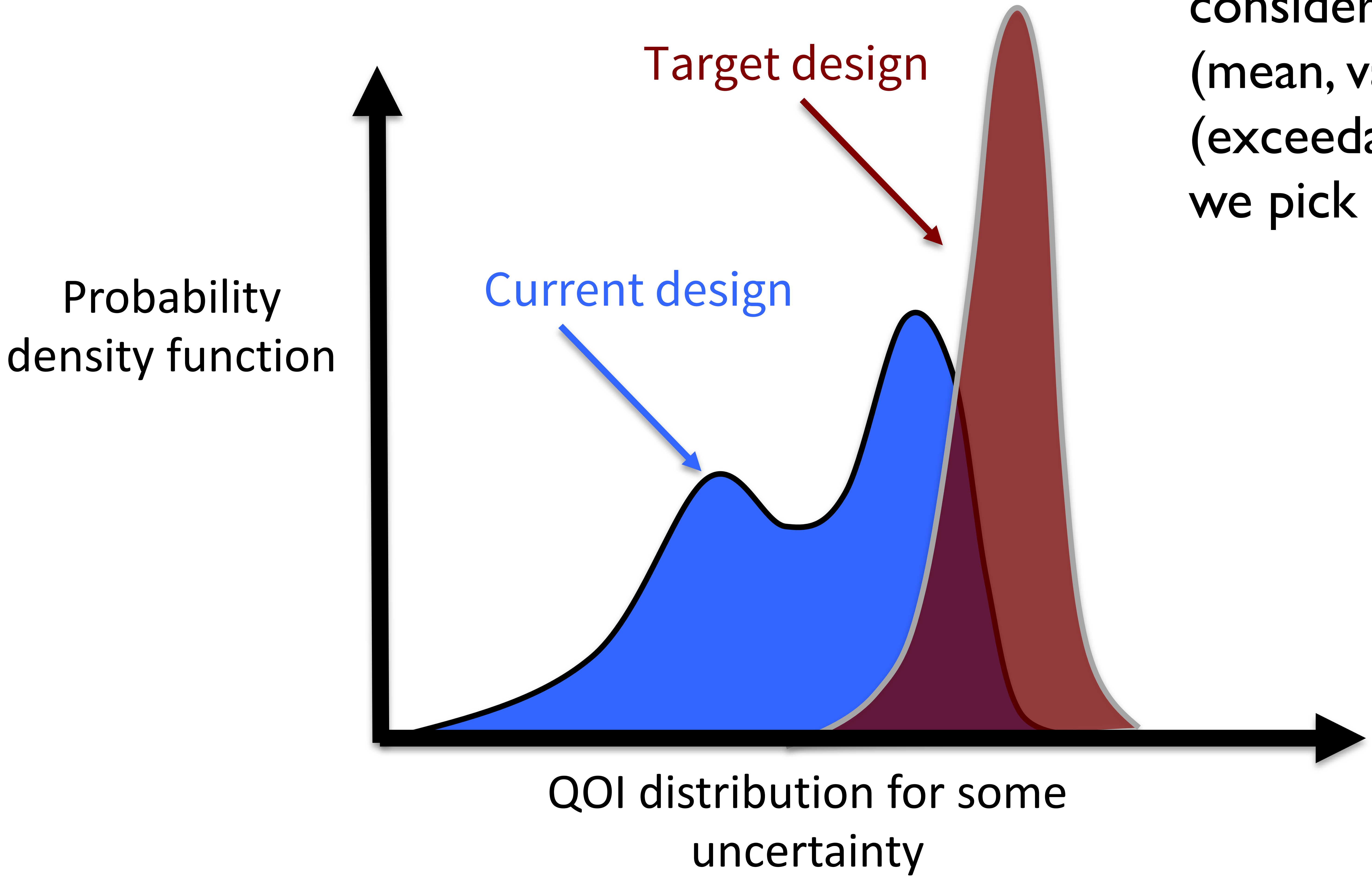
optimization under uncertainty

Accounting for uncertainties lead to performance metric for our system (quantity of interest, QOI) to become probabilistic, i.e. they have an associated distribution



optimization under uncertainty

Accounting for uncertainties lead to performance metric for our system (quantity of interest, QOI) to become probabilistic, i.e. they have an associated distribution but rather than considering moments (mean, variance) or tails (exceedance probability) we pick a target design!



optimization under uncertainty

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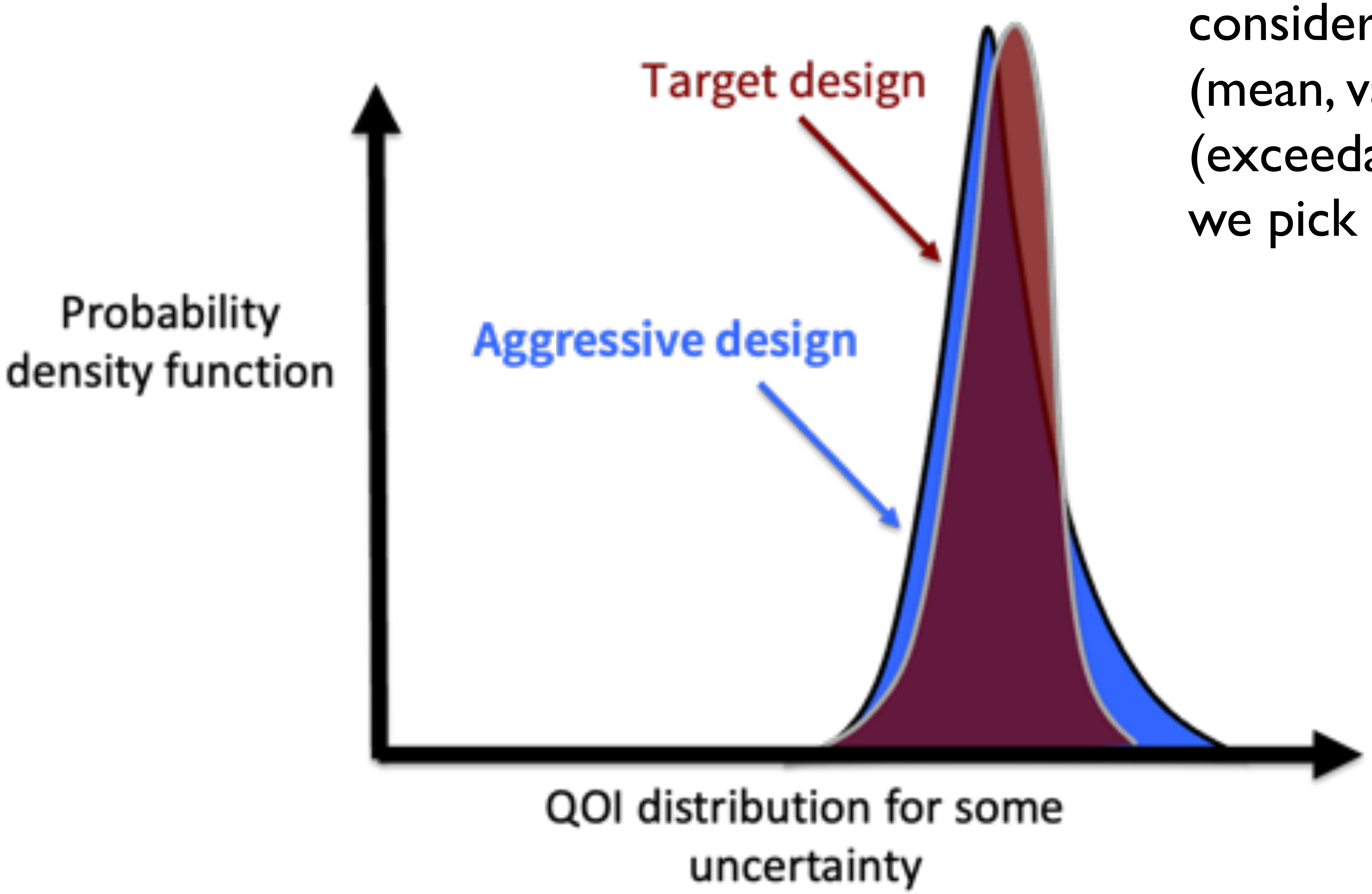


optimization under uncertainty

Goal is to find the design so that model pdf is as close as possible to the designer's target.

$$\underset{s}{\text{minimize}} \quad \delta(t, u_s)$$

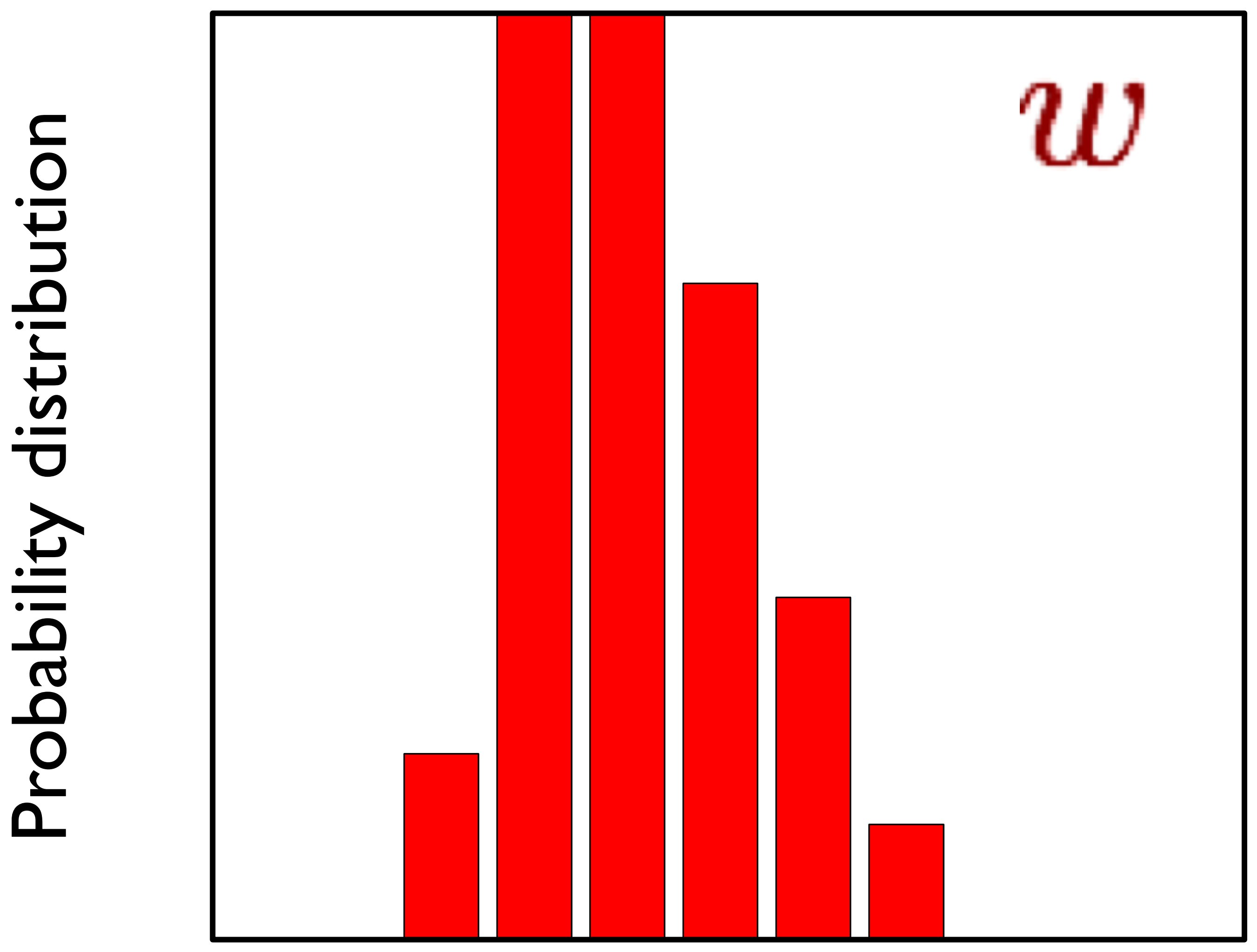
where delta is a distance metric. We choose

$$\delta(t, u_s) = \int (t - u_s)^2 \, df$$

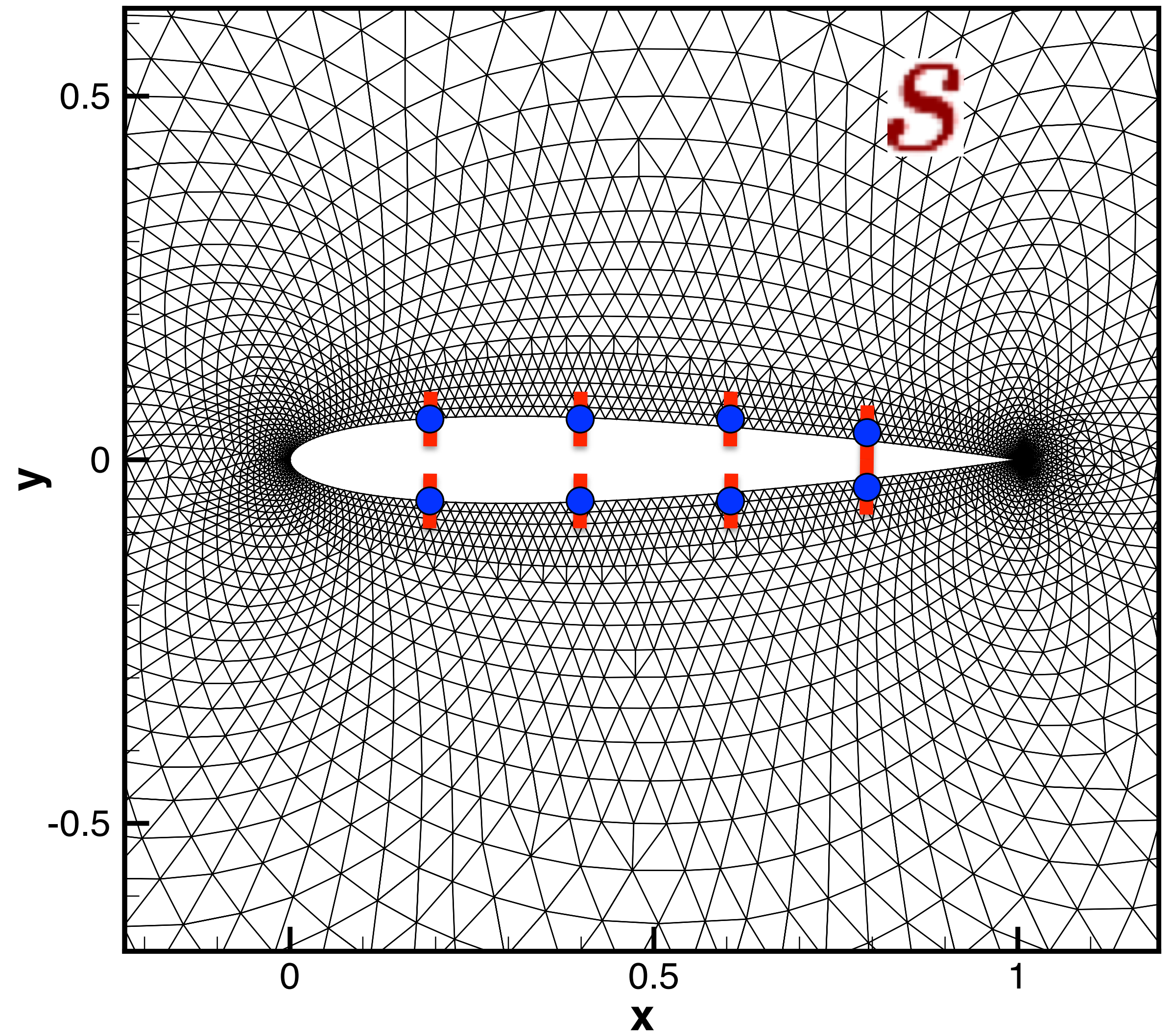
Target PDF

PDF for a given design s

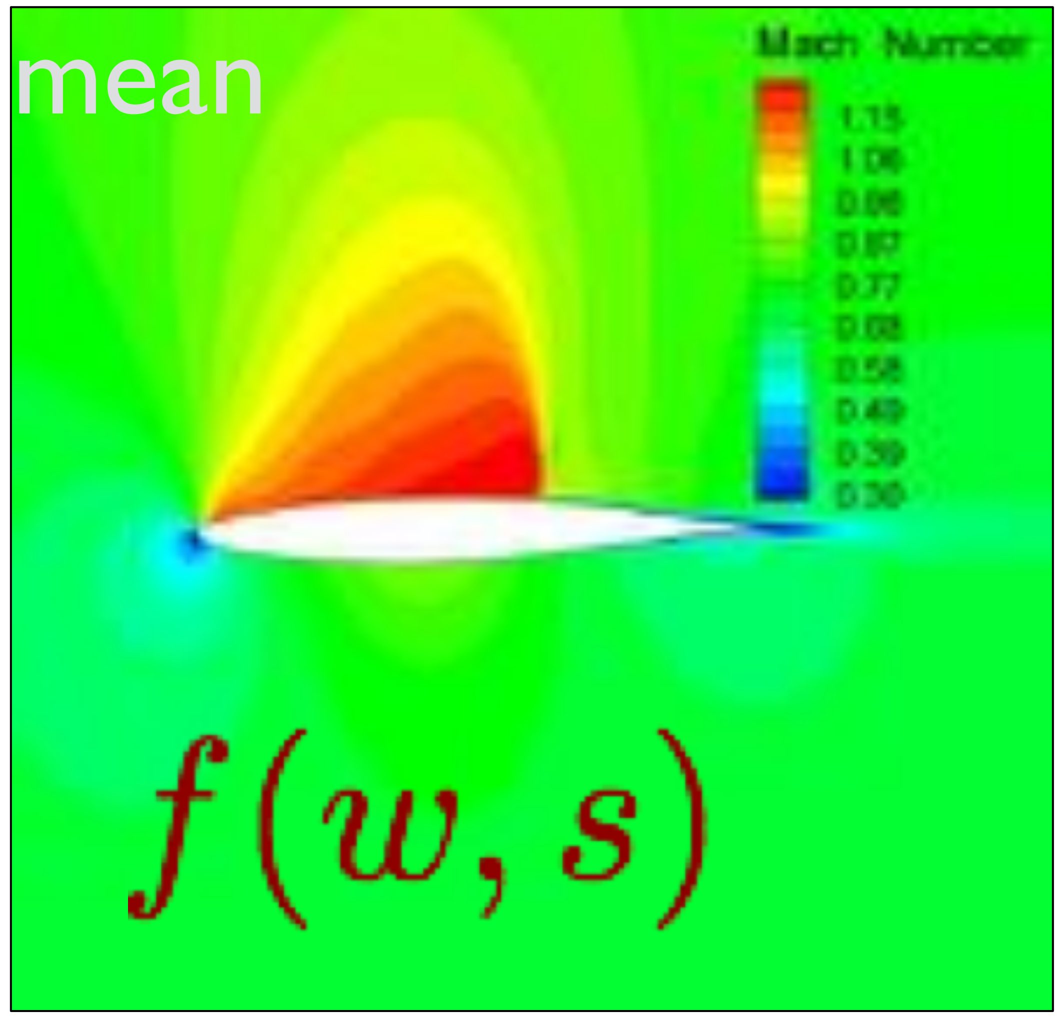
optimization under uncertainty



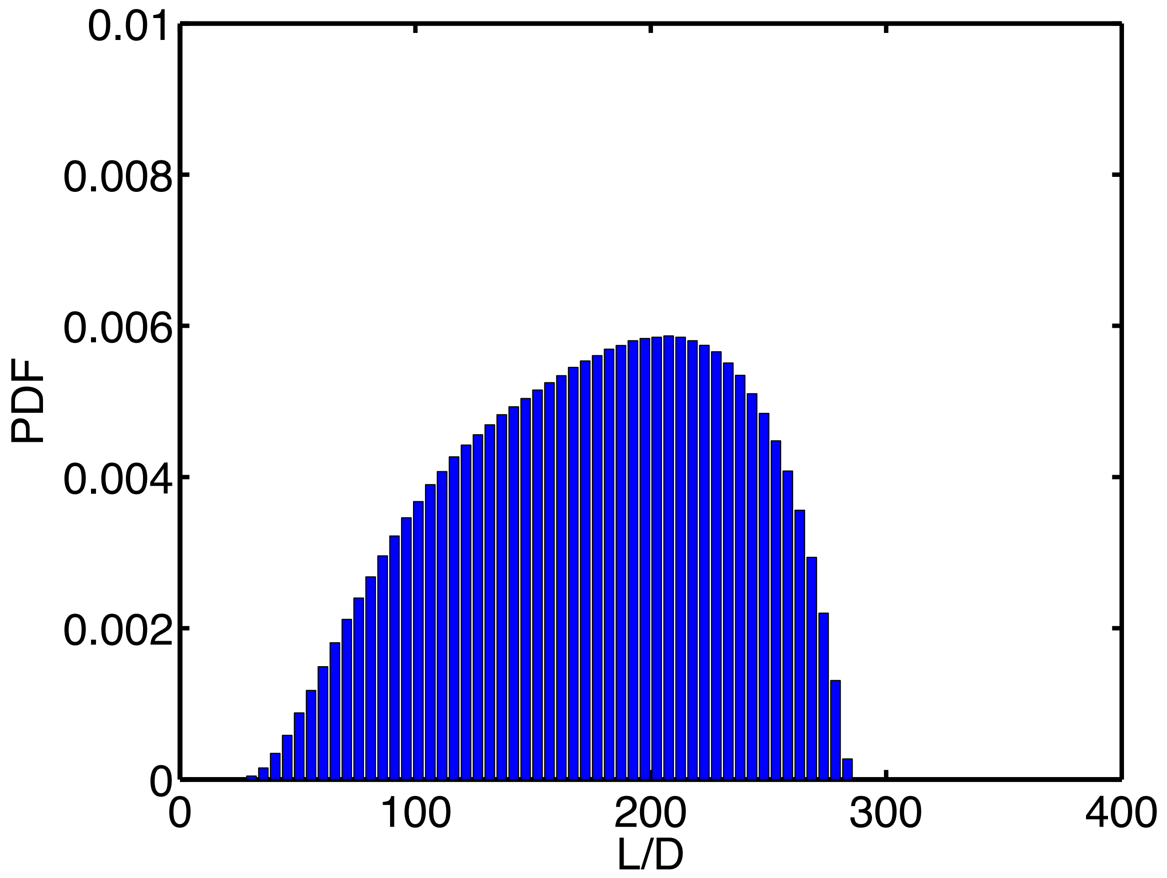
Free-Stream
Mach # uncertainty



Airfoil with Hicks-Henne bump functions

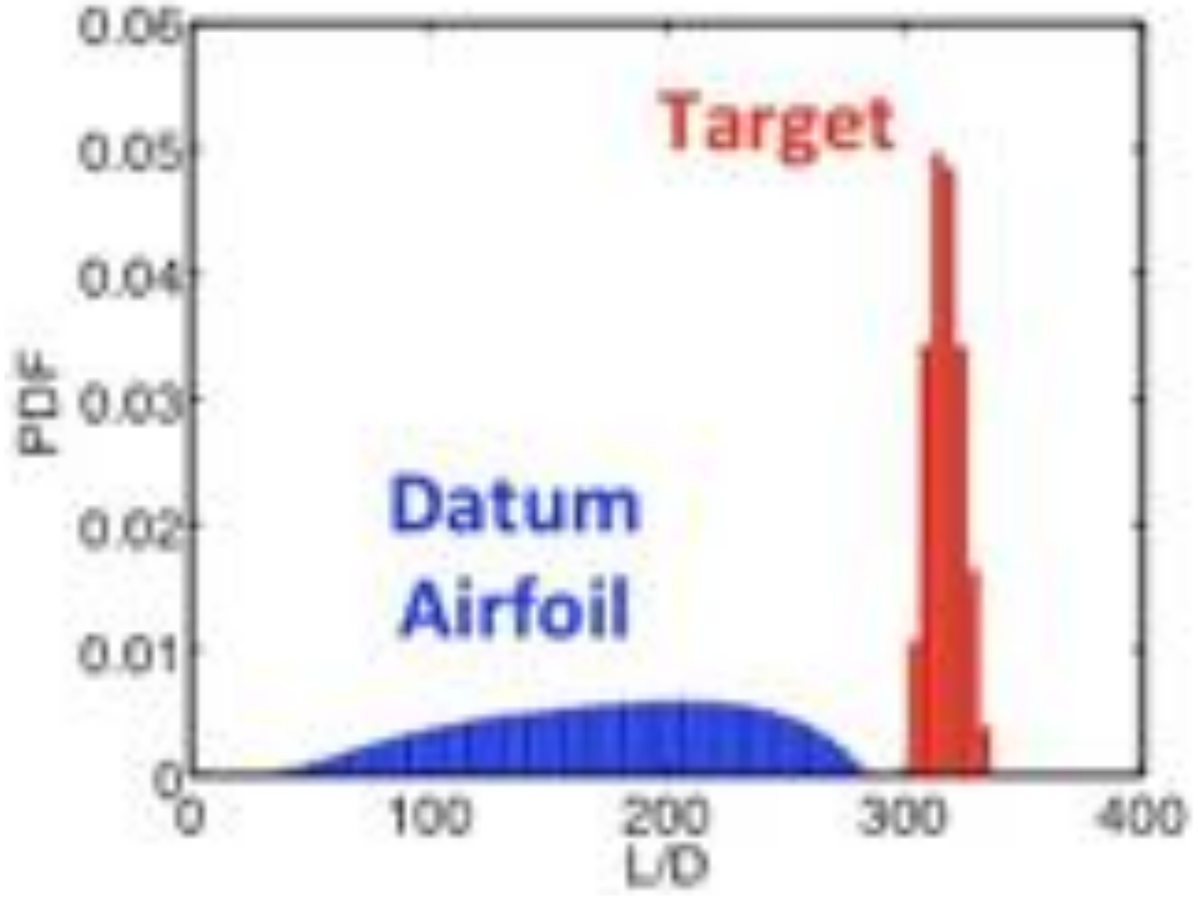


Obtain lift-to-drag ratio

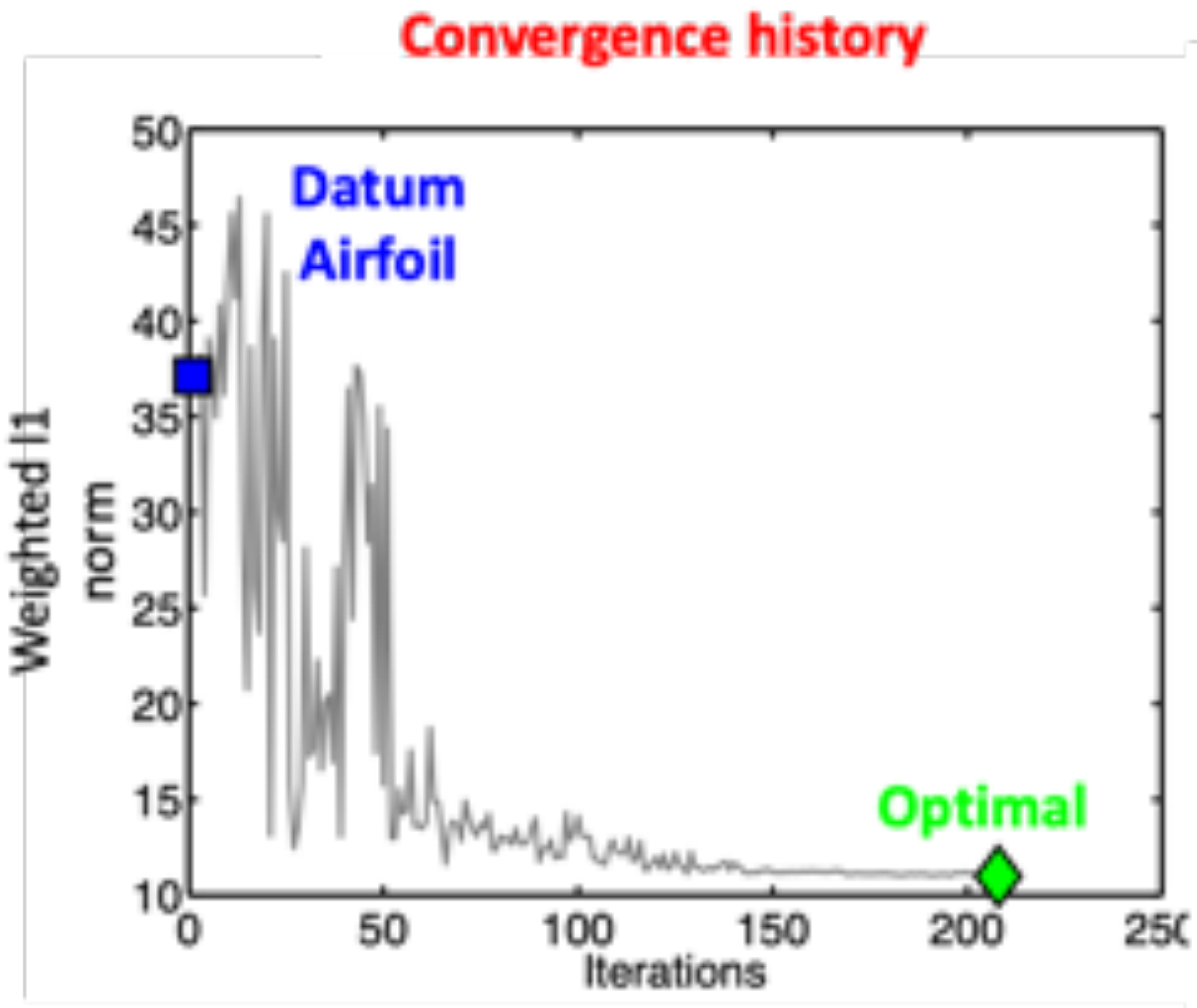


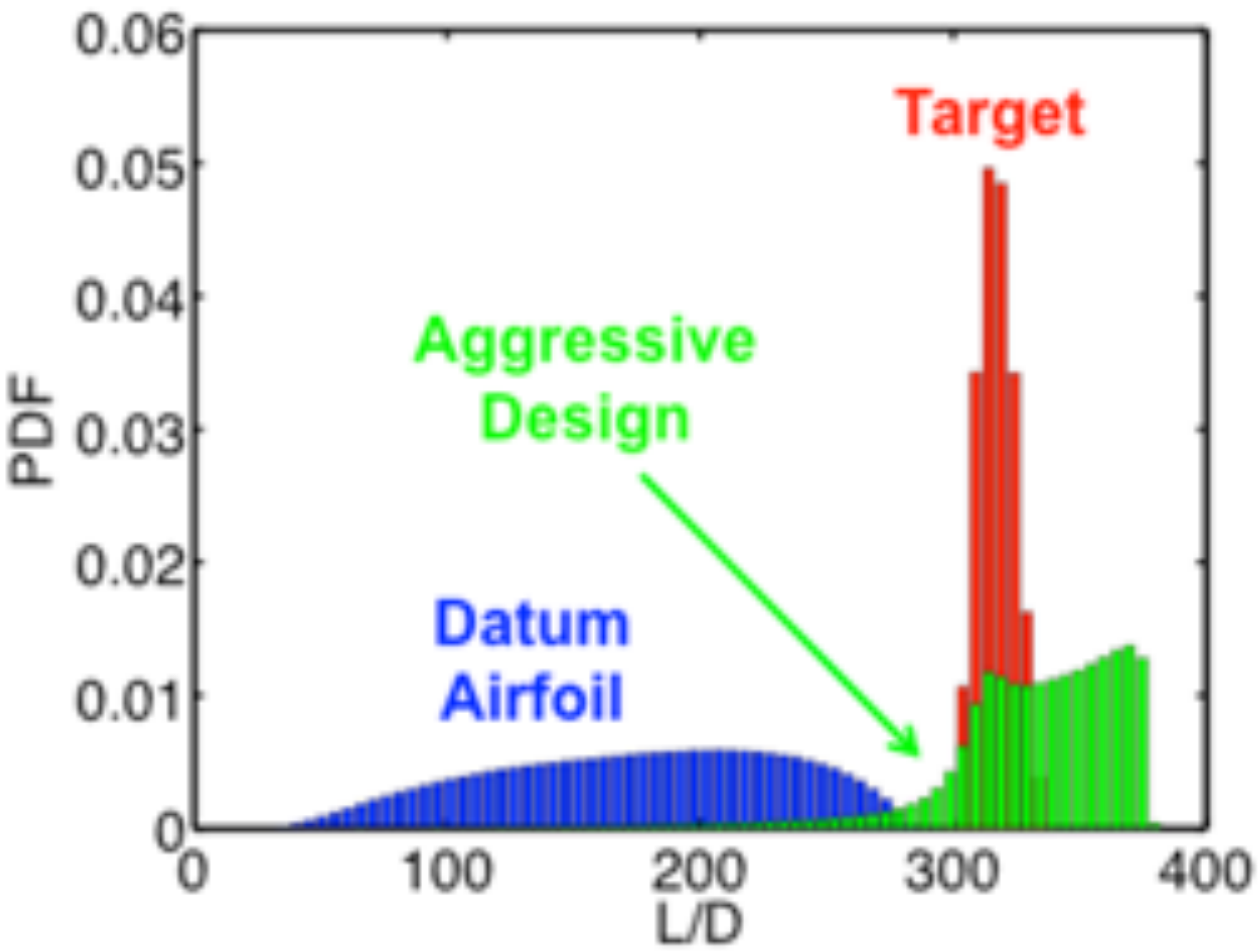
PDF and statistical moments of lift/drag

Optimize



optimization under uncertainty





Property	Datum Airfoil	Target PDF	Aggressive Design
Mean	174.68	317.14	**330.5**
Standard deviation	57.52	7.0	**40.5**

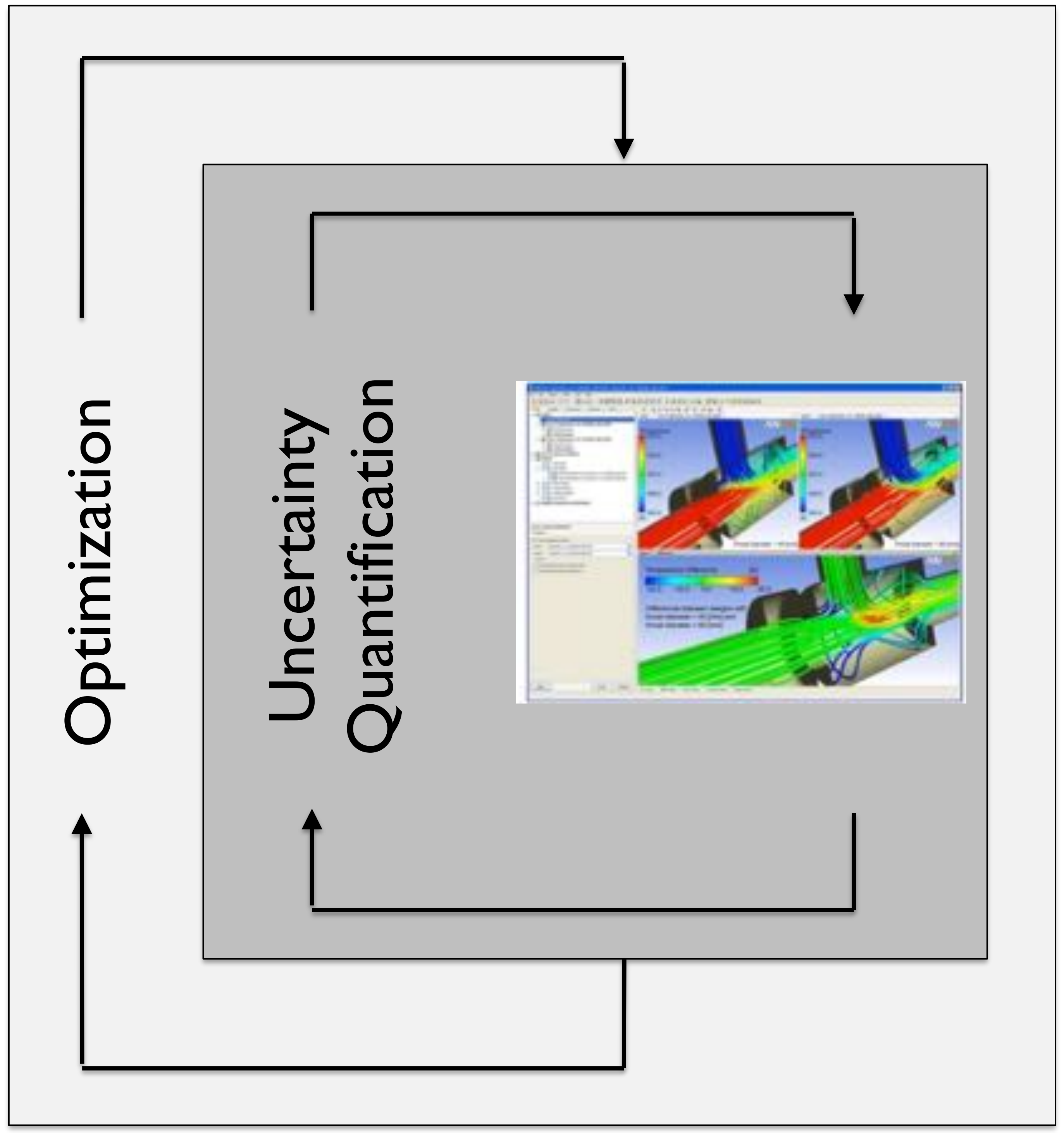
summary

optimization under uncertainty

- formulation of the optimization goal is not straightforward
- solution strategies are complex and more expensive

accounting for uncertainties is critical

- “certain” optimal performance are fragile
- uncertainty quantification leads to natural choice between different trade-offs



uncertainties without probabilities

“basic equation of uncertainty analysis”

Experimental Thermal & Fluid Sciences, 1988

Describing the Uncertainties in Experimental Results

Robert J. Moffat
Professor of Mechanical Engineering, Stanford University, Stanford, California

It is no longer acceptable, in most circles, to present experimental results without describing the uncertainties involved. Besides its obvious role in publishing, uncertainty analysis provides the experimenter a rational way of evaluating the significance of the scatter on repeated trials. This can be a powerful tool in locating the source of trouble in a misbehaving experiment. To the

The partial derivative of R with respect to X_i is the *sensitivity coefficient* for the result R with respect to the measurement X_i.

When several independent variables are used in the function R, the individual terms are combined by a root-sum-square method.

$$\delta R = \left\{ \sum_{i=1}^{N} \left(\frac{\partial R}{\partial X_i} \delta X_i \right)^2 \right\}^{1/2} \tag{4}$$

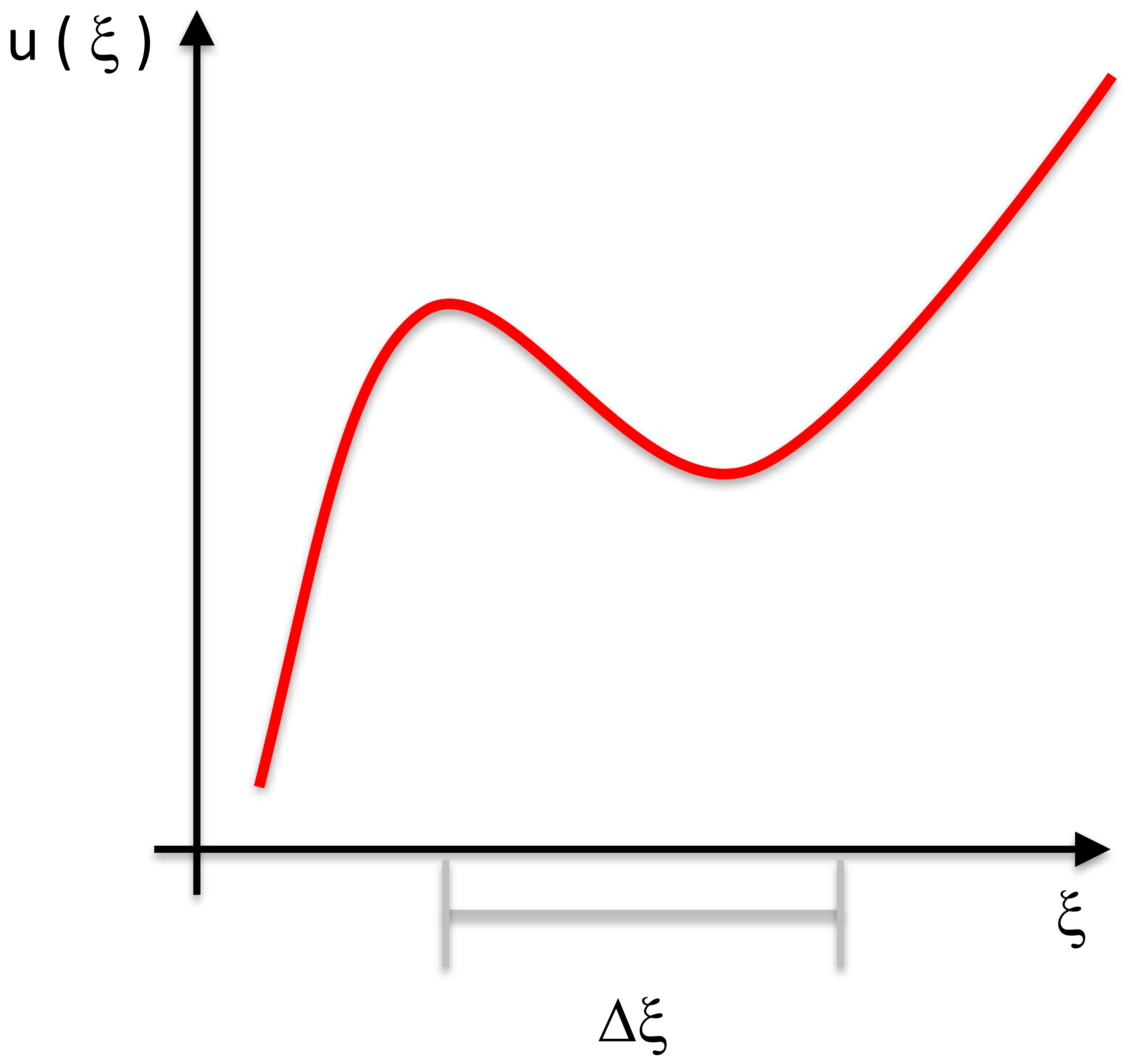
This is the basic equation of uncertainty analysis. Each term

deterministic estimate of uncertainties

model output

model inputs with given ranges $\Delta\xi_i$

$$u = u(\xi_1, \cdots, \xi_d)$$



deterministic estimate of uncertainties

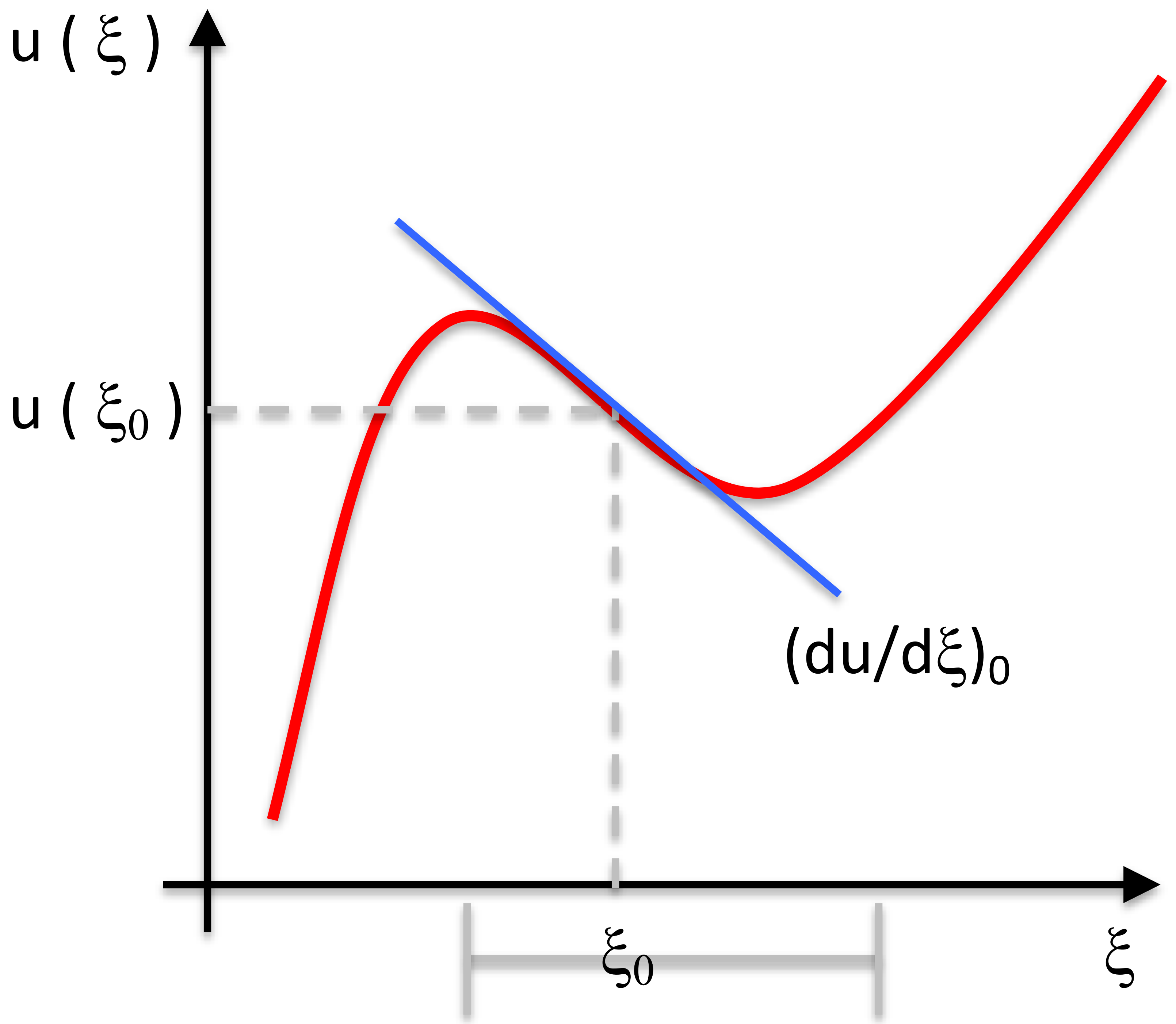
model output

model inputs with given ranges $\Delta\xi_i$

$$u = u(\xi_1, \cdots, \xi_d)$$

Moffat's **basic equation of uncertainty analysis** is simply a first order Taylor series expansion:

$$\Delta u \approx \left[\sum_{i=1}^{d} \left(\frac{\partial u}{\partial \xi_i} \right)^2 \Delta \xi_i^2 \right]^{\frac{1}{2}}$$



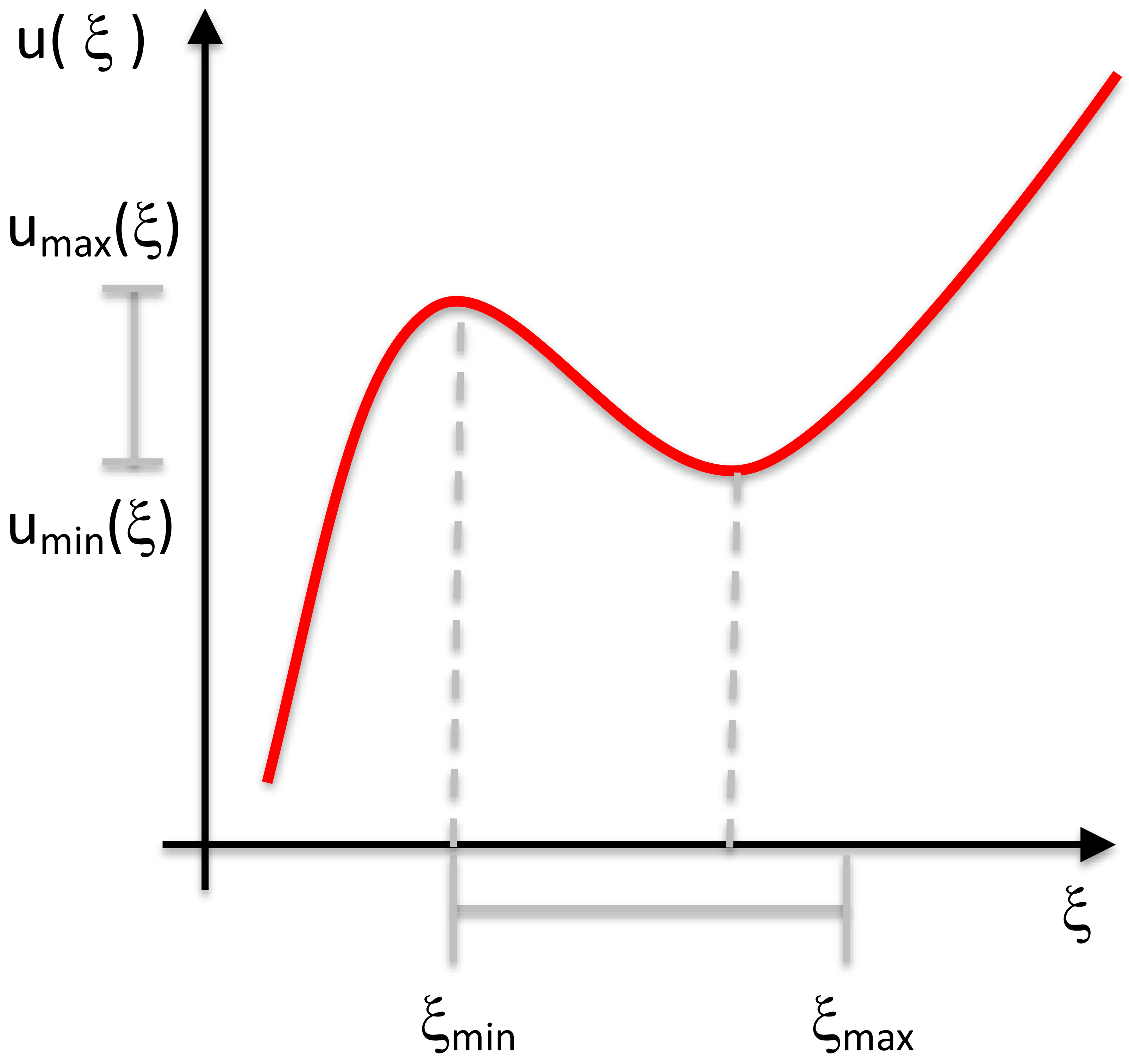
this is also referred to as a local sensitivity, i.e. refers to a local approximation of the function

deterministic estimate of uncertainties

model output

model inputs with given ranges $\Delta\xi_i$

$$u = u(\xi_1, \cdots, \xi_d)$$



The **most general strategy**

given $\xi \in [\xi_{min}, \xi_{max}]$

solve two optimization problems to find:

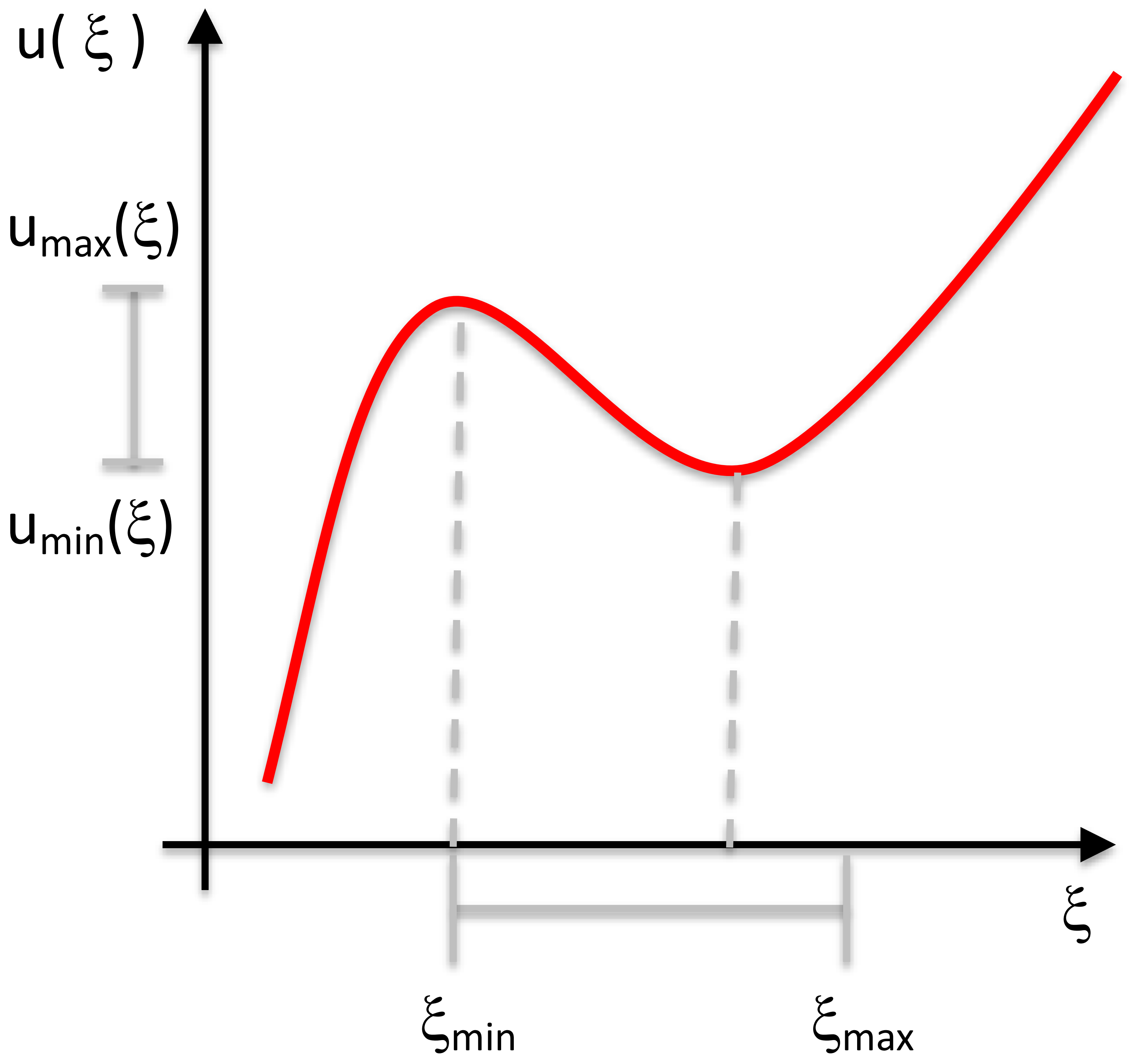
$$u(\xi) \in [u_{min}, u_{max}]$$

deterministic estimate of uncertainties

model output

model inputs with given ranges $\Delta\xi_i$

$$u = u(\xi_1, \cdots, \xi_d)$$



Can we compute intervals directly?

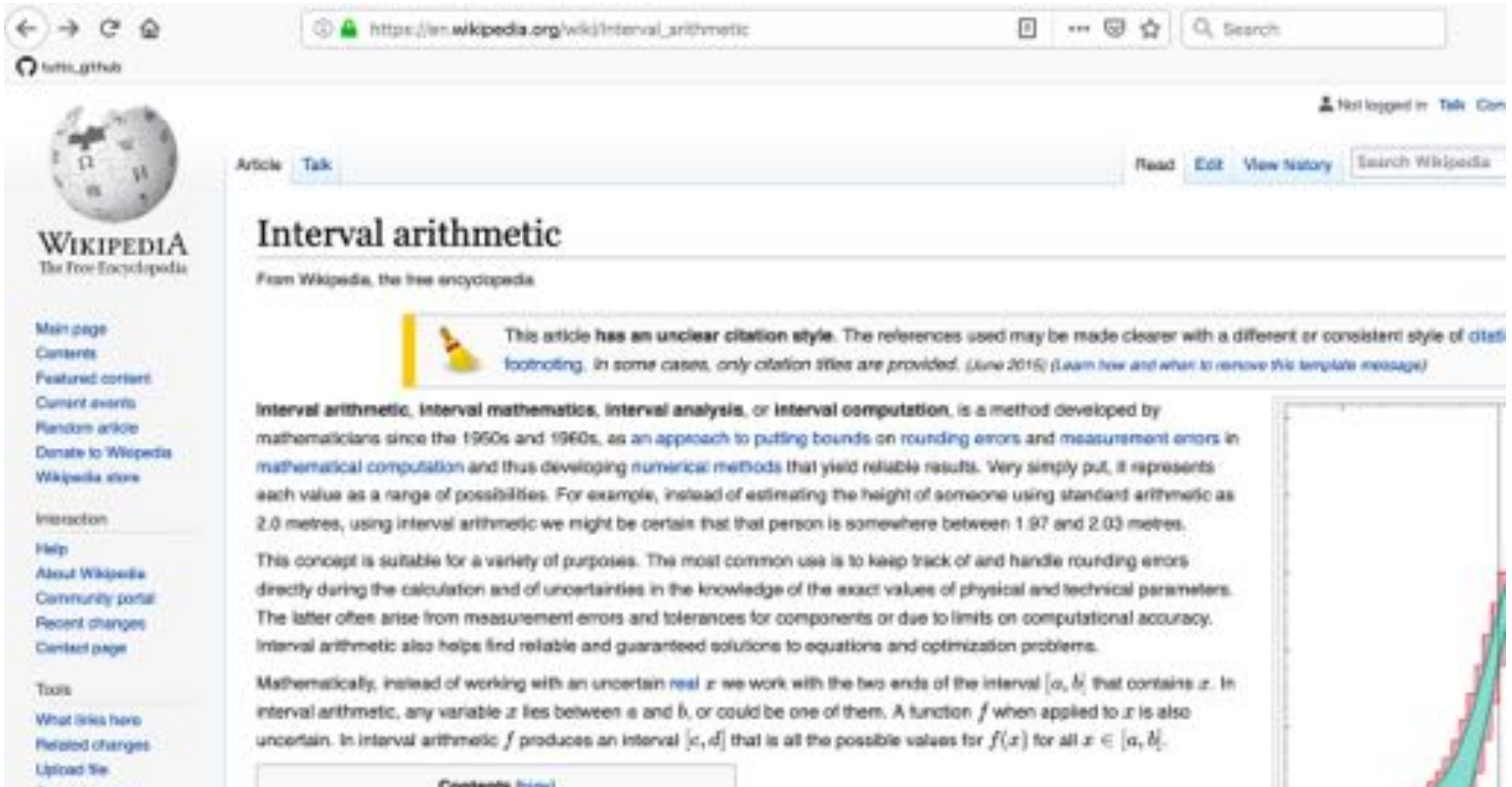
$$\xi \in [\xi_{min}, \xi_{max}] \quad \blacktriangleright \quad u(\xi) \in [u_{min}, u_{max}]$$

Values vs. Intervals

interval arithmetic – given two variables defined as intervals….

- $\xi + \eta = [\xi_a : \xi_b] + [\eta_a : \eta_b] = [\xi_a + \eta_a : \xi_b + \eta_b]$
- $\xi - \eta = [\xi_a : \xi_b] - [\eta_a : \eta_b] = [\xi_a - \eta_b : \xi_b + \eta_a]$
- $\xi \times \eta = [\xi_a : \xi_b] \times [\eta_a : \eta_b] = [min(\xi_a\eta_a, \xi_a\eta_b, \xi_b\eta_a, \xi_b\eta_b) : max(\xi_a\eta_a, \xi_a\eta_b, \xi_b\eta_a, \xi_b\eta_b)]$
- $\xi / \eta = [\xi_a : \xi_b][1/\eta_a : 1/\eta_b]$

resulting intervals are rigorous and relatively inexpensive to evaluate…but



Problems with Intervals Arithmetic

Dependency Problem

$$\xi \in [1 : 2] \quad \blacktriangleright \quad \xi - \xi = [-1 : 3]$$

$$f(x) = \frac{x}{1+x}$$

$$g(x) = \frac{1}{1+1/x}$$

$$x = \bar{x}[1 - 1/10 : 1 + 1/10]$$

▶

$\bar{x}$	x	$f(\bar{x})$	$g(\bar{x})$	$f(x)$	$g(x)$	$\frac{\lVert f(x) \rVert}{\lVert g(x) \rVert}$
1	$\left[\frac{9}{10} : \frac{11}{10}\right]$	$\frac{1}{2}$	$\frac{1}{2}$	$\left[\frac{3}{7} : \frac{11}{19}\right]$	$\left[\frac{9}{19} : \frac{11}{21}\right]$	3
$\frac{5}{4}$	$\left[\frac{9}{8} : \frac{11}{8}\right]$	$\frac{5}{9}$	$\frac{5}{9}$	$\left[\frac{9}{19} : \frac{11}{17}\right]$	$\left[\frac{9}{17} : \frac{11}{19}\right]$	$\frac{7}{2}$
$\frac{3}{2}$	$\left[\frac{27}{20} : \frac{33}{20}\right]$	$\frac{3}{5}$	$\frac{3}{5}$	$\left[\frac{27}{53} : \frac{33}{47}\right]$	$\left[\frac{27}{47} : \frac{33}{53}\right]$	4
$\frac{7}{4}$	$\left[\frac{63}{40} : \frac{77}{40}\right]$	$\frac{7}{11}$	$\frac{7}{11}$	$\left[\frac{7}{13} : \frac{77}{103}\right]$	$\left[\frac{63}{103} : \frac{77}{117}\right]$	$\frac{9}{2}$
2	$\left[\frac{9}{5} : \frac{11}{5}\right]$	$\frac{2}{3}$	$\frac{2}{3}$	$\left[\frac{9}{16} : \frac{11}{14}\right]$	$\left[\frac{9}{14} : \frac{11}{16}\right]$	5

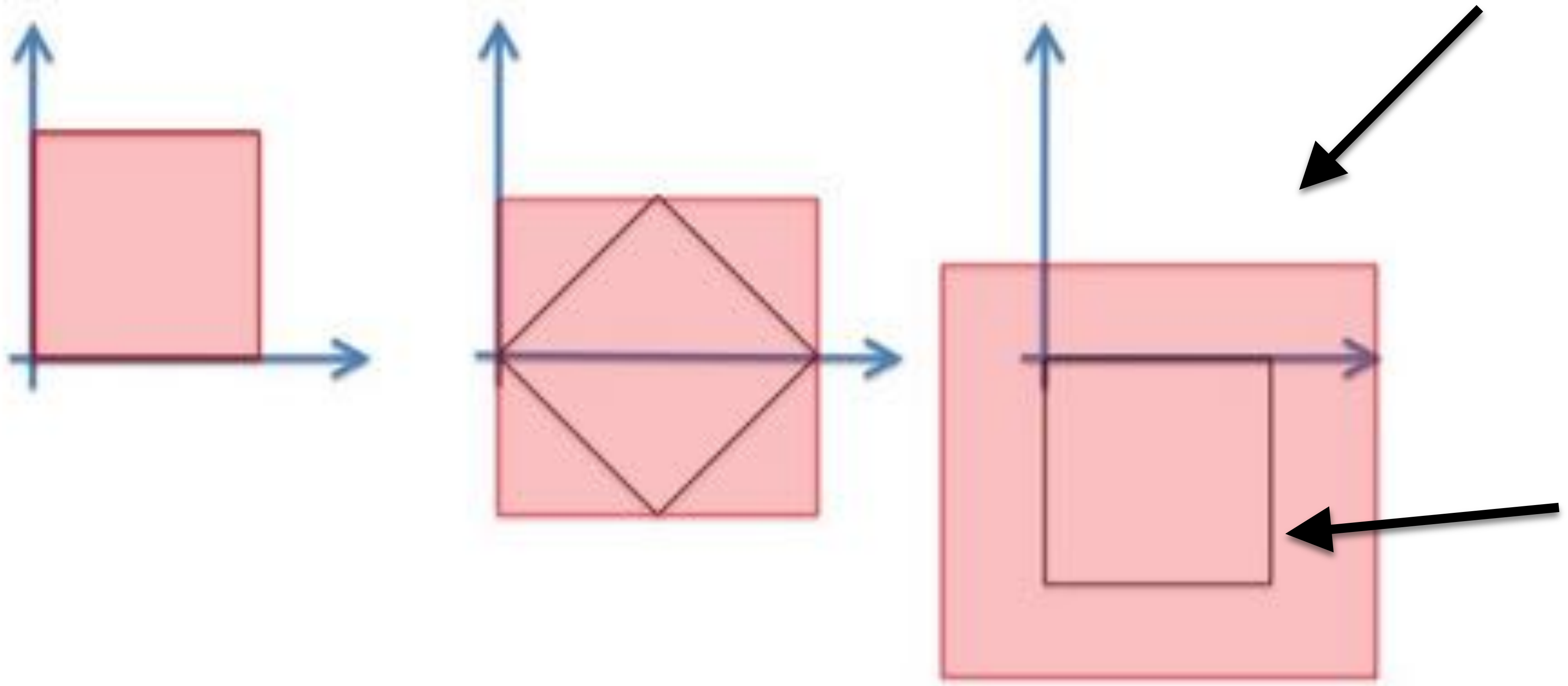
Problems with Intervals Arithmetic

Wrapping Problem

consider the iteration

$$(\xi, \eta) \to \frac{\sqrt{2}}{2}(\xi + \eta, \eta - \xi)$$

interval arithmetic



exact

Iteration 0 1 2

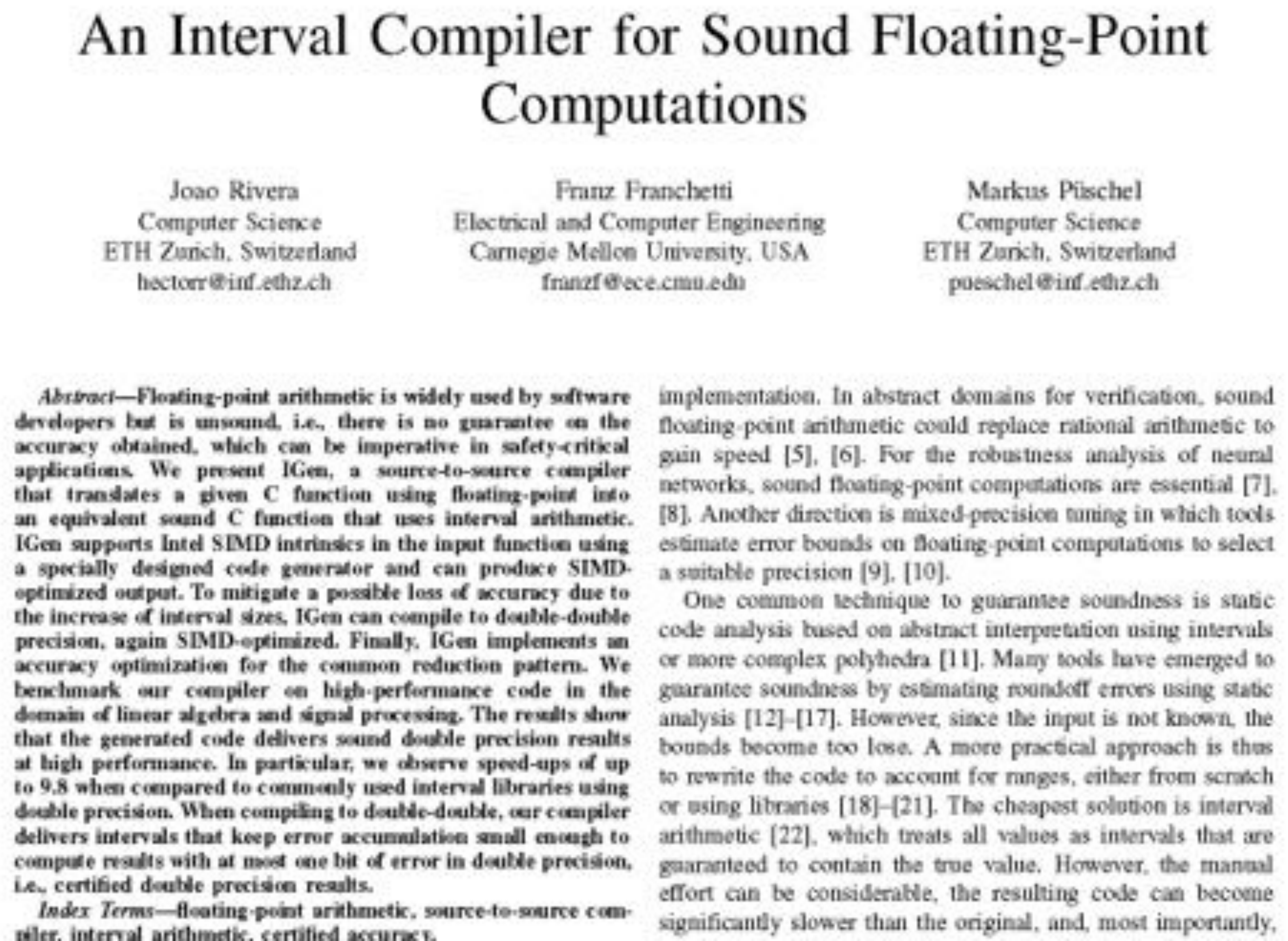
intervals arithmetic produces accurate bounds that are, in general, not optimally tight

summary

non-probabilistic methods for uncertainty quantification don't have a rich theoretical foundation but they are useful when no information is available to justify a probabilistic assumption

question: is an interval equal to a uniform random variable?

interval arithmetic is mostly the focus of computer scientists aiming a building error control within compilers



An Interval Compiler for Sound Floating-Point Computations

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Abstract—Floating-point arithmetic is widely used by software developers but is unsound, i.e., there is no guarantee on the accuracy obtained, which can be imperative in safety-critical applications. We present IGen, a source-to-source compiler that translates a given C function using floating-point into an equivalent sound C function that uses interval arithmetic. IGen supports Intel SIMD intrinsics in the input function using a specially designed code generator and can produce SIMD-optimized output. To mitigate a possible loss of accuracy due to the increase of interval sizes, IGen can compile to double-double precision, again SIMD-optimized. Finally, IGen implements an accuracy optimization for the common reduction pattern. We benchmark our compiler on high-performance code in the domain of linear algebra and signal processing. The results show that the generated code delivers sound double precision results at high performance. In particular, we observe speed-ups of up to 9.8 when compared to commonly used interval libraries using double precision. When compiling to double-double, our compiler delivers intervals that keep error accumulation small enough to compute results with at most one bit of error in double precision, i.e., certified double precision results.

Index Terms—floating-point arithmetic, source-to-source compiler, interval arithmetic, certified accuracy.

implementation. In abstract domains for verification, sound floating-point arithmetic could replace rational arithmetic to gain speed [5], [6]. For the robustness analysis of neural networks, sound floating-point computations are essential [7], [8]. Another direction is mixed-precision tuning in which tools estimate error bounds on floating-point computations to select a suitable precision [9], [10].

One common technique to guarantee soundness is static code analysis based on abstract interpretation using intervals or more complex polyhedra [11]. Many tools have emerged to guarantee soundness by estimating roundoff errors using static analysis [12]–[17]. However, since the input is not known, the bounds become too lose. A more practical approach is thus to rewrite the code to account for ranges, either from scratch or using libraries [18]–[21]. The cheapest solution is interval arithmetic [22], which treats all values as intervals that are guaranteed to contain the true value. However, the manual effort can be considerable, the resulting code can become significantly slower than the original, and, most importantly,

ME270

advances in computing with uncertainties

topics (briefly) covered for today

communicating uncertainties

optimization with uncertainties

uncertainties without probabilities

overall summary

errors are uncertainties are NOT the same

uncertainties come from diverse sources and require different representations (intervals, random variables) thus leading to mutliple quantification strategies

context and intended use of the model estimates (and uncertainties) is an important component of the communication strategy

uncertainties are always present in engineering design and can lead to different choices among various trade-offs

uncertainty quantification should be explicit, principled and free of errors

Questions?

ME270 – Fall 2021

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