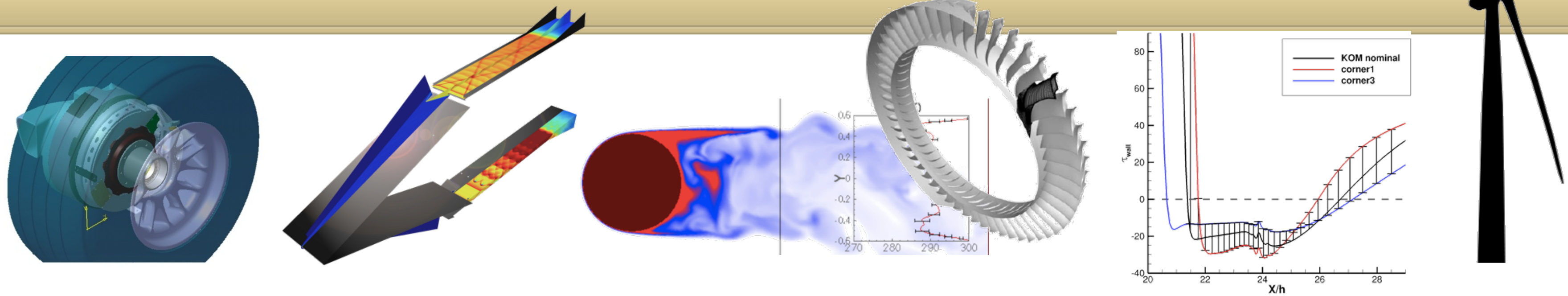
STANFORD UNIVERSITY | UNCERTAINTY QUANTIFICATION LABORATORY



Quantifying Uncertainties in Turbulent Flow Simulations

Gianluca Iaccarino

Mechanical Engineering Department

Institute for Computational Math & Engineering

Stanford University

MUSAF II Colloquium, September 2013 Toulouse, France

Outline

- **Why UQ?**
- **How to Quantify Uncertainties? AUQ and EUQ**
- **The UQ Experiment**
- **Conclusions**

Outline

- **Why UQ?**
- How to Quantify Uncertainties? AUQ and EUQ
- The UQ Experiment
- Conclusions

Why Uncertainty Quantification?

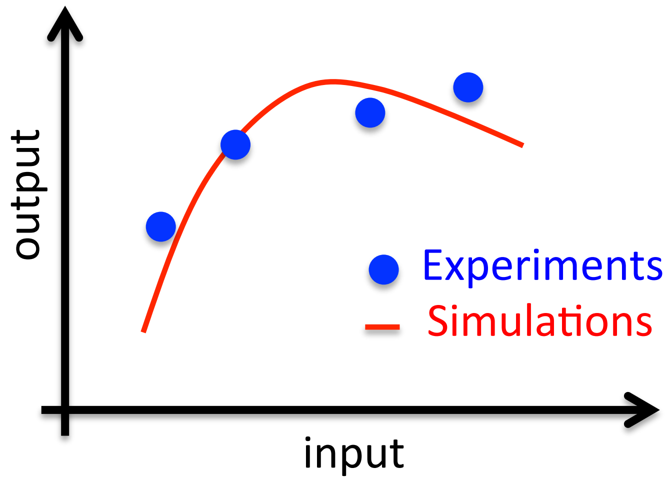
Why Uncertainty Quantification?

#1: UQ is an essential part of **Validation**

Why Uncertainty Quantification?

#1: UQ is an essential part of **Validation**

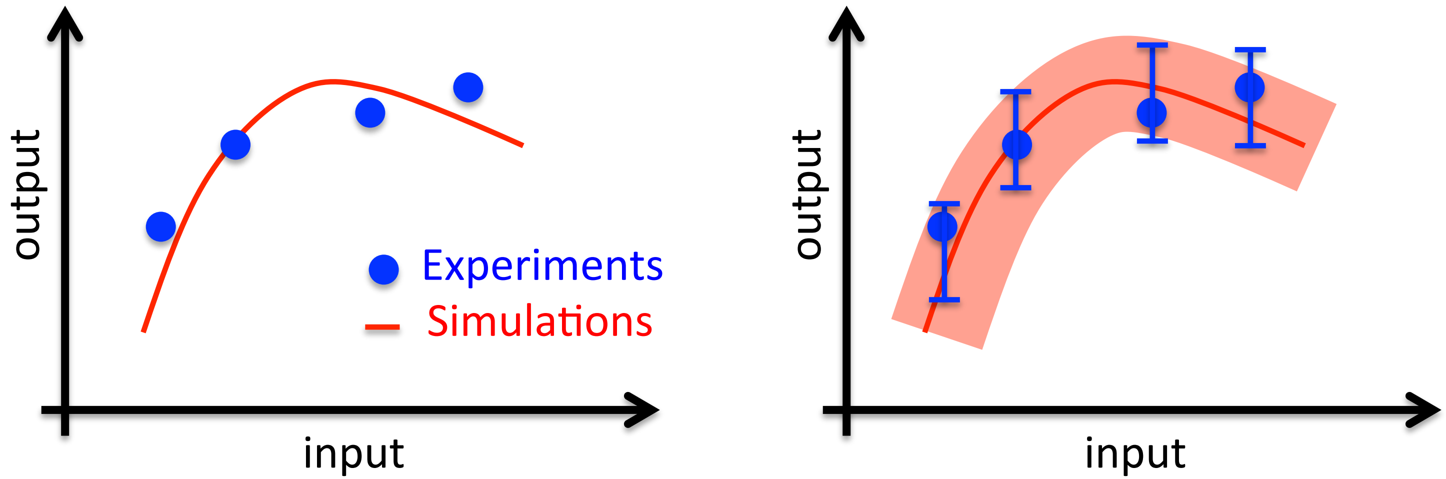
Validation = Comparisons of simulations with experiments



Why Uncertainty Quantification?

#1: UQ is an essential part of **Validation**

Validation = Comparisons of simulations with experiments
Experimentalists are "required" to provide uncertainty measures,
Computationalists will have to follow (very soon)!

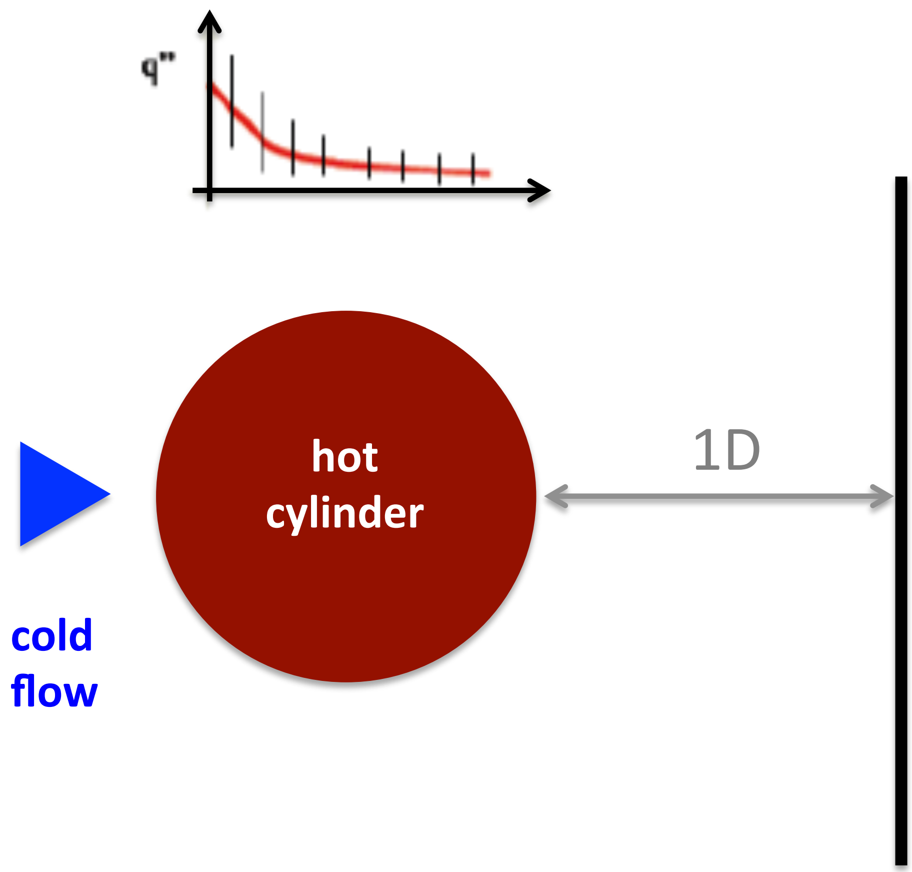


Why Uncertainty Quantification?

#2: UQ can provide a **rigorous measure of confidence**

Why Uncertainty Quantification?

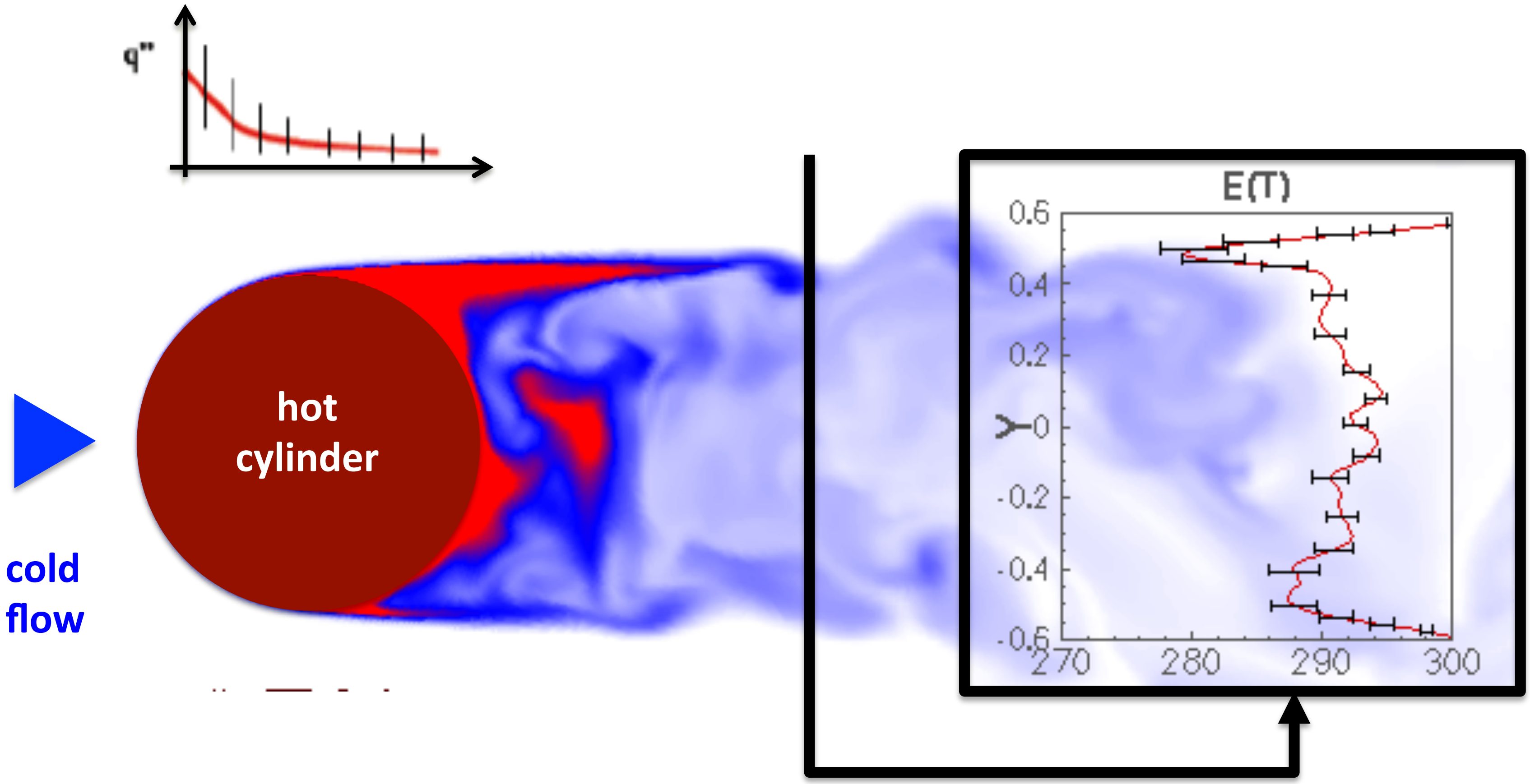
#2: UQ can provide a **rigorous measure of confidence**



If we have uncertainty in the conditions of the cylinder wall (e.g. material inhomogeneity) what it the resulting temperature in the wake?

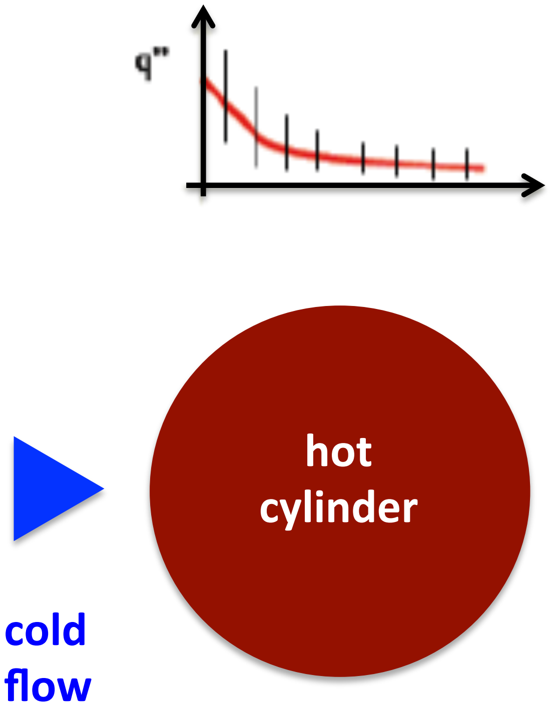
Why Uncertainty Quantification?

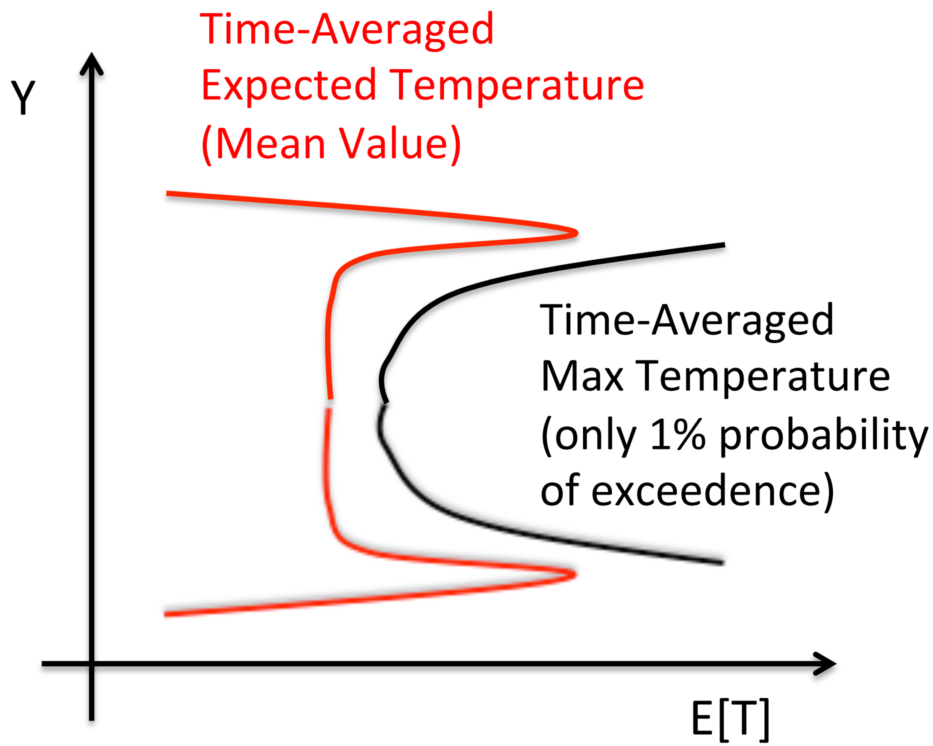
#2: UQ can provide a **rigorous measure of confidence**



Why Uncertainty Quantification?

#2: UQ can provide a **rigorous measure of confidence**





Constantine, Doostan & Iaccarino
JCP 2009, IJNME 2009

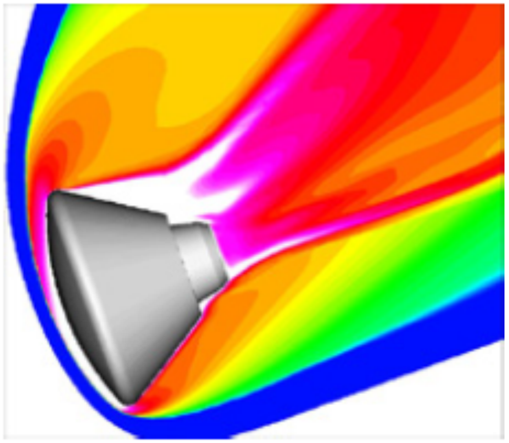
Why Uncertainty Quantification?

#3: UQ indicates **priorities** and supports decision making

Why Uncertainty Quantification?

#3: UQ indicates **priorities** and supports decision making

Computations of peak heating at the stagnation point requires detailed modeling of the high-temperature non-equilibrium effects



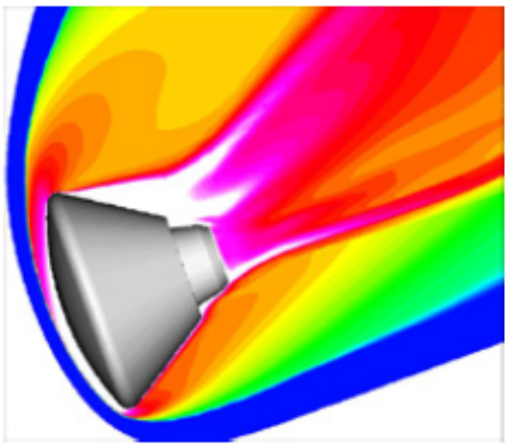
For Titan entry a model including 13 species and 26 reactions was employed: the reaction rates are based on measurements

	Dissociation reactions $k_f = A_r T^{b_r} \exp(-C_r/T)$	A_r(cc/mol-s)	b_r	C_r (K)	95% conf. limit [Ref.]
1	$N_2 + M \Leftrightarrow 2N + M$	7.00×10^{21}	-1.60	113200	See Table 2
	M=N,C,H	3.00×10^{22}	-1.60	113200	
2	$CH_4 + M \Leftrightarrow CH_3 + H + M$	4.70×10^{47}	-8.20	59200	±0.30[22]
3	$CH_3 + M \Leftrightarrow CH_2 + H + M$	1.02×10^{16}	0.00	45600	±0.35[22]
4	$CH_3 + M \Leftrightarrow CH + H_2 + M$	5.00×10^{15}	0.00	42800	±0.30[23]
5	$CH_2 + M \Leftrightarrow CH + H + M$	4.00×10^{15}	0.00	41800	±0.30[23]
6	$CH_2 + M \Leftrightarrow C + H_2 + M$	1.30×10^{14}	0.00	29700	±0.30[23]
7	$CH + M \Leftrightarrow C + H + M$	1.90×10^{14}	0.00	33700	±0.30[23]
8	$C_2 + M \Leftrightarrow 2C + M$	1.50×10^{16}	0.00	71600	±0.30[24]
9	$H_2 + M \Leftrightarrow 2H + M$	2.23×10^{14}	0.00	48350	±0.30[22,25]
10	$CN + M \Leftrightarrow C + N + M$	2.53×10^{14}	0.00	71000	±0.30[26,27]
11	$NH + M \Leftrightarrow N + H + M$	1.80×10^{14}	0.00	37600	±0.30[28]
12	$HCN + M \Leftrightarrow CN + H + M$	3.57×10^{26}	-2.60	62845	±0.30[29]
	Exchange reactions				
13	$CH_3 + H \Leftrightarrow CH_2 + H_2$	6.03×10^{13}	0.00	7600	±1.00[25]
14	$CH_3 + N_2 \Leftrightarrow HCN + NH$	4.82×10^{12}	0.00	18000	±1.00[28]
15	$CH_2 + N \Leftrightarrow HCN + H$	5.00×10^{13}	0.00	0	±1.00[30]
16	$CH_2 + H \Leftrightarrow CH + H_2$	6.03×10^{12}	0.00	-900	±0.87[25,28]
17	$CH + N_2 \Leftrightarrow HCN + N$	4.40×10^{12}	0.00	11060	±0.35[30]
18	$CH + C \Leftrightarrow C_2 + H$	2.00×10^{14}	0.00	0	±1.00[23]
19	$C_2 + N_2 \Leftrightarrow 2CN$	1.50×10^{13}	0.00	21000	±0.30[31]
20	$CN + H_2 \Leftrightarrow HCN + H$	2.95×10^{5}	0.00	1130	±0.60[32]
21	$CN + C \Leftrightarrow C_2 + N$	5.00×10^{13}	0.00	13000	±0.54[18]
22	$N + H_2 \Leftrightarrow NH + H$	1.60×10^{14}	0.00	12650	±0.30[33]
23	$C + N_2 \Leftrightarrow CN + N$	5.24×10^{13}	0.00	22600	±0.50[T]
24	$C + H_2 \Leftrightarrow CH + H$	4.00×10^{14}	0.00	11700	±0.30[34]
25	$H + N_2 \Leftrightarrow NH + N$	3.00×10^{12}	0.50	71400	±0.50[T]
26	$CH_4 + H \Leftrightarrow CH_3 + H_2$	1.32×10^{4}	3.00	4045	±0.30[22,25]

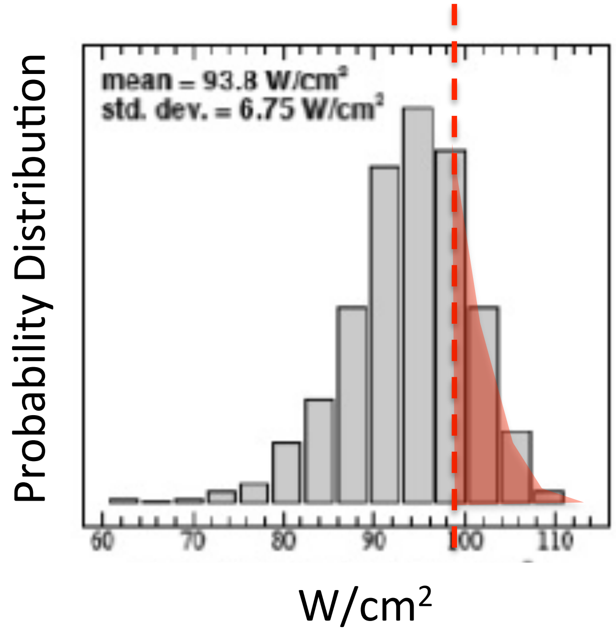
Why Uncertainty Quantification?

#3: UQ indicates **priorities** and supports decision making

Computations of peak heating at the stagnation point requires detailed modeling of the high-temperature non-equilibrium effects



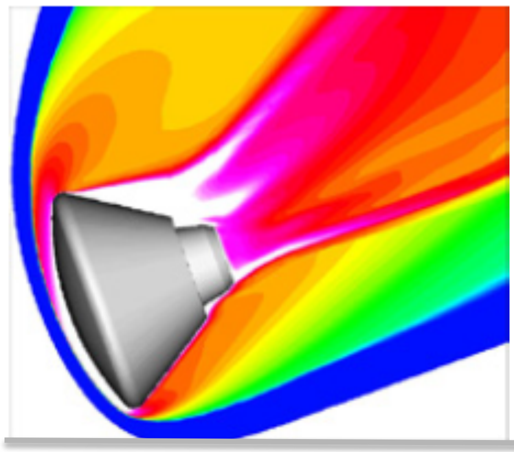
Effect of the reaction rate uncertainties on the stagnation point heat flux



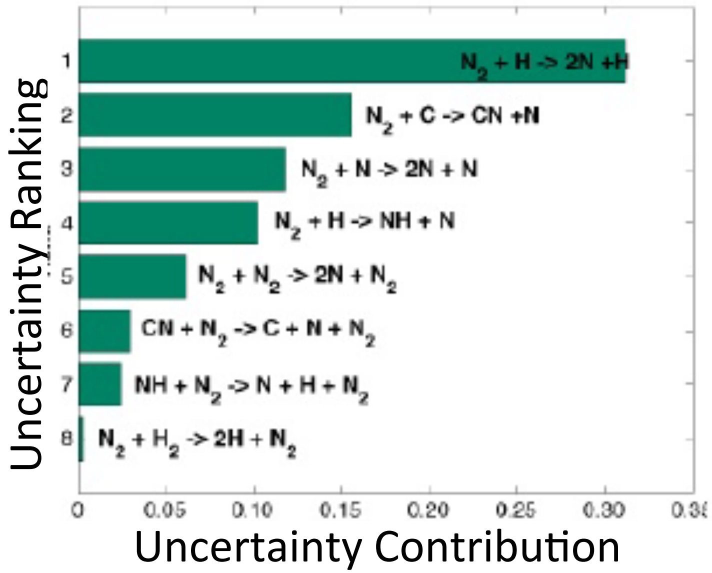
Why Uncertainty Quantification?

#3: UQ indicates **priorities** and supports decision making

Computations of peak heating at the stagnation point requires detailed modeling of the high-temperature non-equilibrium effects



UQ indicates the reactions rates dominating the output uncertainty



Ghaffari, Magin & Iaccarino AIAA 2009

Why Uncertainty Quantification?

#1: UQ is an essential part of **Validation**

#2: UQ can provide a **rigorous measure of confidence**

#3: UQ indicates **priorities** and supports decision making

#4: UQ enables **robust design/reliability analysis**

#5: Quantification of **margins** and **risk analysis**

....

Why Uncertainty Quantification?

#1: UQ is an essential part of **Validation**

#2: UQ can provide a **rigorous measure of confidence**

#3: UQ indicates **priorities** and supports decision making

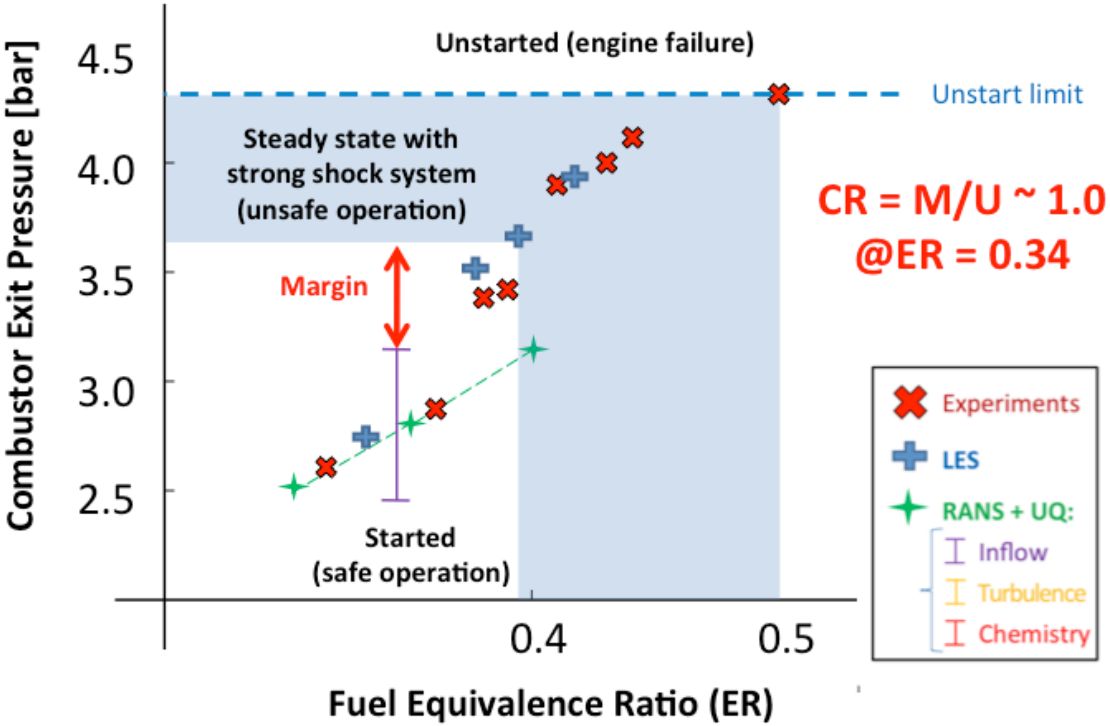
#4: UQ enables **robust design/reliability analysis**

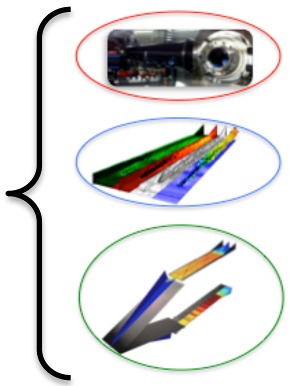
#5: Quantification of **margins** and **risk analysis**

….

Quantification of Margin to Failure

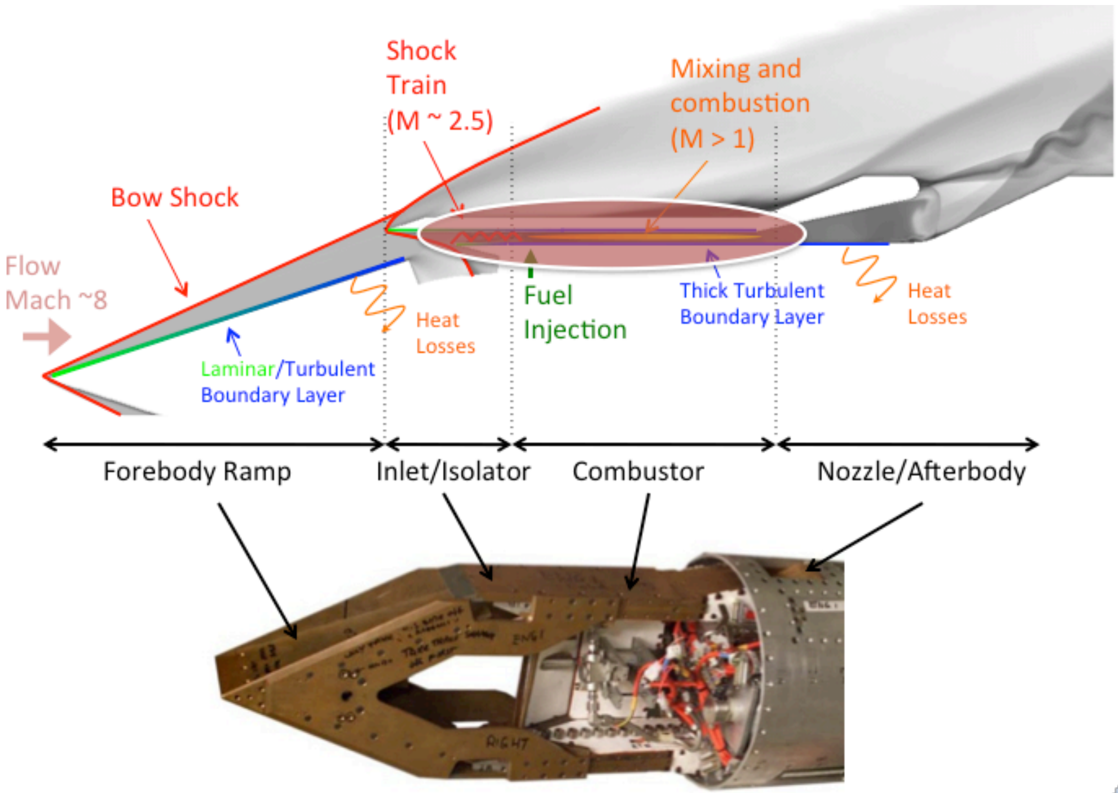
PSAAP: Predictive Science Academic Alliance Program @ Stanford

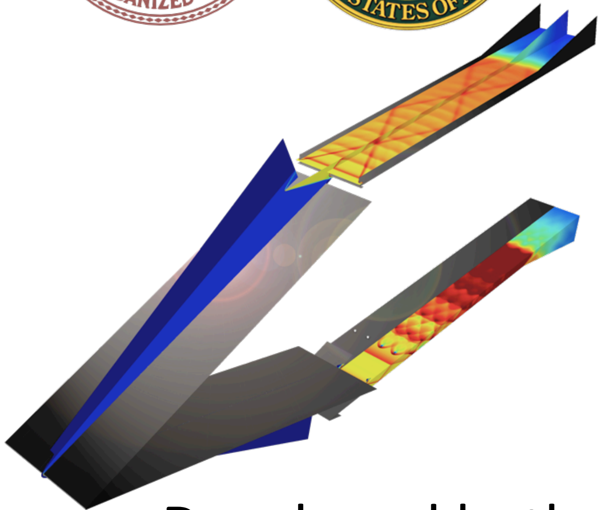




Multi-fidelity Assessment of Margin and Uncertainties to SCRAMJET Unstart

Scramjet





Developed both engineering codes (RANS) and high-fidelity simulation capabilities

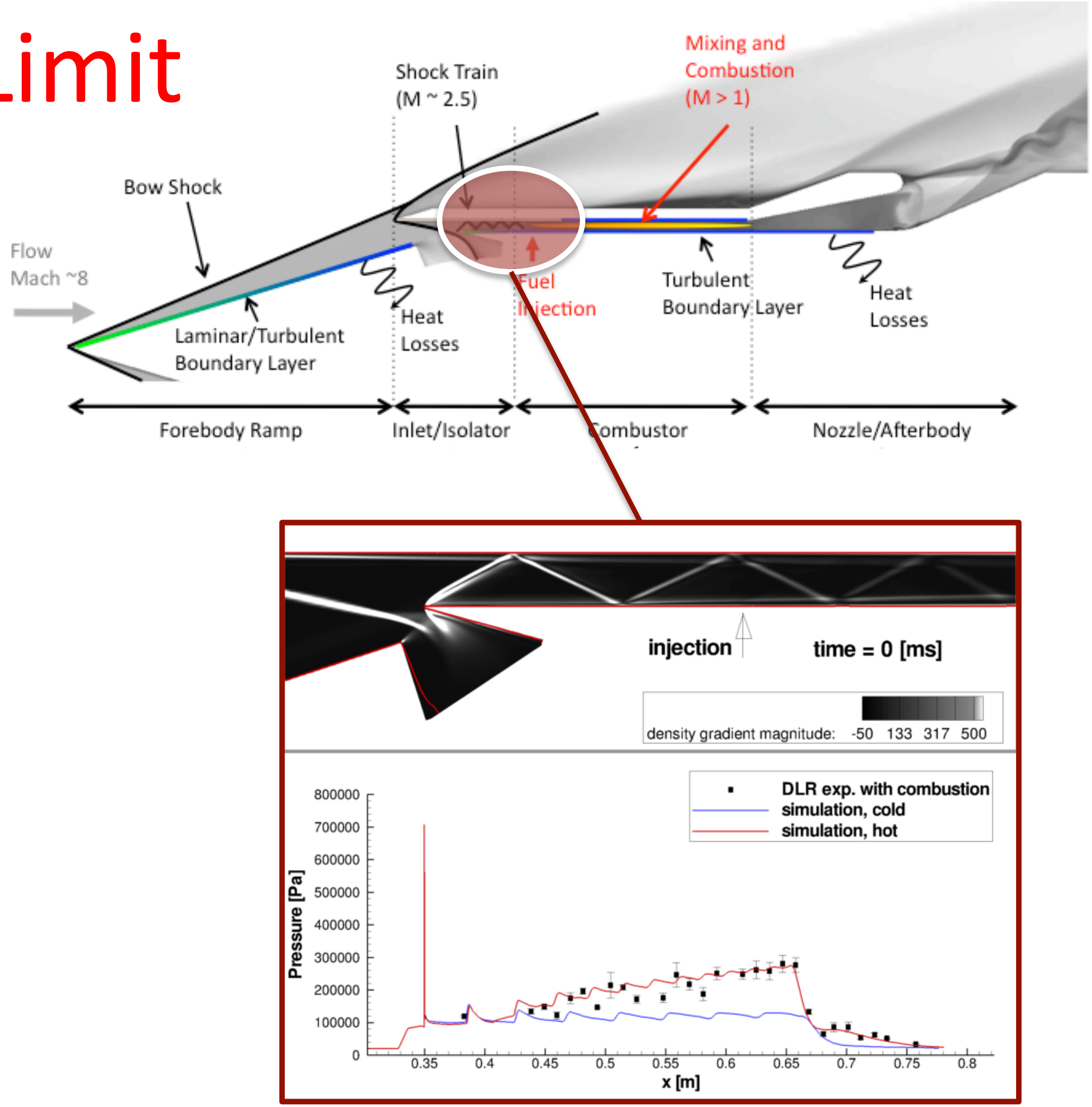
PSAAP: Predictive Science Academic Alliance Program

Operability Limit

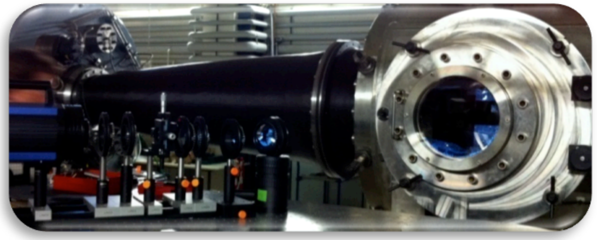
- An increase in the fuel injection leads to more thrust via an increased level of heat release in the combustor

- Excessive heat can lead to a violent ejection of the shock system from the started engine

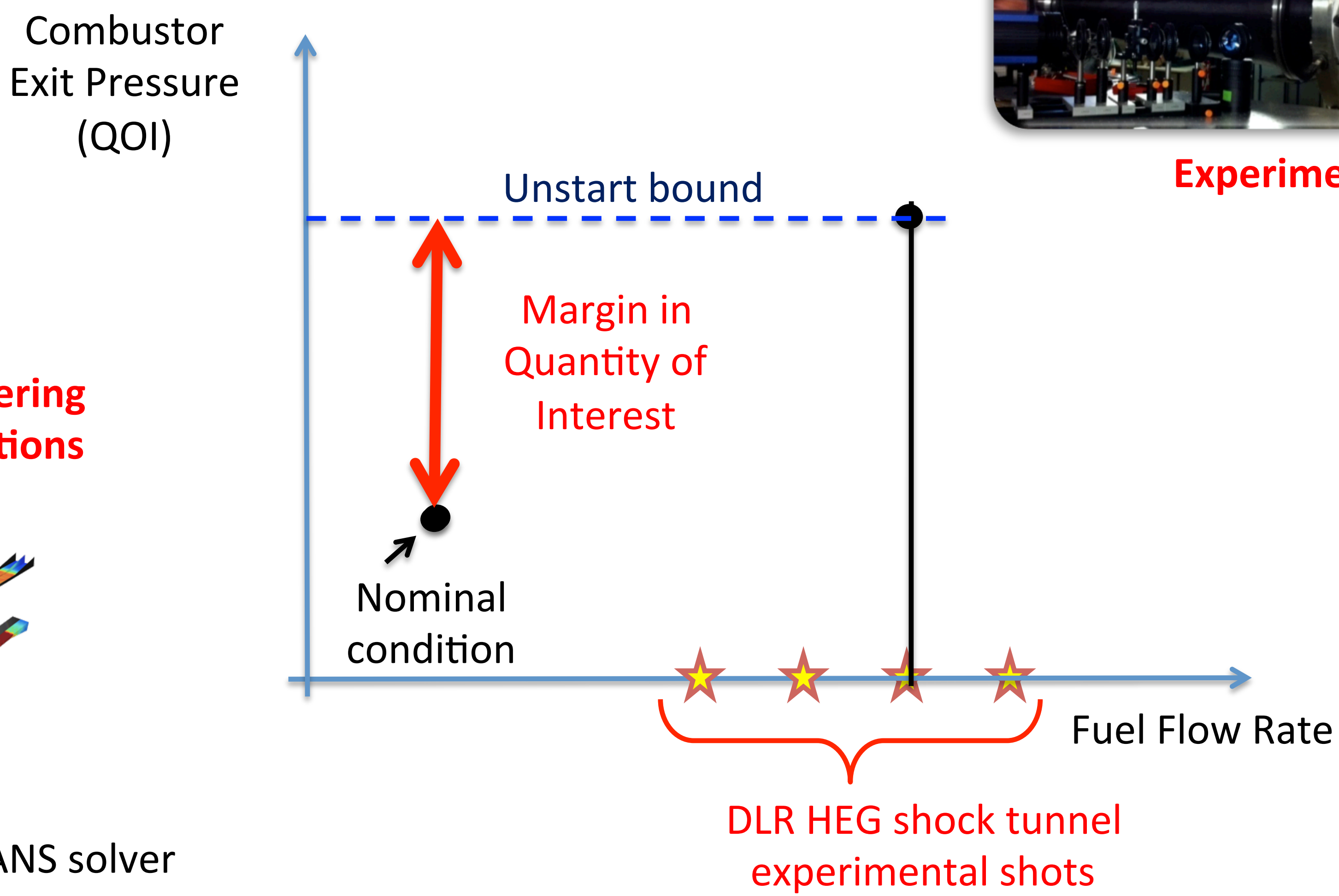
- The result is a loss of oxygen for combustion, large flow separation, excessive structural loads, subsonic flow



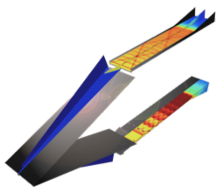
Operability Limits



Experiments

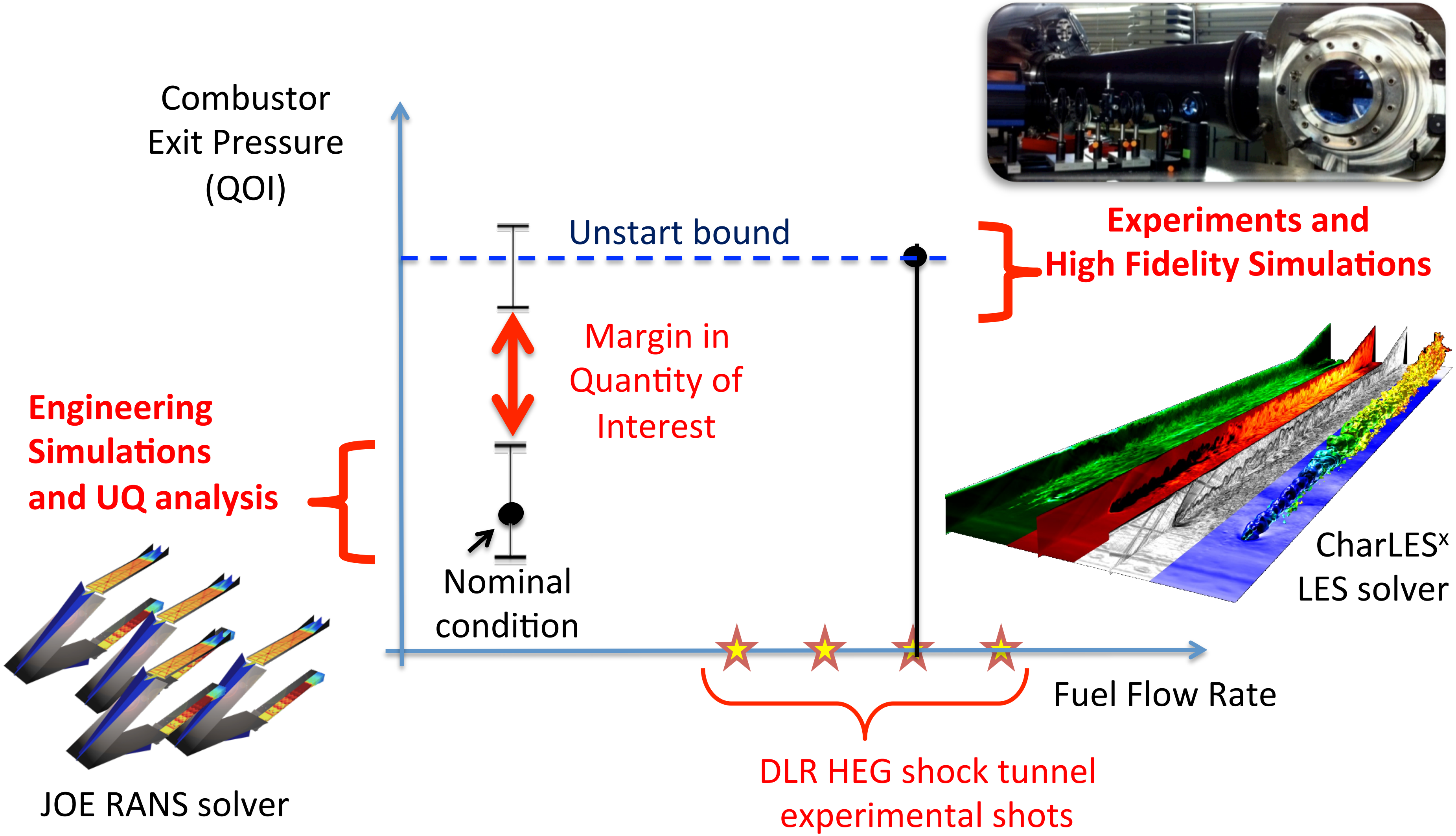


Engineering Simulations



JOE RANS solver

Operability Limits

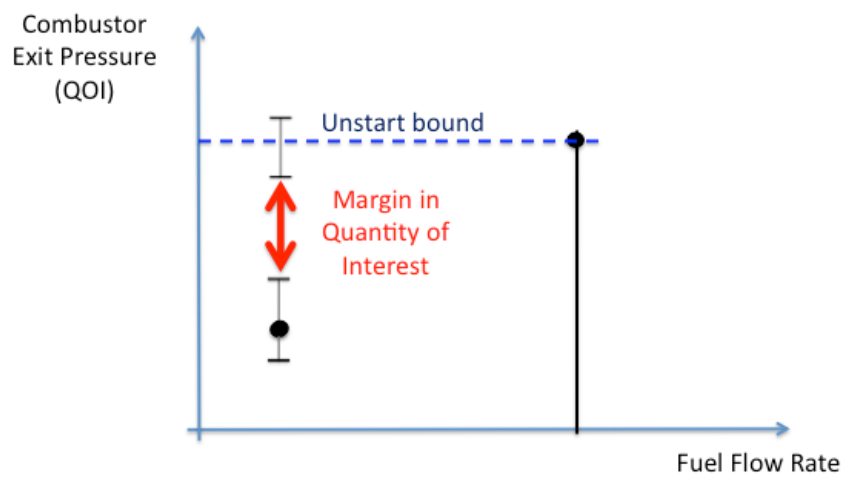


Operability Limits Using QMU

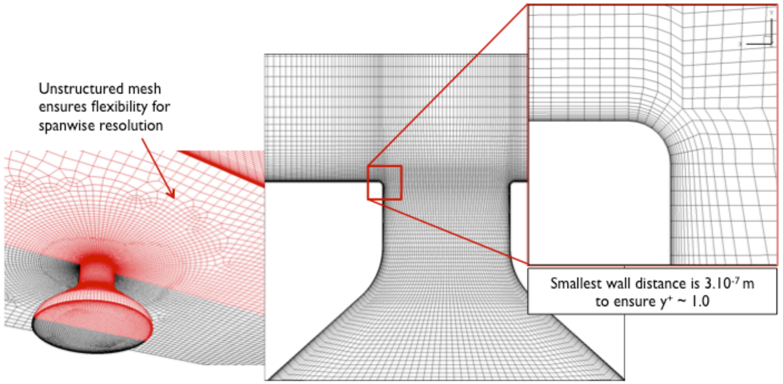
- Quantification of Margins and Uncertainties (QMU) defines the operability limit in terms of both safety and confidence
  - **Safety** in characterized by a given **margin**
  - Explicit inclusion of **uncertainties** leads to quantified level of **confidence**

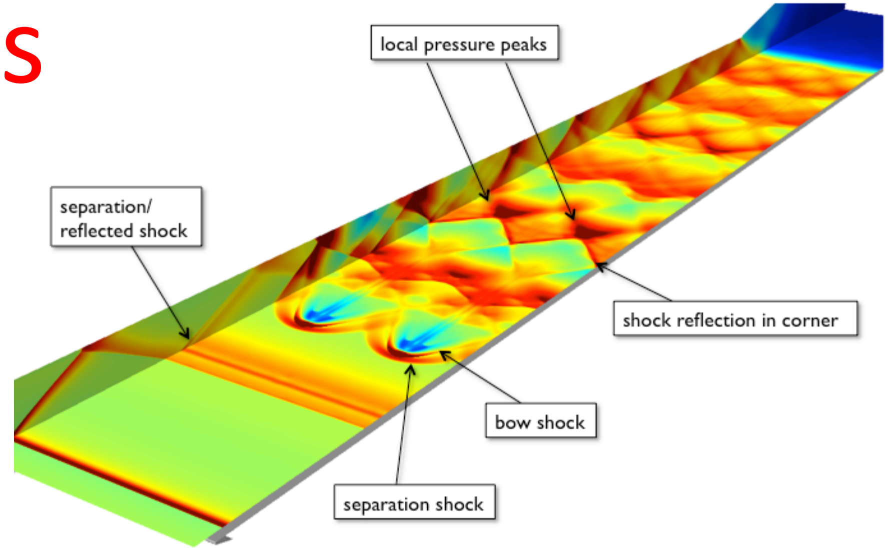
Confidence Ratio = CR = M/U

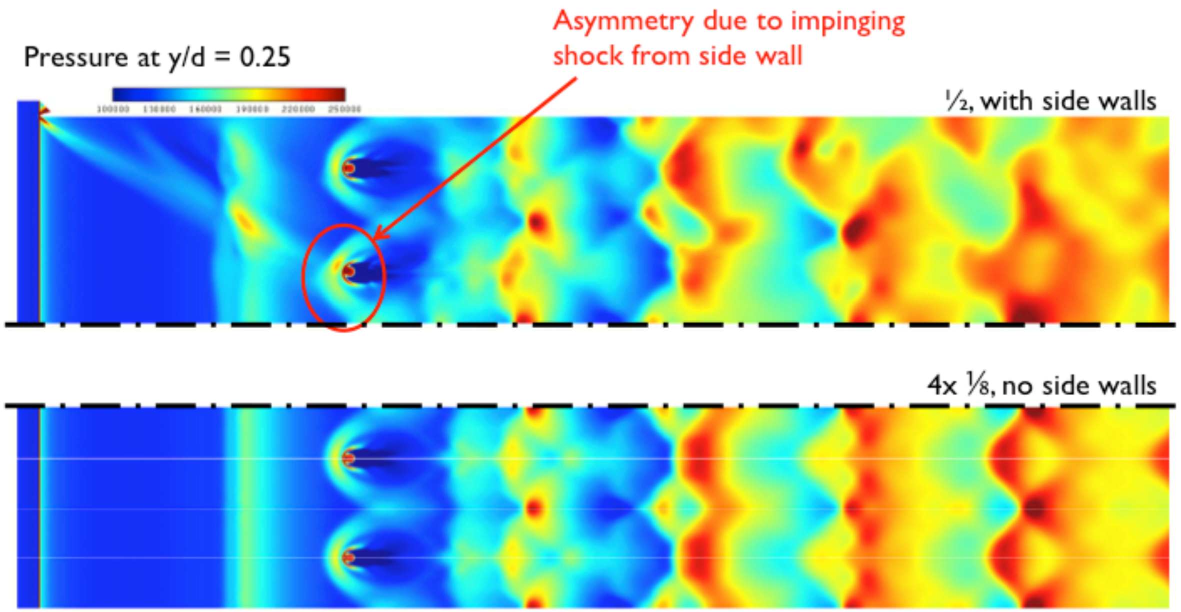
- Our approach is to generate operability maps using V&V-ed computations and explicit UQ assessment



Scramjet Simulations





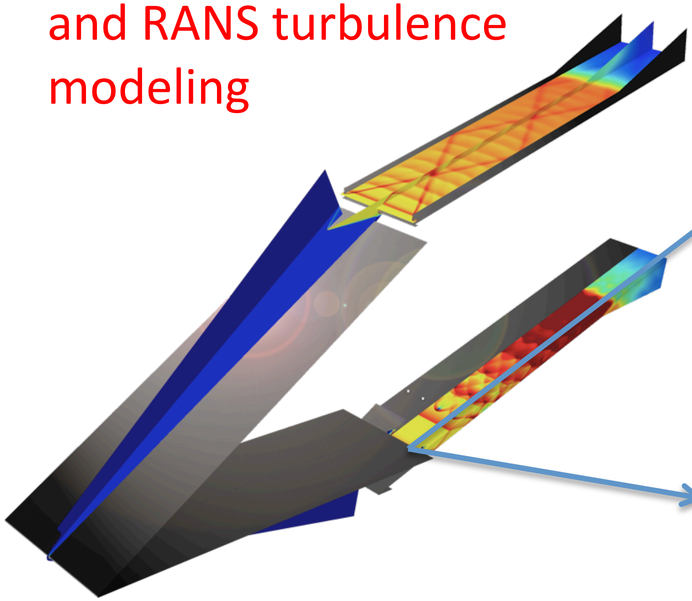


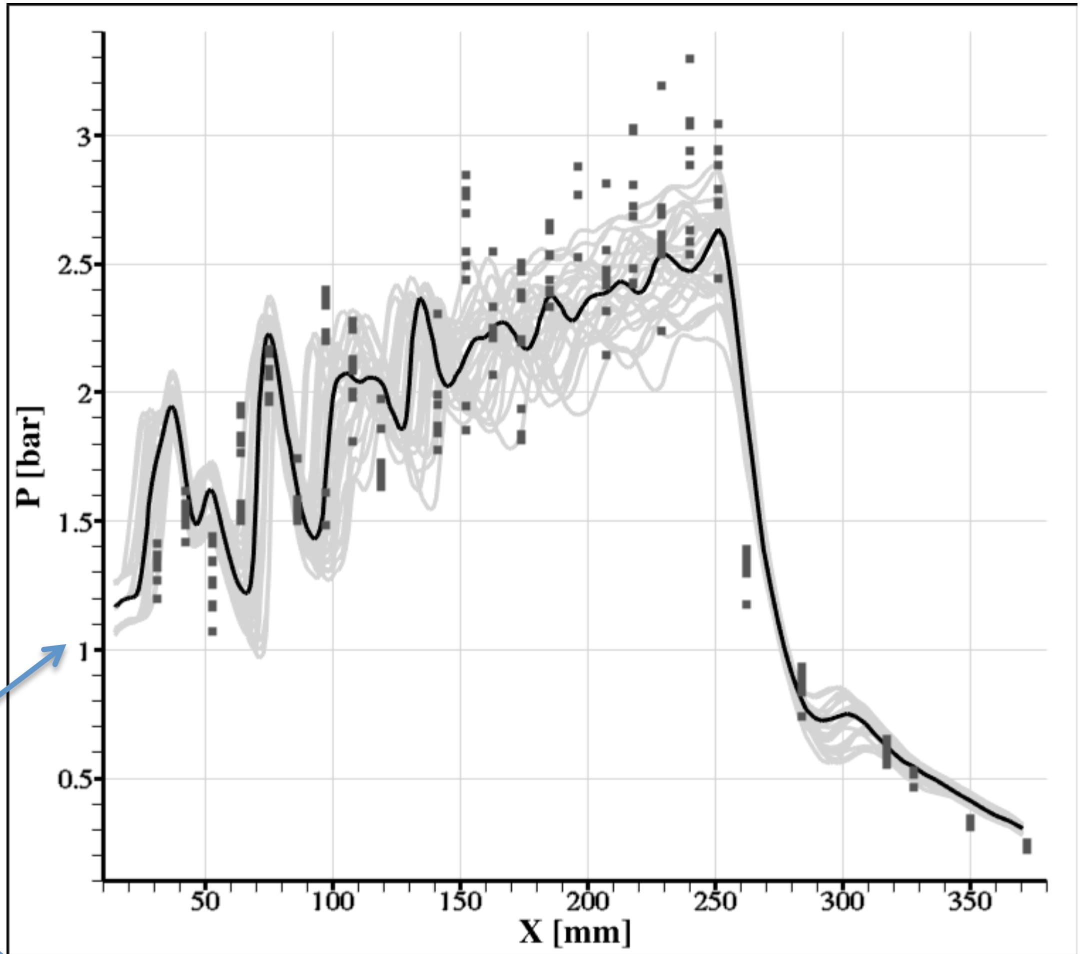
Mesh size

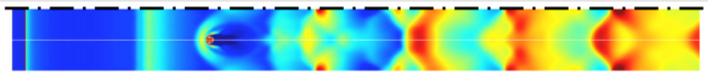
- 2D 0.2 million
- 3D, ⅛ : 2.6 million
- 3D, ½ (side wall) 12.5 million

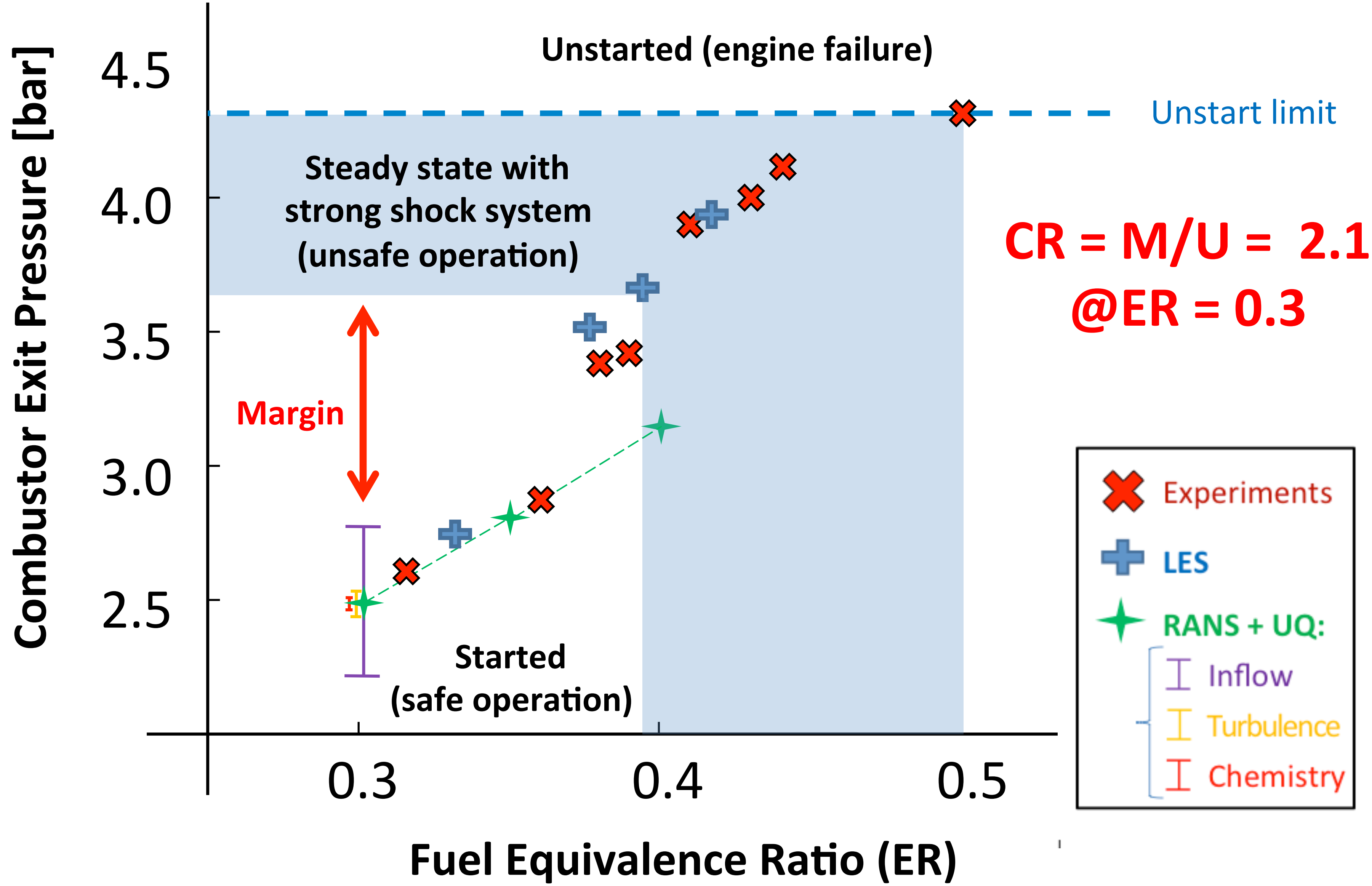
Scramjet Simulations

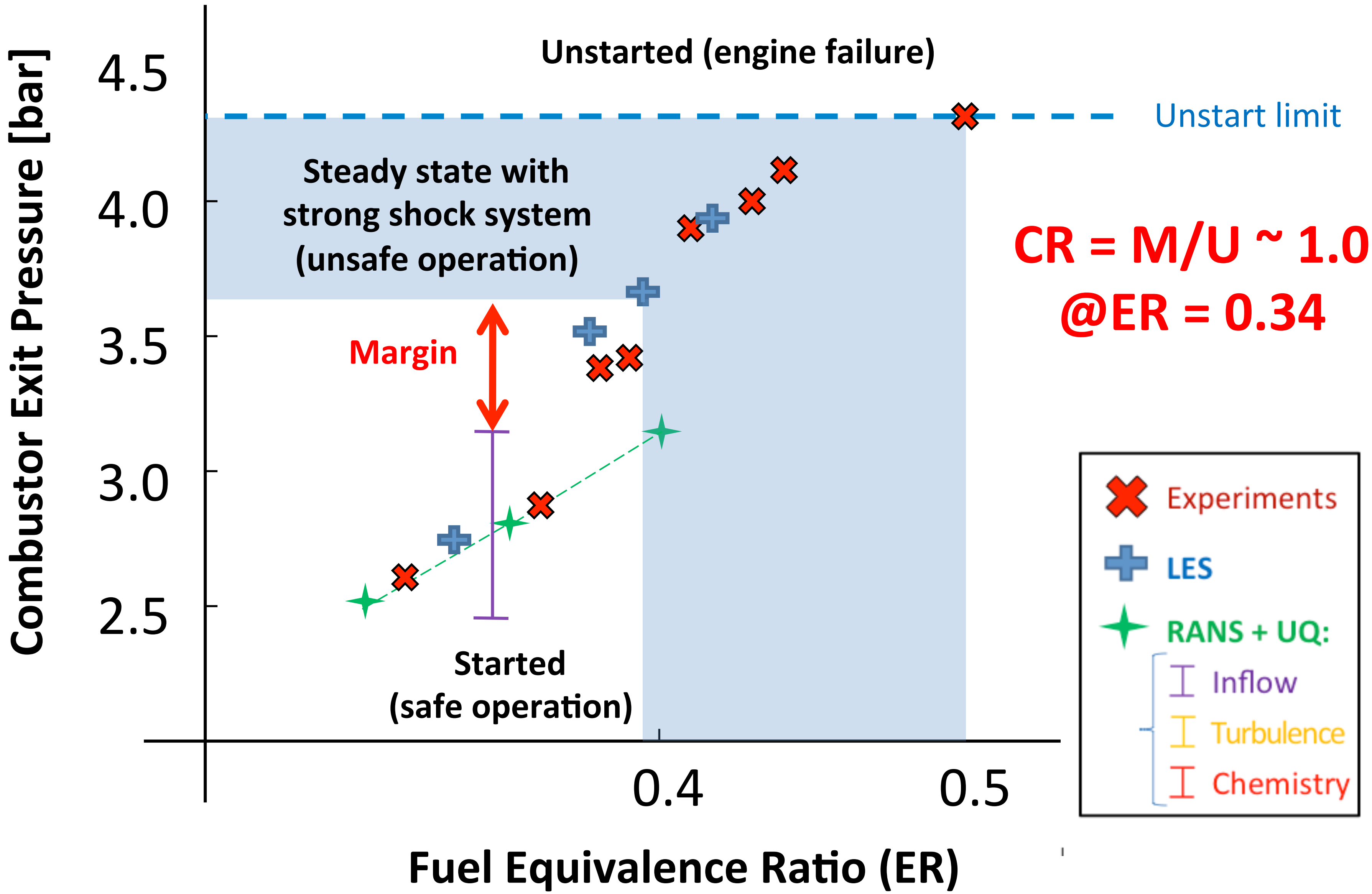
- Pressure distribution in the fueled combustor (low equivalence ratio)
- Uncertainty in the flow/ fuel conditions (DLR HEG facility), chemical rates and RANS turbulence modeling








Unstarted (engine failure)
Unstart limit
Steady state with strong shock system (unsafe operation)
Margin
Started (safe operation)
CR = M/U = 2.1
@ER = 0.3
Experiments
LES
RANS + UQ:
Inflow
Turbulence
Chemistry
Combustor Exit Pressure [bar]
Fuel Equivalence Ratio (ER)
4.5
4.0
3.5
3.0
2.5
0.3
0.4
0.5



CR = M/U ~ 1.0
@ER = 0.34

Outline

- Why UQ?
- **How to Quantify Uncertainties? AUQ and EUQ**
- The UQ Experiment
- Conclusions

How to Quantify Uncertainty?

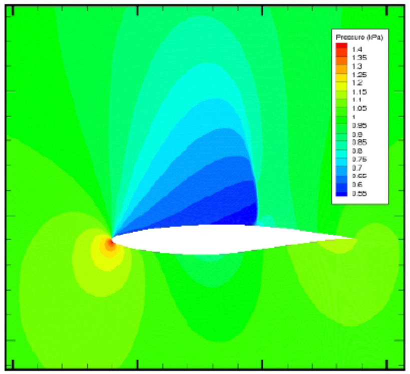
How to Quantify Uncertainty?

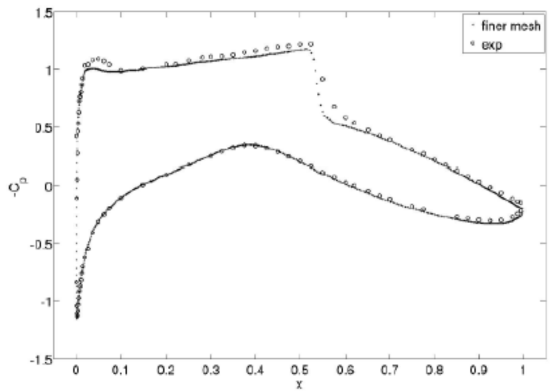
Consider a computational model for investigating the transonic turbulent flow around an airfoil….

$M_\infty = 0.734$

$\alpha = 2.79^o$

$Re = 6.5 \times 10^6$





How to Quantify Uncertainty?

Consider a computational model for investigating the transonic turbulent flow around an airfoil….

$M_\infty = 0.734$
$\alpha = 2.79^o$
$Re = 6.5 \times 10^6$

inputs outputs

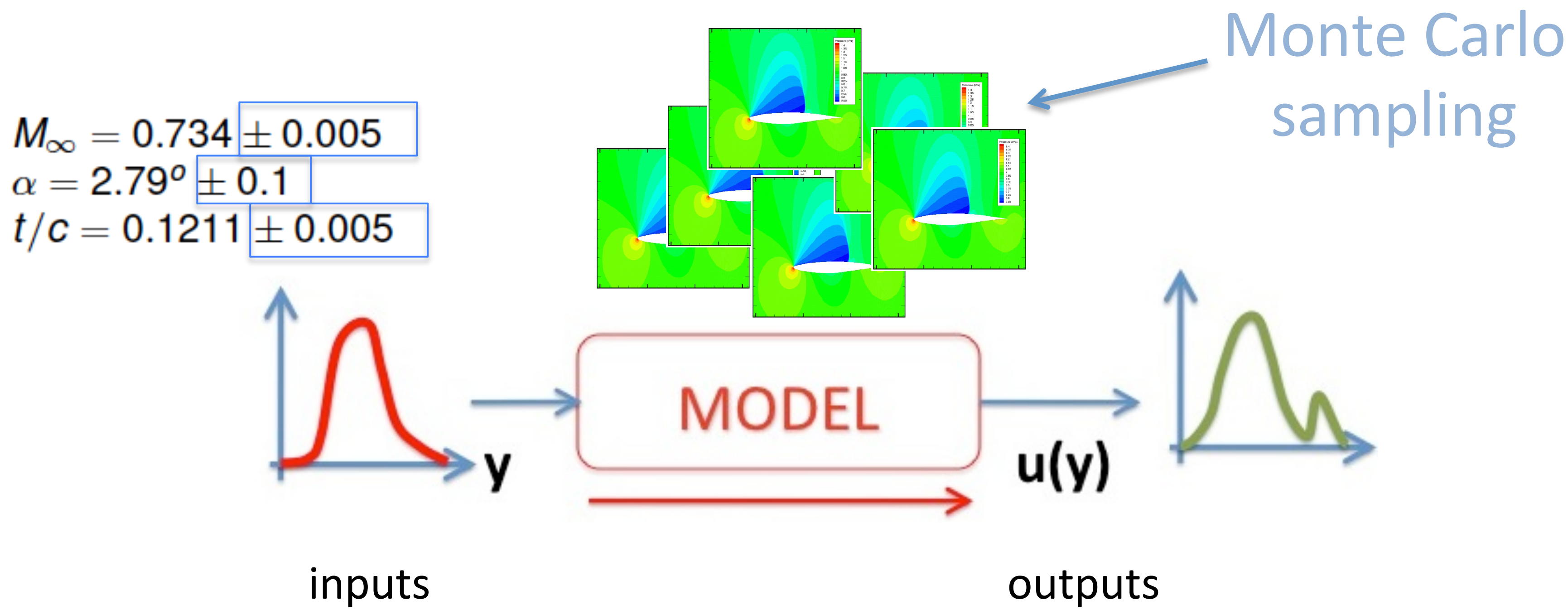
How to Quantify Uncertainty?

Now suppose that the free stream conditions and geometry are not precisely known…

$$M_\infty = 0.734 \boxed{\pm 0.005}$$
$$\alpha = 2.79^o \boxed{\pm 0.1}$$
$$t/c = 0.1211 \boxed{\pm 0.005}$$

How to Quantify Uncertainty?

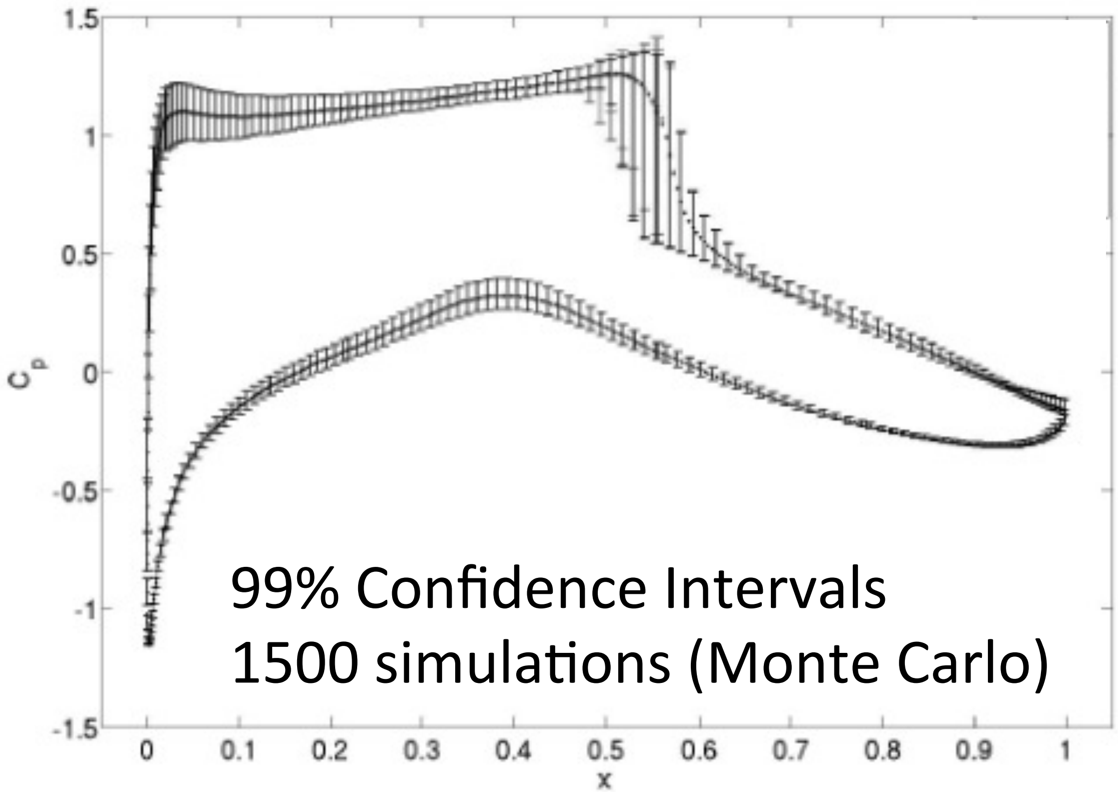
If we can describe the uncertainties in probabilistic terms, e.g. interpret the input ranges as confidence intervals



How to Quantify Uncertainty?

Compute an ensemble of simulations and determine confidence bounds on outputs

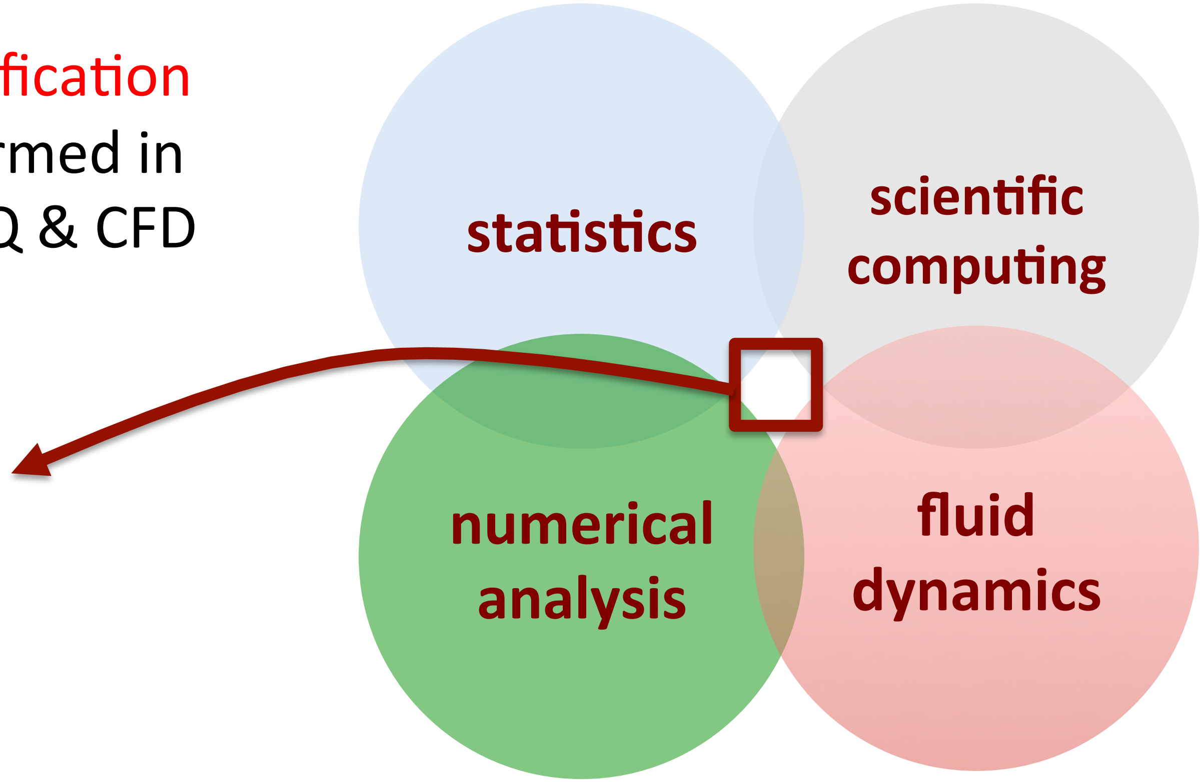
$$M_\infty = 0.734 \pm 0.005$$
$$\alpha = 2.79^o \pm 0.1$$
$$t/c = 0.1211 \pm 0.005$$



The Need for UQ Science

Monte Carlo was "invented" in the 40s…and is not feasible for any realistic numerical simulations

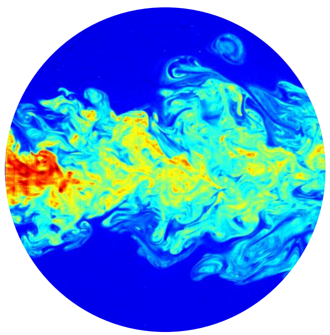
The Uncertainty Quantification Lab at Stanford was formed in 2007 and focuses on UQ & CFD



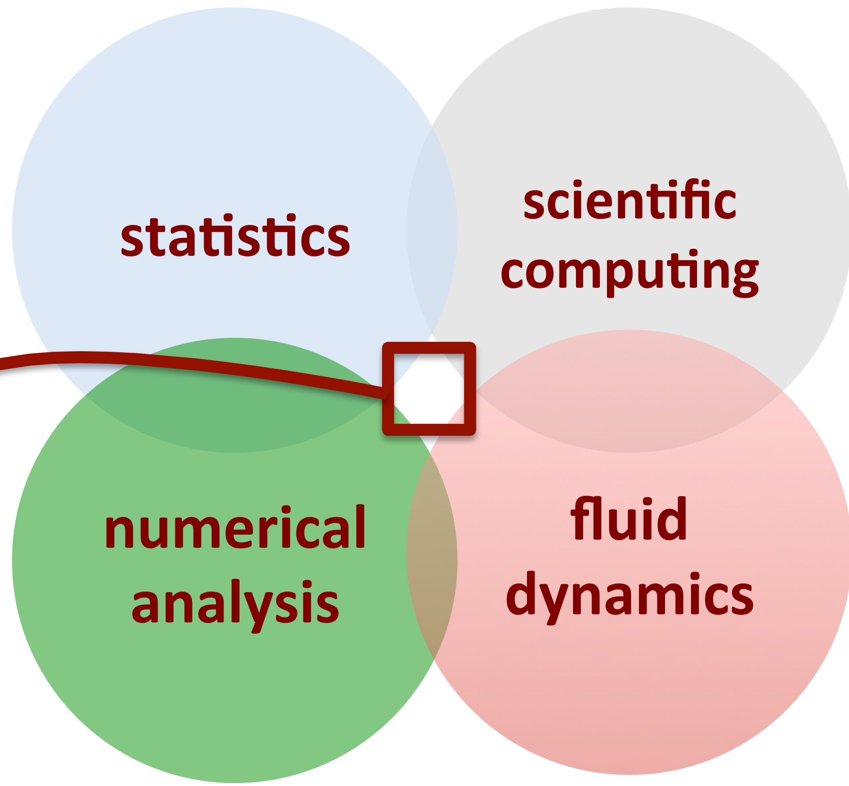
The Need for UQ Science

Monte Carlo was "invented" in the 40s…and is not feasible for any realistic numerical simulations

The Uncertainty Quantification Lab at Stanford was formed in 2007 and focuses on UQ & CFD



Center for Turbulence Research

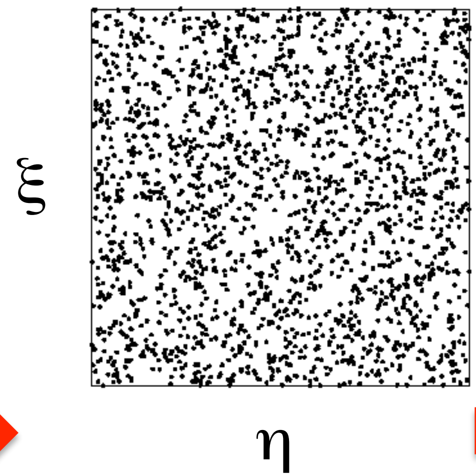


Better than Monte Carlo

In a probabilistic framework the objective is to compute statistics of the output of interest

Input: ξ, η

Output: Q(ξ, η)



$$Var[Q] = \sum_{k=1}^{N} \frac{(Q(\xi_k, \eta_k) - E[Q])^2}{N-1}$$

$$E[Q] = \sum_{k=1}^{N} \frac{Q(\xi_k, \eta_k)}{N}$$

Better than Monte Carlo

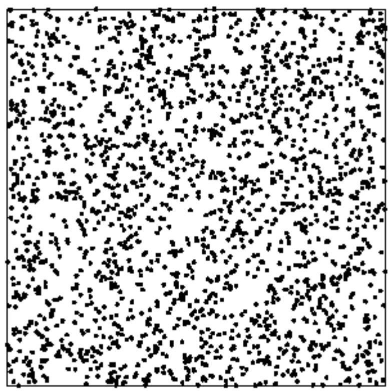
In a probabilistic framework the objective is to compute statistics of the output of interest

…these statistics can be represented in terms of continuous (random) variables and integrals

Input: ξ, η

Output: Q(ξ, η)

ξ



η

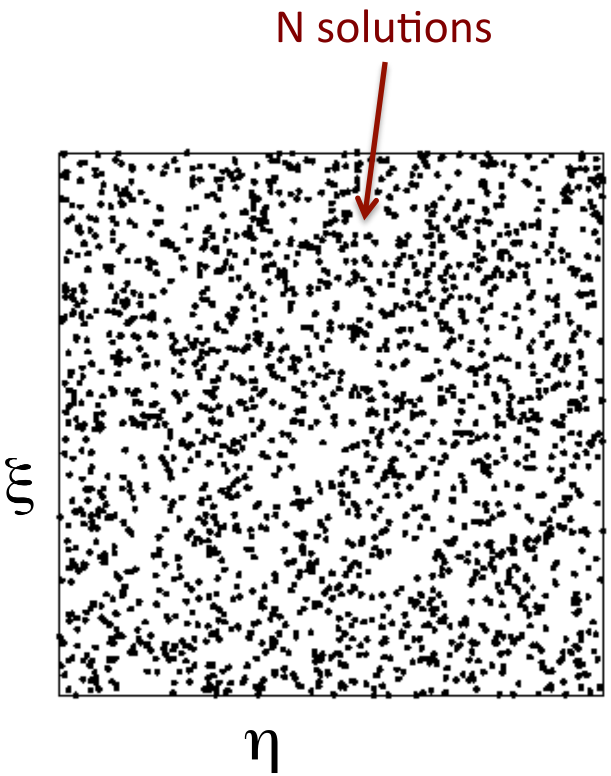
$$Var[Q] = \sum_{k=1}^{N} \frac{(Q(\xi_k, \eta_k) - E[Q])^2}{N-1}$$

$$= \int\int (Q(\xi, \eta) - E[Q])^2 f_{\xi,\eta}\, d\xi d\eta$$

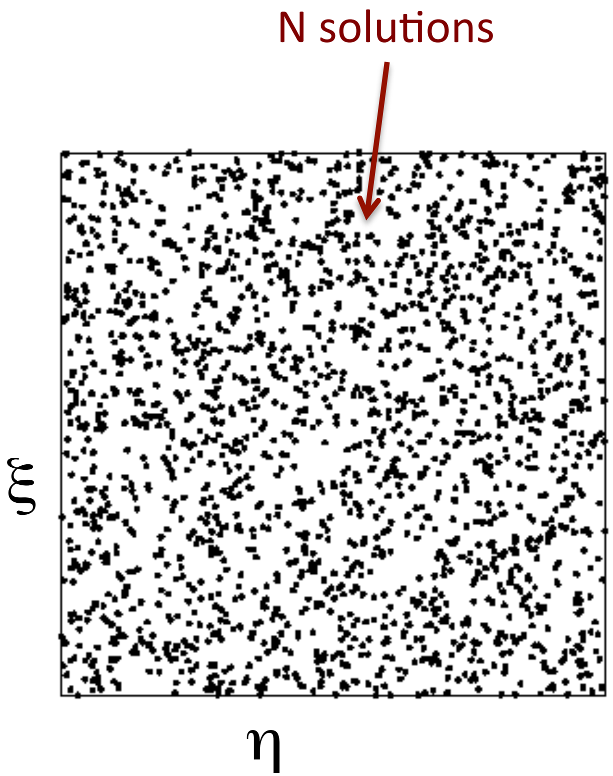
$$E[Q] = \sum_{k=1}^{N} \frac{Q(\xi_k, \eta_k)}{N}$$

$$= \int\int Q(\xi, \eta) f_{\xi,\eta}\, d\xi d\eta$$

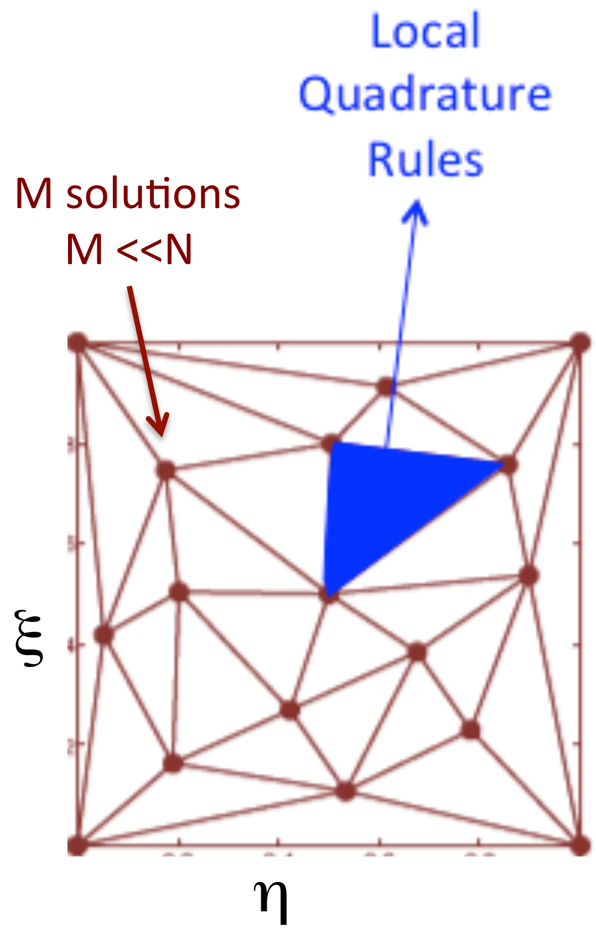
Better than Monte Carlo



Better than Monte Carlo



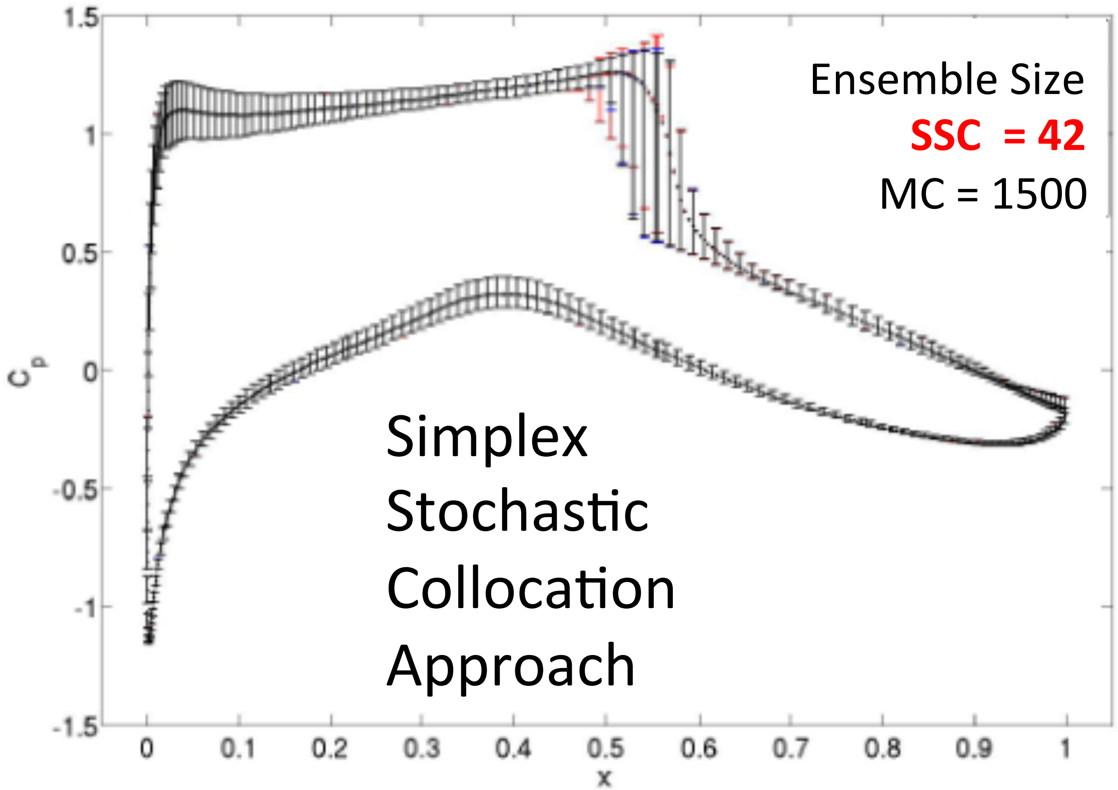
Simplex
Stochastic
Collocation
Approach



Better than Monte Carlo

Modern UQ algorithms blend numerical analysis and classical statistics

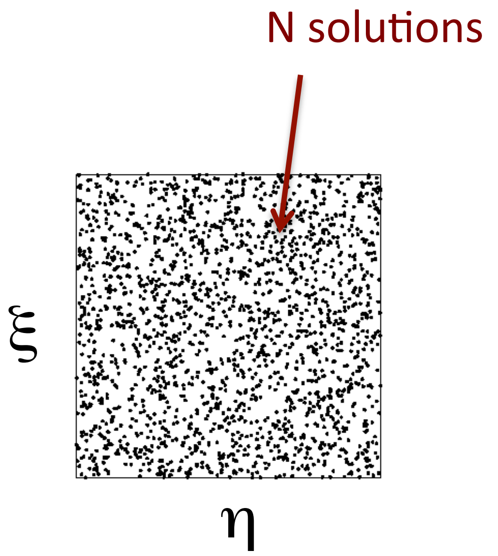
$$M_\infty = 0.734 \pm 0.005$$
$$\alpha = 2.79^o \pm 0.1$$
$$t/c = 0.1211 \pm 0.005$$

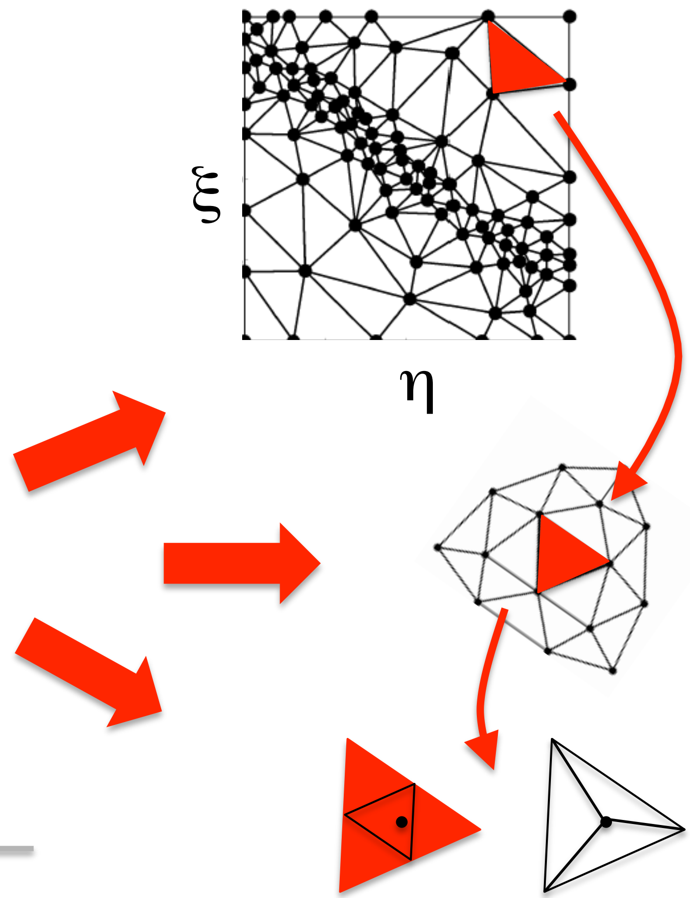


Witteveen & Iaccarino
SIAM 2012,2013, JCP 2011, 2012

Better than Monte Carlo

Key UQ enablers:





Adaptivity

High-order quadrature

Randomized refinement

Witteveen & Iaccarino
SIAM 2012,2013, JCP 2011, 2012

Need for UQ Science (cont'd)

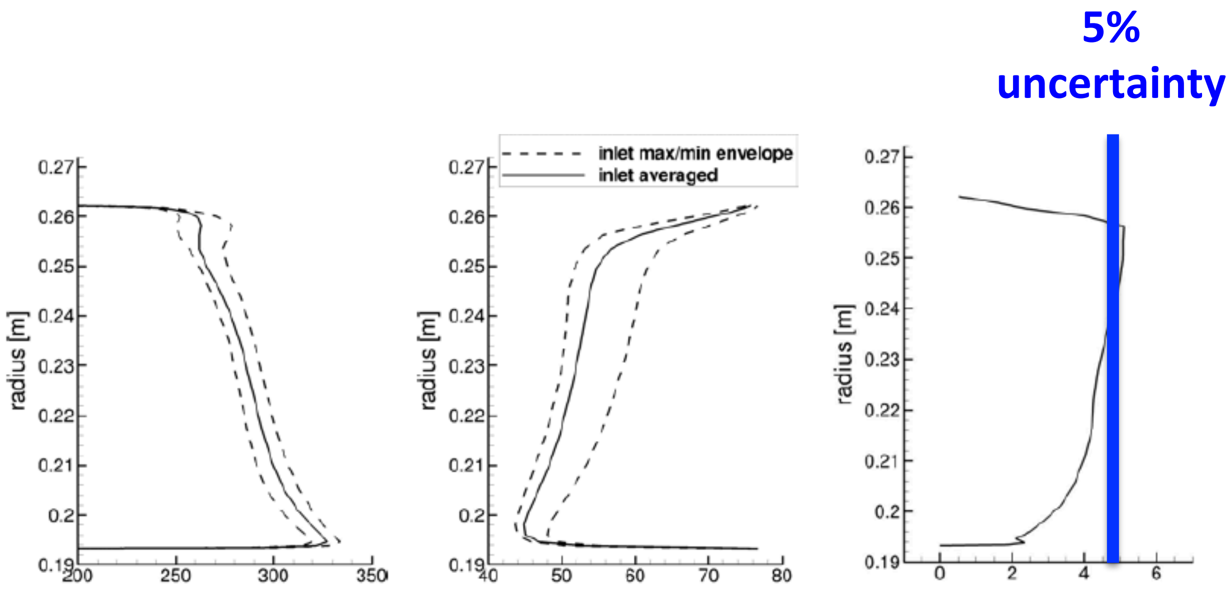
Input Uncertainty ≠ Output Uncertainties

Fluid mechanics equations are strongly non-linear, so a small input uncertainties can be amplified dramatically

Need for UQ Science (cont'd)

Input Uncertainty ≠ Output Uncertainties

High-Pressure Compressor Stator



(a) velocity v (m/s) (b) flow angle α (deg) (c) COV of flow angle α

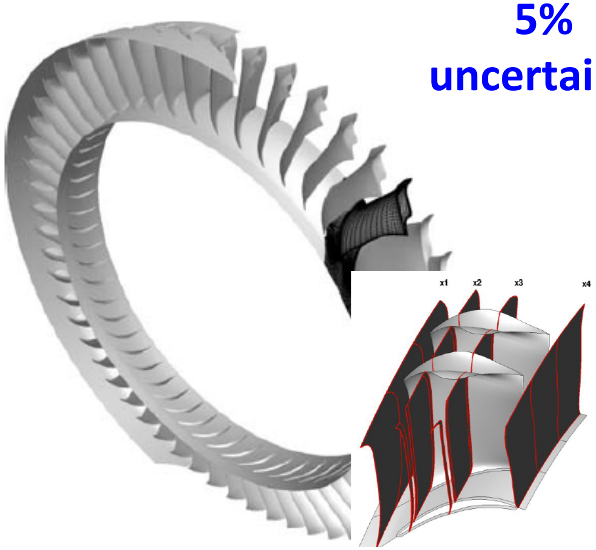
Input uncertainty: Inlet Turning Angle

Need for UQ Science (cont'd)

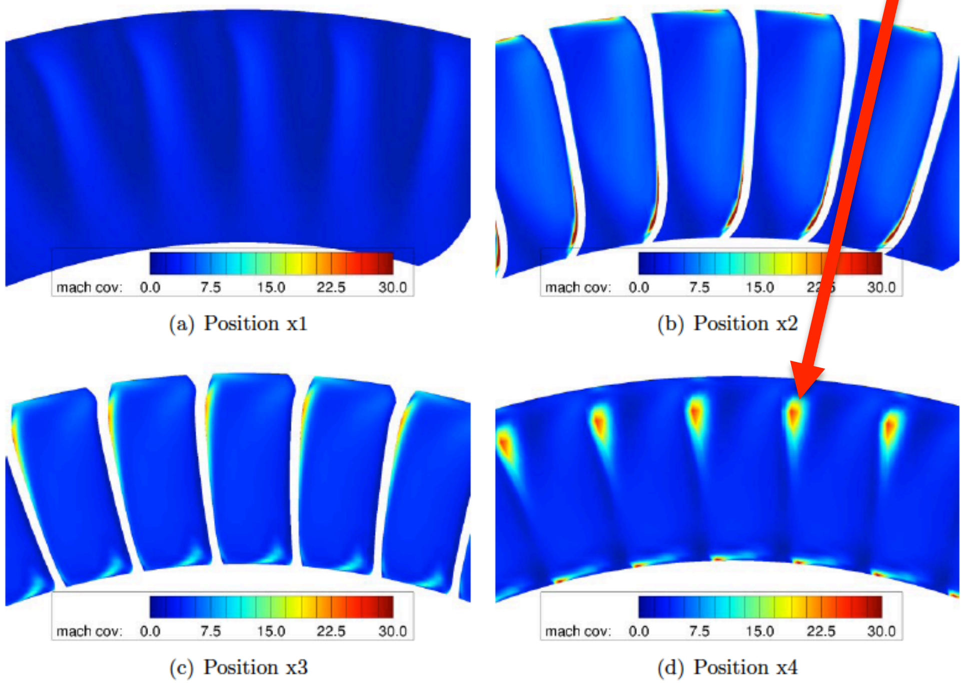
Input Uncertainty ≠ Output Uncertainties

30% uncertainty

High-Pressure Compressor Stator



5% uncertainty



Output Uncertainty: Mach Number

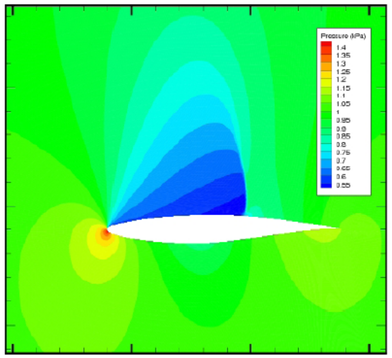
Need for UQ Science (cont'd)

The **definition** of the Input Uncertainty is **critical**

Need for UQ Science (cont'd)

The **definition** of the Input Uncertainty is **critical**

Probabilistic uncertainty quantification requires the statistical description of ALL the uncertainties and their correlation!



$$M_\infty = 0.734 \pm 0.005$$
$$\alpha = 2.79^o \pm 0.1$$
$$t/c = 0.1211 \pm 0.005$$

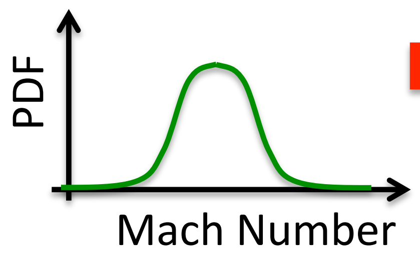
Conditions characterized in terms of a range, are not uniquely defined!

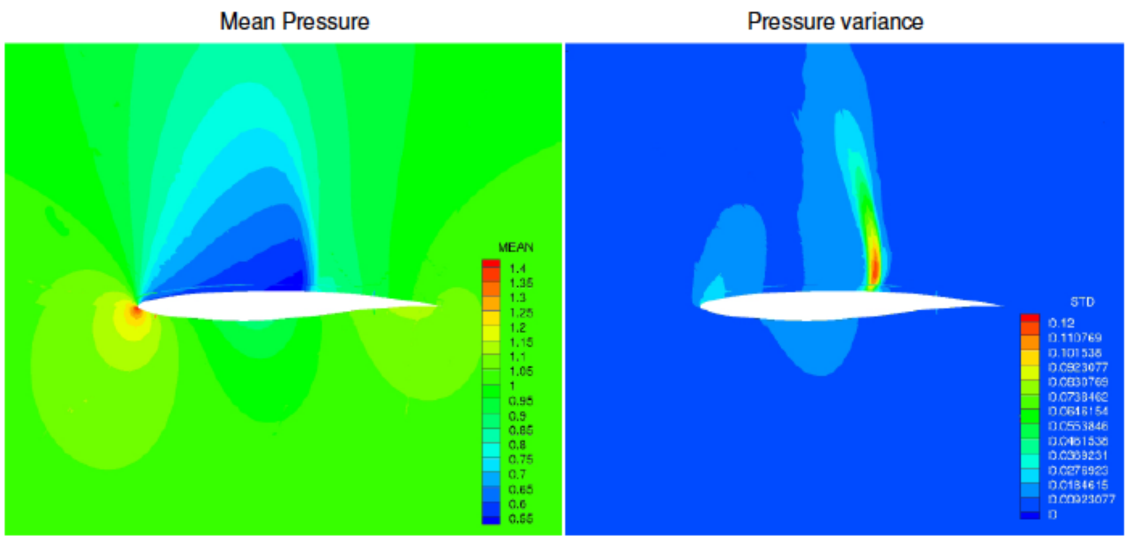
Need for UQ Science (cont'd)

The **definition** of the Input Uncertainty is **critical**

Assuming that the range is a 95% confidence interval and that the distributions are Gaussian random variables

$$M_\infty = 0.734 \pm 0.005$$
$$\alpha = 2.79^o \pm 0.1$$
$$t/c = 0.1211 \pm 0.005$$



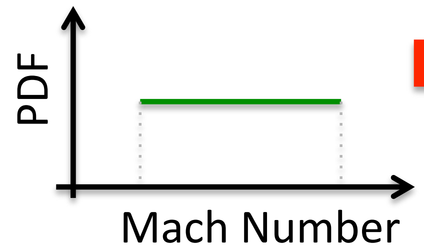


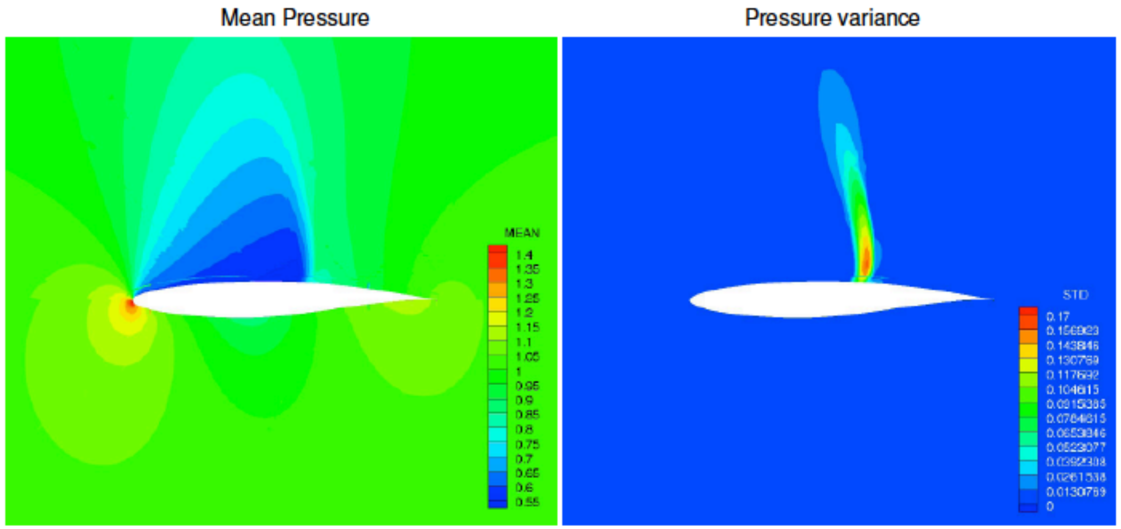
Need for UQ Science (cont'd)

The **definition** of the Input Uncertainty is **critical**

Assuming that the range is a likely set of scenarios and that the distributions are uniform random variables

$$M_\infty = 0.734 \pm 0.005$$
$$\alpha = 2.79^o \pm 0.1$$
$$t/c = 0.1211 \pm 0.005$$



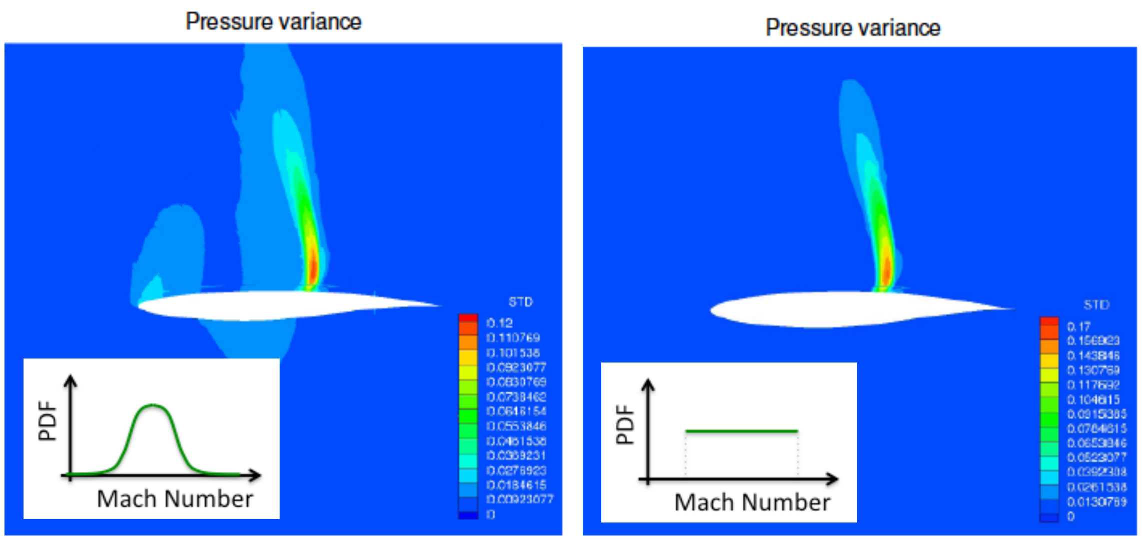


Need for UQ Science (cont'd)

The **definition** of the Input Uncertainty is **critical**

Normal vs uniform distributed uncertainties

$$M_\infty = 0.734 \pm 0.005$$
$$\alpha = 2.79^o \pm 0.1$$
$$t/c = 0.1211 \pm 0.005$$



UQLab Algorithmic Research

- GI - Quantification of Margins and Uncertainties – RESS 2009, 2013
- T. Chatrasmi - Pade-Legendre Method – JCP 2009, IJUQ 2011
- J. Witteveen - Simplex Stochastic Collocation – JCP 2009, 2011, SIAM SISC 2009
- A. Doostan - Low-rank Tensorization – JCP 2009, 2013
- P. Pettersson - Polynomial Chaos for Hyperbolic PDEs – JCP 2009, 2012
- G. Tang - Compressed Sensing Stochastic Expansions – SIAM JUQ 2013
- P. Constantine - Hybrid Galerkin Projection – IJNME 2009
- P. Congedo - Backward UQ – CMAME 2011
- A. Mittal - Gradient Enhanced Quadratures – SIAM JUQ 2013 submitted
- D. Schiavazzi - Adaptive Multiresolution Wavelet – SIAM JUQ submitted
- N. Kseib – Fast MCMC for Data Assimilation – CF 2013, CF to be completed

http://uq.stanford.edu

AUQ vs EUQ

The uncertainties sources **are not all the same**

AUQ vs EUQ

The uncertainties sources **are not all the same**

The examples illustrated so far have uncertainties that are identified in:

- Boundary conditions: free stream state, wall temperatures, etc.
- Material properties: inhomogeneity, reaction rates, etc.
- Geometry: manufacturing tolerances, contamination, etc.

AUQ vs EUQ

The uncertainties sources **are not all the same**

The examples illustrated so far have uncertainties that are identified in:

- Boundary conditions: free stream state, wall temperatures, etc.
- Material properties: inhomogeneity, reaction rates, etc.
- Geometry: manufacturing tolerances, contamination, etc.

What about:

- Numerical errors, bugs

AUQ vs EUQ

The uncertainties sources **are not all the same**

The examples illustrated so far have uncertainties that are identified in:

- Boundary conditions: free stream state, wall temperatures, etc.
- Material properties: inhomogeneity, reaction rates, etc.
- Geometry: manufacturing tolerances, contamination, etc.

What about:

- ~~Numerical errors, bugs~~ >>> not uncertainties >>> use verification

AUQ vs EUQ

The uncertainties sources **are not all the same**

The examples illustrated so far have uncertainties that are identified in:

- Boundary conditions: free stream state, wall temperatures, etc.
- Material properties: inhomogeneity, reaction rates, etc.
- Geometry: manufacturing tolerances, contamination, etc.

What about:

- ~~Numerical errors, bugs~~ >>> not uncertainties >>> use verification
- Physical modeling assumptions

AUQ vs EUQ

Uncertainties in physical models are abundant and potentially critical, e.g. turbulence closures in RANS

Boussinesq Hypothesis

$$\overline{u_i' u_j'} \approx \frac{2}{3} k \delta_{ij} - 2\nu_T S_{ij} = \frac{2}{3} k \delta_{ij} - 2 C_\mu \frac{k^2}{\epsilon} S_{ij}$$

AUQ vs EUQ

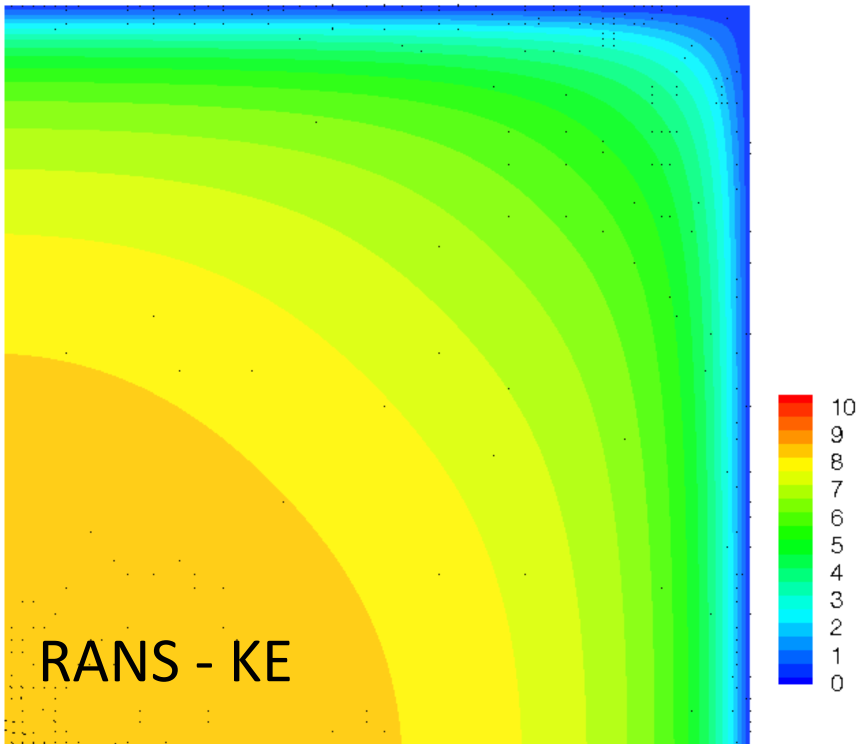
Uncertainties in physical models are abundant and potentially critical, e.g. turbulence closures in RANS

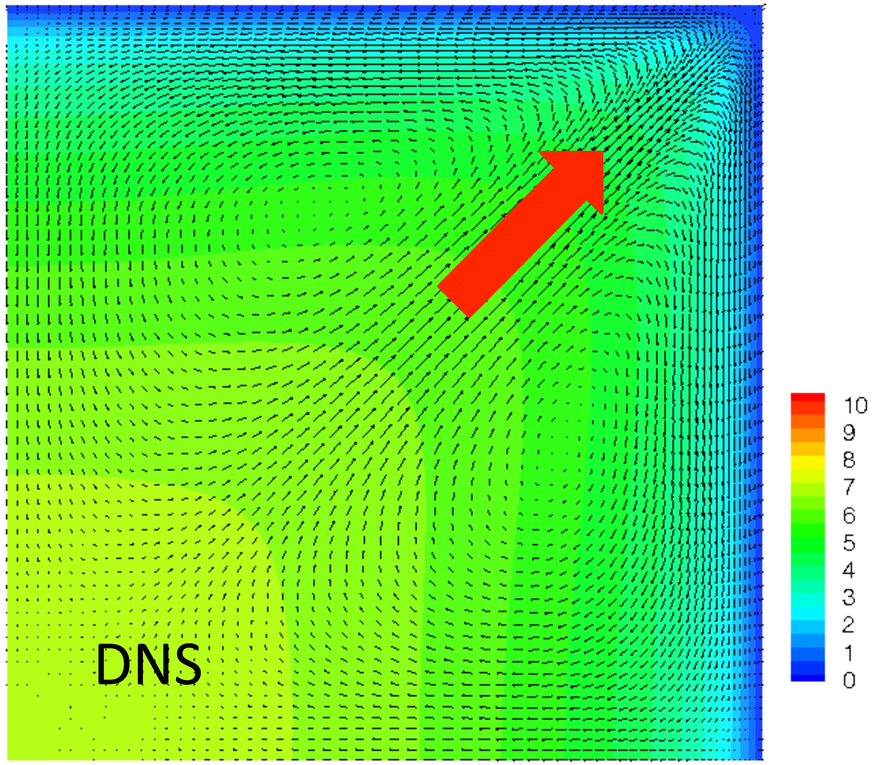
Boussinesq Hypothesis

$$\overline{u_i' u_j'} \approx \frac{2}{3} k \delta_{ij} - 2\nu_T S_{ij} = \frac{2}{3} k \delta_{ij} - 2 C_\mu \frac{k^2}{\epsilon} S_{ij}$$

Simply making the coefficient(s) **uncertain (=probabilistic)** does not address the structural assumptions, for example that Reynolds stress and mean strain are linearly dependent

Turbulent square duct





A catastrophic failure of parametric UQ/sensitivity analysis (C_μ)

EUQ: Epistemic Uncertainty Quantification

(AUQ = Aleatoric UQ = Probabilistic-based UQ)

We are developing a novel methodology based on

- Non-probabilistic representation of the assumptions – as a **bias**
- Introduction of turbulence theory constraints, e.g. realizability
- Independent of the turbulence closure
- Work in progress…

EUQ: Epistemic Uncertainty Quantification

(AUQ = Aleatoric UQ = Probabilistic-based UQ)

We are developing a novel methodology based on

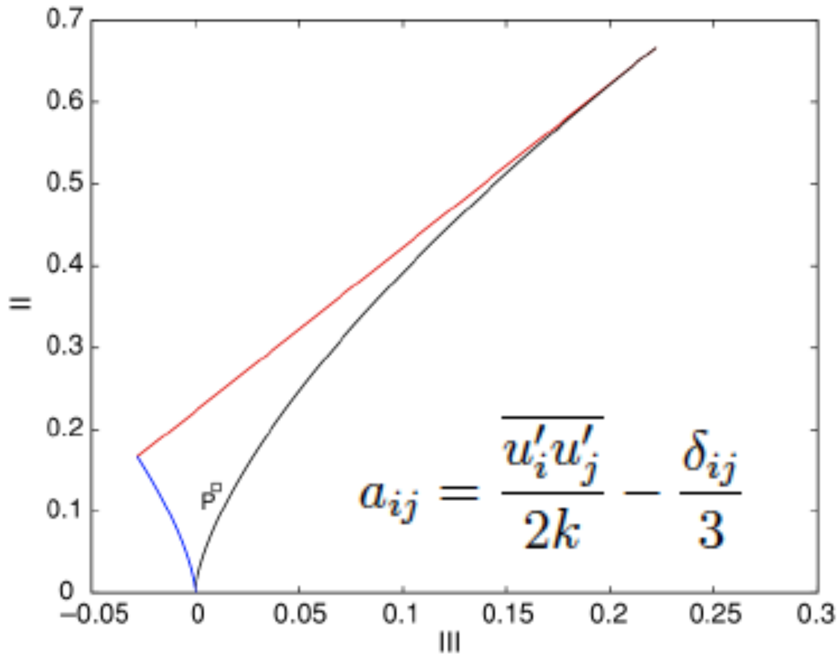
- Non-probabilistic representation of the assumptions – as a **bias**
- Introduction of turbulence theory constraints, e.g. realizability
- Independent of the turbulence closure
- Work in progress…

Reynolds stress decomposition $$R^*_{ij} = 2k^* \left(v^*_{in}\Lambda^*_{nl}v^*_{jl} + \frac{\delta_{ij}}{3} \right)$$

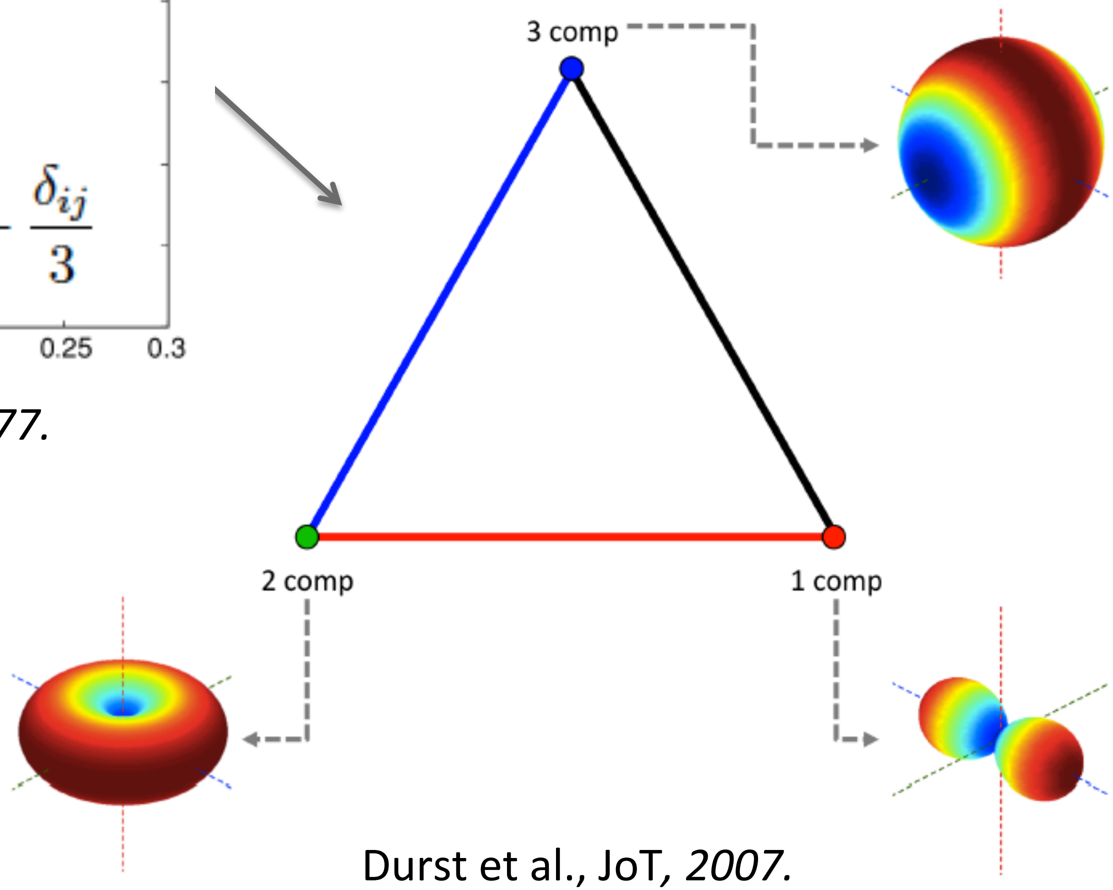
$k^* = k + \Delta k$ $\quad$ $k^* \geq 0$

$v^*_{in} = q_{id}v_{nd}$ $\quad$ remains orthonormal

$\Lambda^*_{nl} = \Lambda_{nl} + \Delta\Lambda_{nl}$ $\quad$ within constraints of anisotropy maps

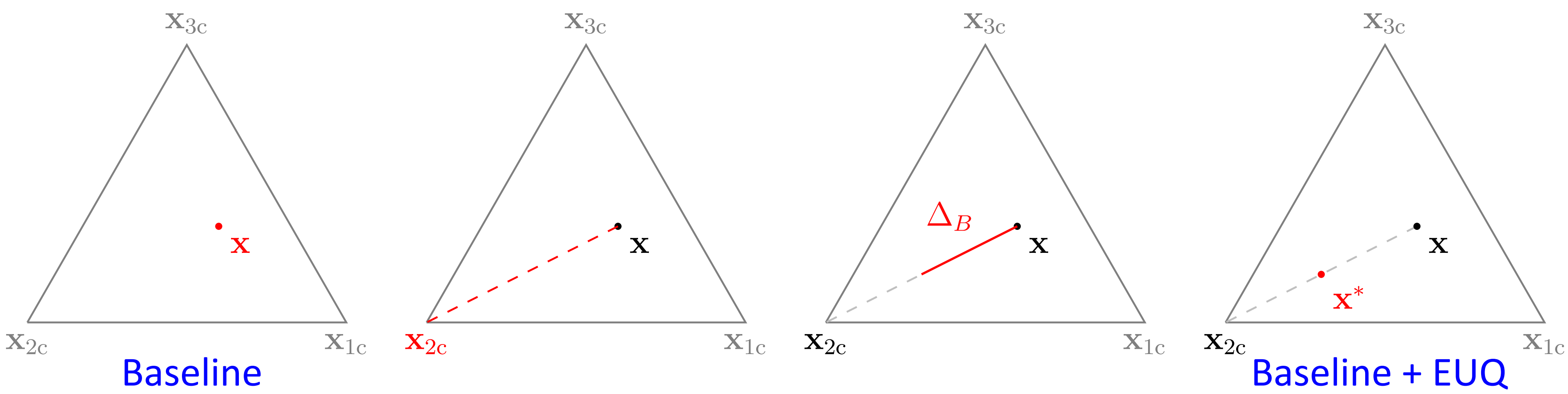


Lumley & Newman, JFM, *1977.*



Durst et al., JoT, *2007.*

Bias (perturbations) introduced in the anisotropy eigenvalues



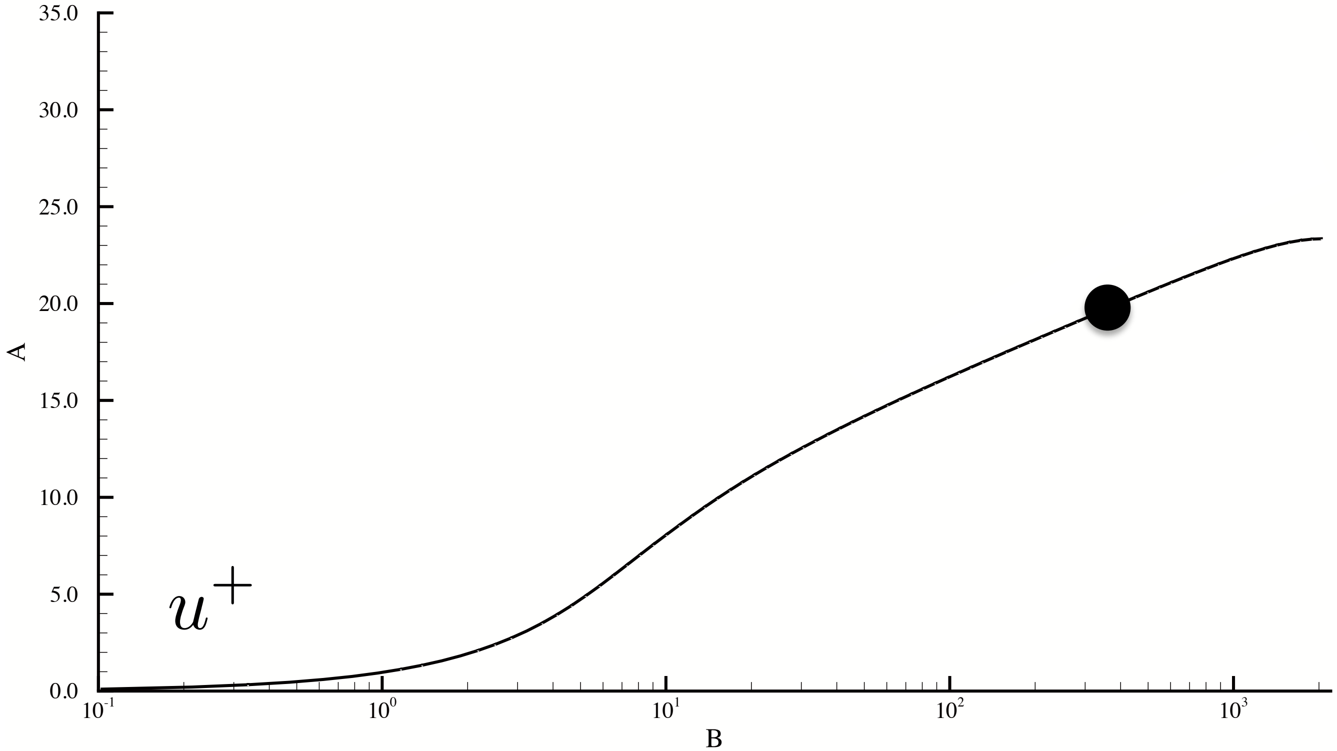
Parametrized by $x^{(t)}, \Delta_B$ ➡ $\Lambda^* = (1 - \Delta_B)\Lambda + \Delta_B \Lambda\big|_{\mathbf{x}^{(t)}}$

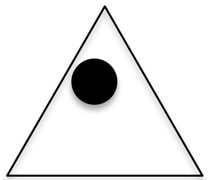
Further work on TKE and eigenvector perturbations has been carried out by C. Gorle (also worked on mixing models)

Emory, Larsson & Iaccarino, POF 013, Gorle & Iaccarino, POF 2013

Turbulent Channel Flow

$$Re_\tau = 2003$$
$$y_1^+ = 0.1$$
$$\mathrm{ny} = 80$$

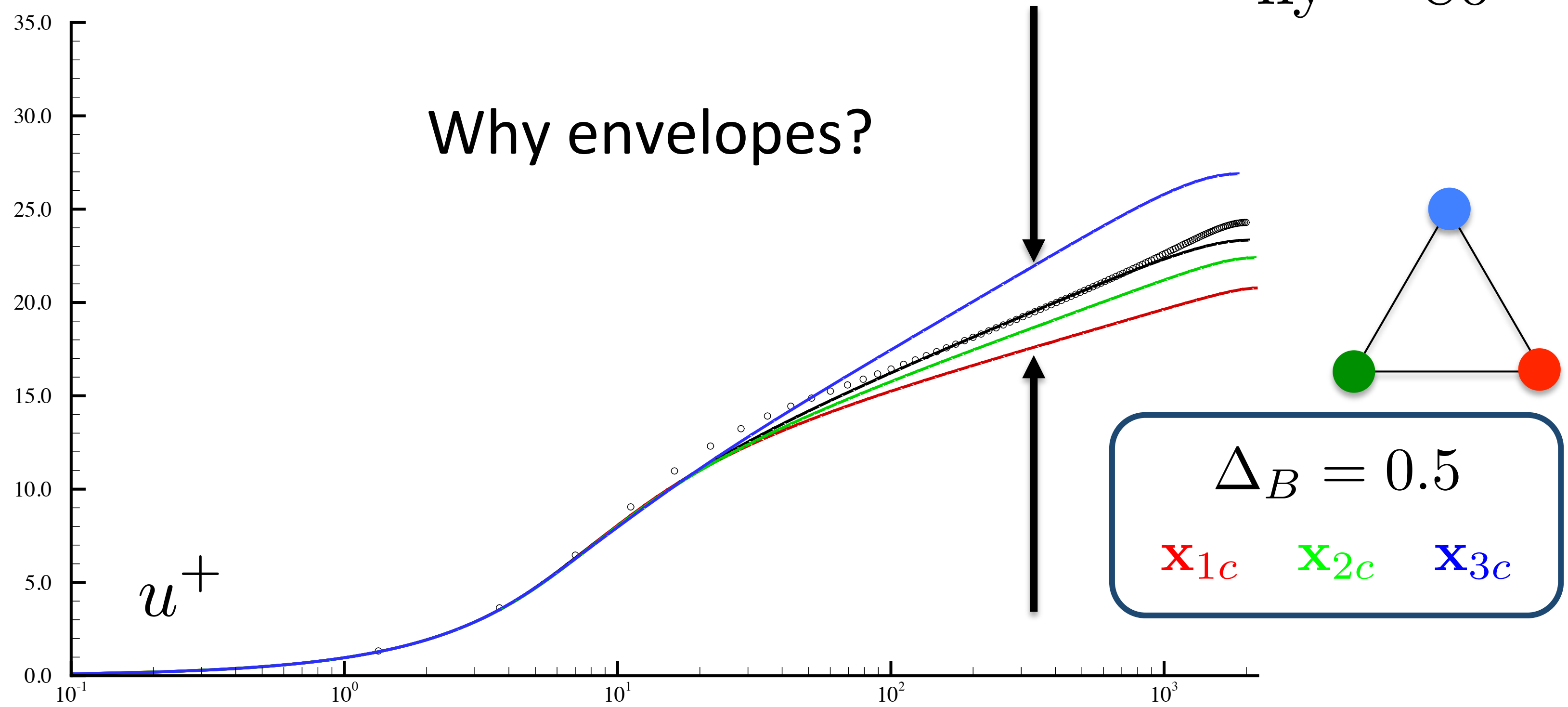




kwSST Baseline

Turbulent Channel Flow

$$Re_\tau = 2003$$
$$y_1^+ = 0.1$$
$$\text{ny} = 80$$



kwSST Baseline + EUQ

For a channel flow:

$$R^*_{12} = 2k\left(v_{1n}\Lambda^*_{nl}v_{2l}\right) \quad \text{with} \quad \begin{cases} \Lambda^* = (1-\Delta_B)\Lambda + \Delta_B \Lambda\big|_{\mathbf{x}^{(t)}} \\ v_{ik} = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ -\sin\theta & 0 & \cos\theta \\ 0 & 1 & 0 \end{bmatrix} \end{cases}$$

$$R^*_{12}\big|_{\mathbf{x}^{(t)}} = (1-\Delta_B)R_{12} + \Delta_B 2k\left(a_{12}\big|_{\mathbf{x}^{(t)}}\right)$$

$$R^*_{12}\big|_{\mathbf{x}^{(t)}} = (1-\Delta_B)R_{12} + \Delta_B k\left(\lambda_3^{(t)} - \lambda_1^{(t)}\right)$$

For a channel flow:

$$R^*_{12} = 2k\left(v_{1n}\Lambda^*_{nl}v_{2l}\right) \quad \text{with} \quad \begin{cases} \Lambda^* = (1-\Delta_B)\Lambda + \Delta_B \Lambda\big|_{\mathbf{x}^{(t)}} \\ v_{ik} = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ -\sin\theta & 0 & \cos\theta \\ 0 & 1 & 0 \end{bmatrix} \end{cases}$$

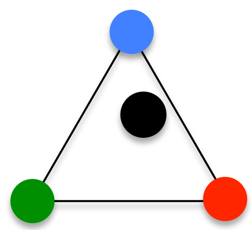
$$R^*_{12}\big|_{\mathbf{x}^{(t)}} = (1-\Delta_B)R_{12} + \Delta_B 2k\left(a_{12}\big|_{\mathbf{x}^{(t)}}\right)$$

$$R^*_{12}\big|_{\mathbf{x}^{(t)}} = (1-\Delta_B)R_{12} + \Delta_B k\left(\lambda_3^{(t)} - \lambda_1^{(t)}\right)$$

$$R^*_{12}\big|_{\mathbf{x}_{1c}} = (1-\Delta_B)R_{12} - \Delta_B k$$

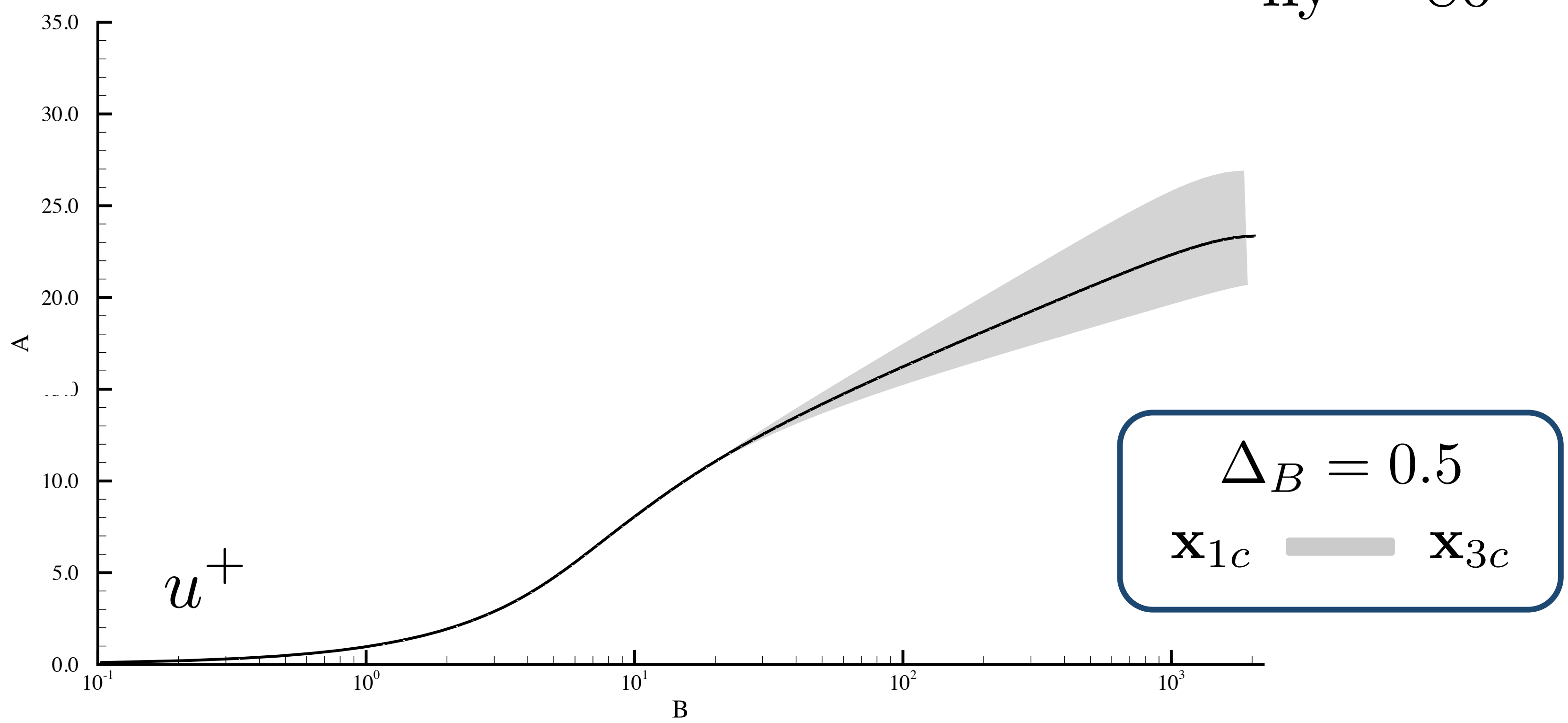
$$R^*_{12}\big|_{\mathbf{x}_{2c}} = (1-\Delta_B)R_{12} - 0.5\Delta_B k$$

$$R^*_{12}\big|_{\mathbf{x}_{3c}} = (1-\Delta_B)R_{12}$$



Turbulent Channel Flow

$$Re_\tau = 2003$$
$$y_1^+ = 0.1$$
$$\text{ny} = 80$$



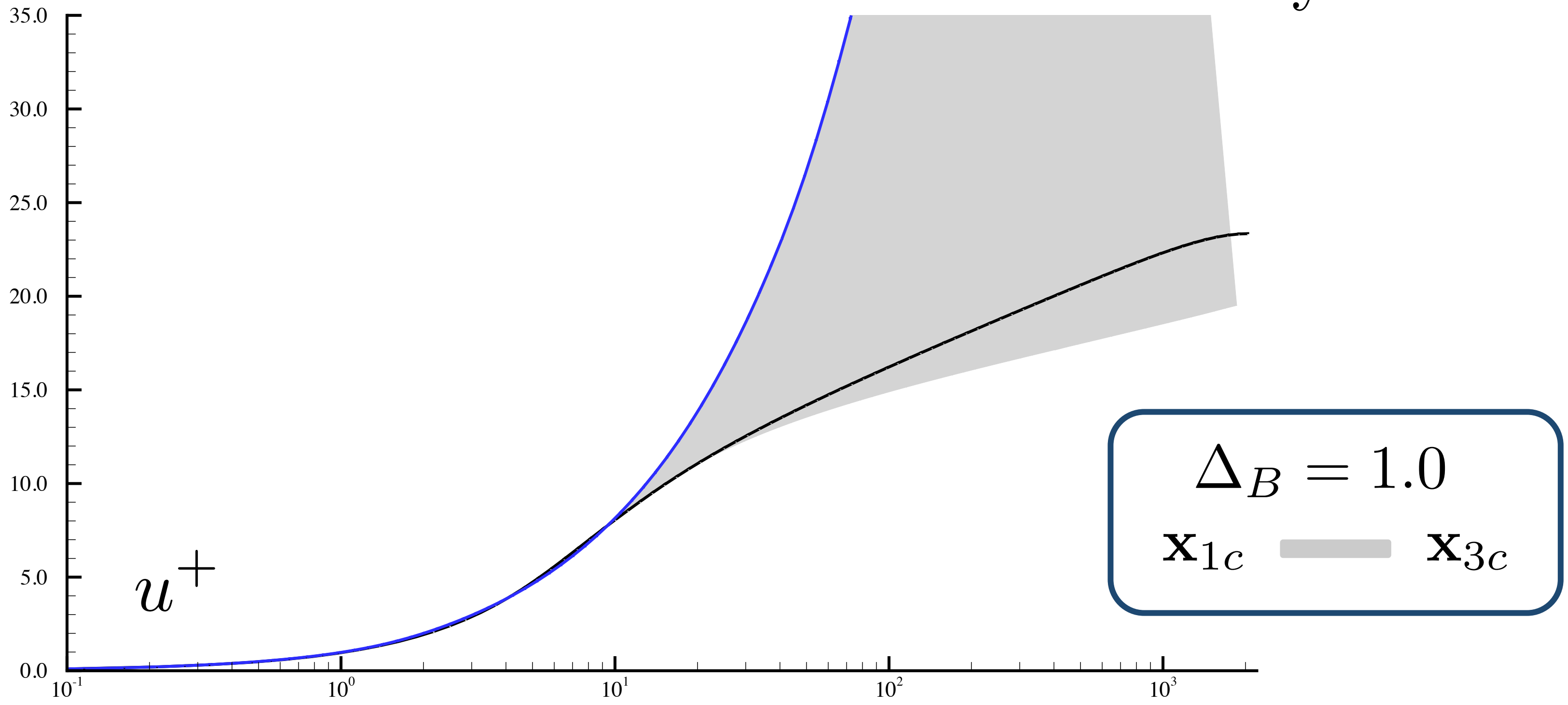
kwSST Baseline + EUQ

Turbulent Channel Flow

$Re_\tau = 2003$

$y_1^+ = 0.1$

$\text{ny} = 80$



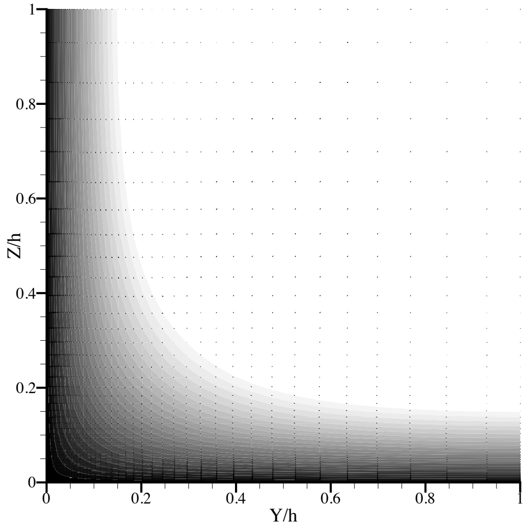
kwSST Baseline + EUQ

Turbulent Square Duct

$$Re_\tau = 2000$$

$$y_1^+ = 0.1$$

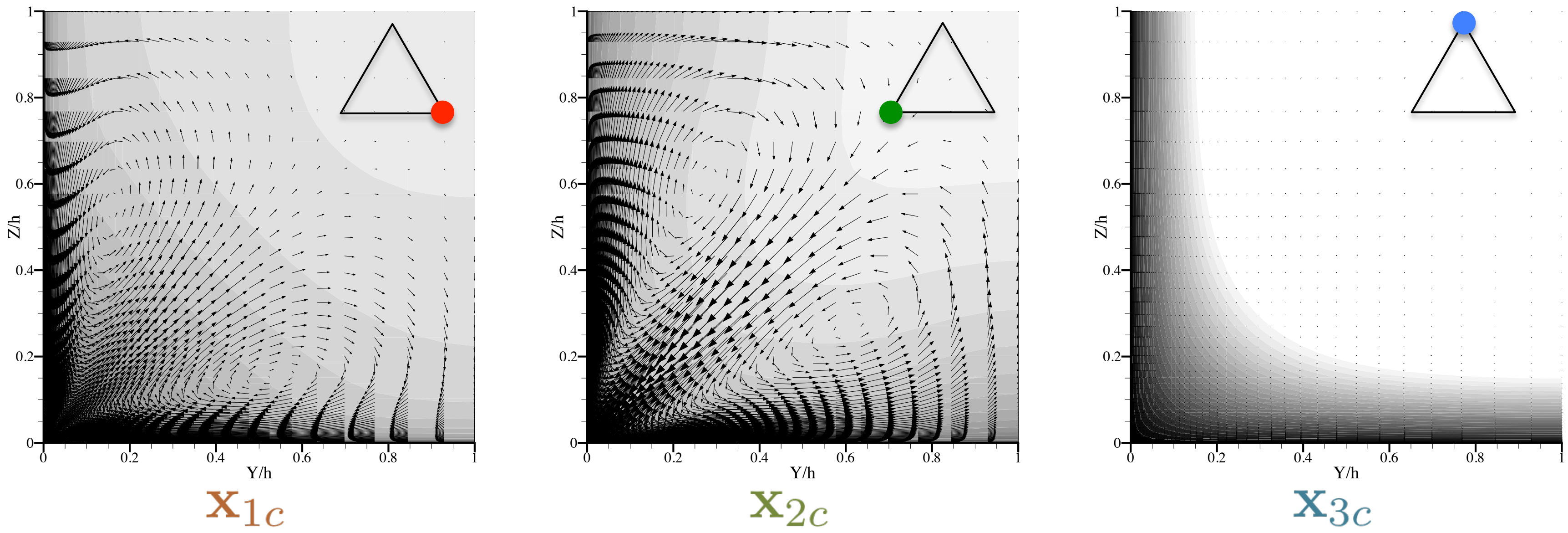
$$ny = nz = 160$$



kwSST Baseline

Turbulent Square Duct

$$Re_\tau = 2000$$
$$y_1^+ = 0.1$$
$$ny = nz = 160$$

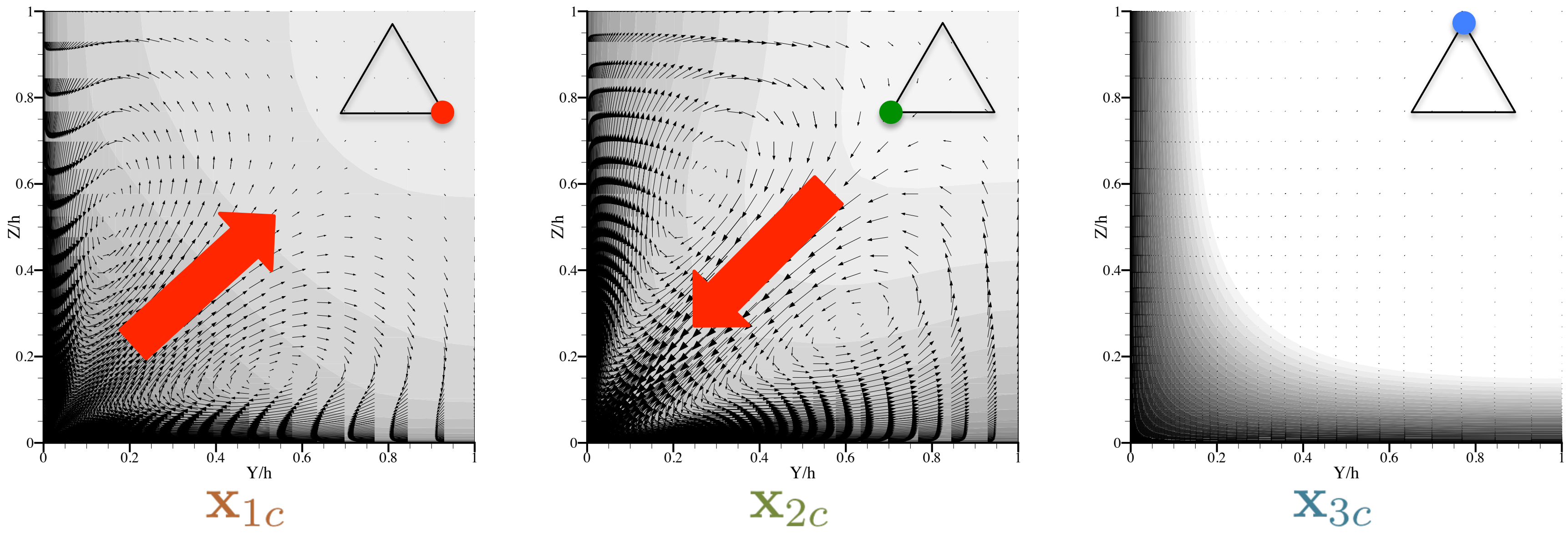


kwSST Baseline + EUQ

$$\Delta_B = 0.5$$

Turbulent Square Duct

$$Re_\tau = 2000$$
$$y_1^+ = 0.1$$
$$ny = nz = 160$$

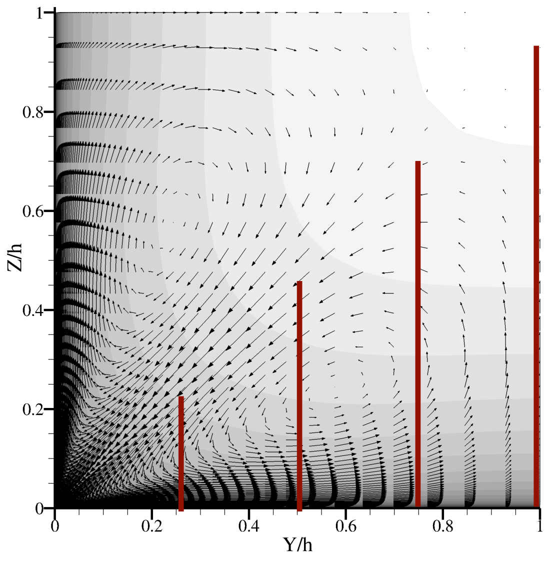


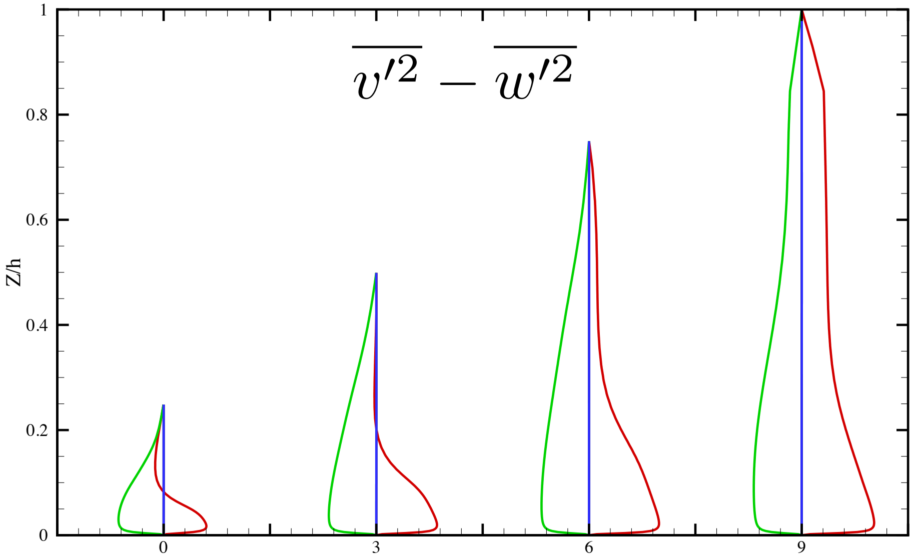
$$\Delta_B = 0.5$$

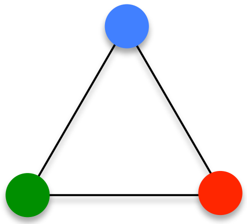
kwSST Baseline + EUQ

Turbulent Square Duct

$$Re_\tau = 2000$$
$$y_1^+ = 0.1$$
$$ny = nz = 160$$



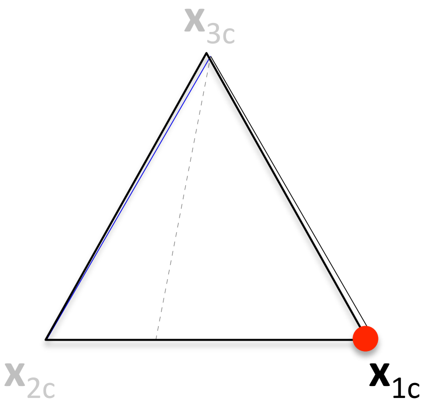


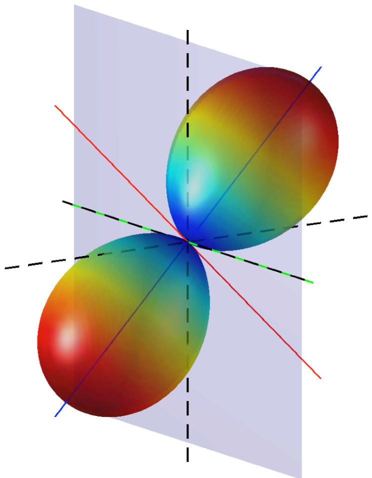


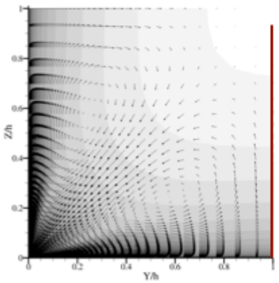
$$\Delta_B = 0.5$$

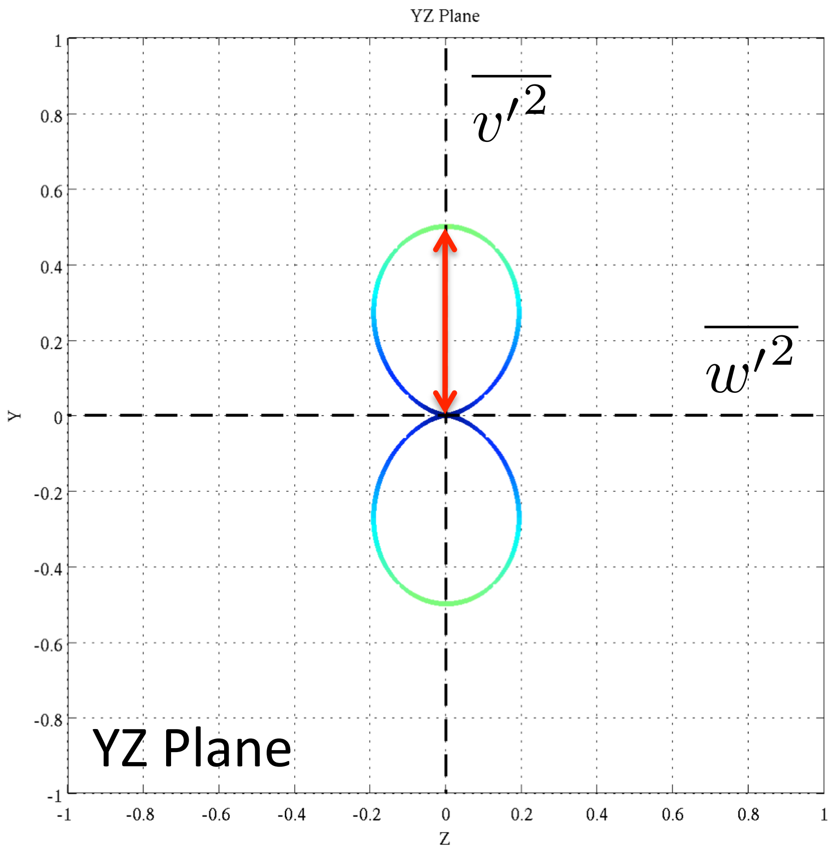
Why envelopes?

$$\overline{v'^2} - \overline{w'^2} > 0$$



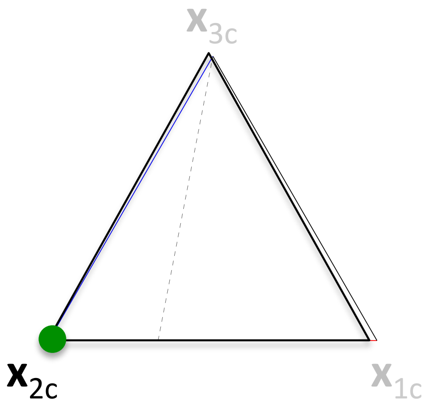


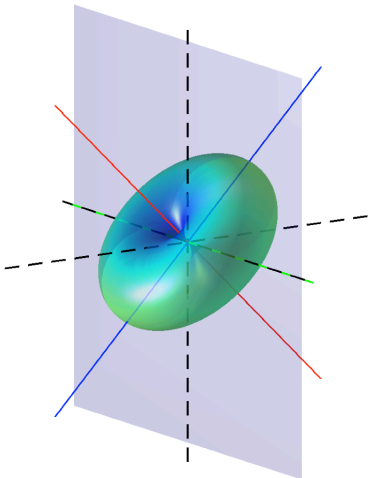




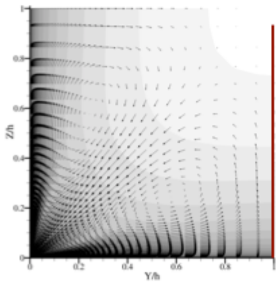
Why envelopes?

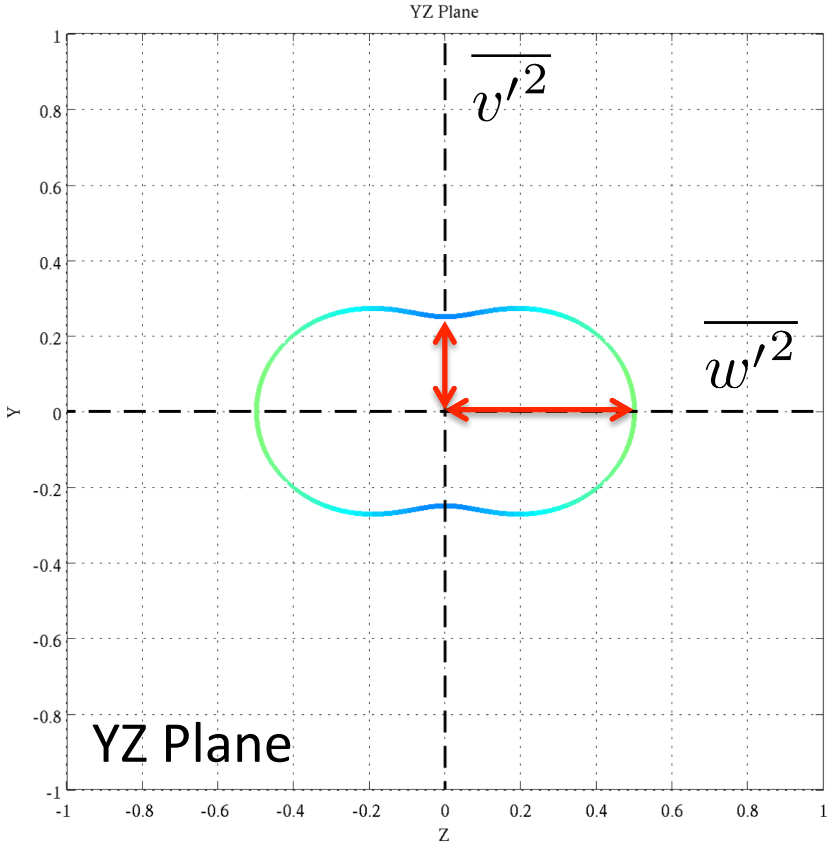
$$\overline{v'^2} - \overline{w'^2} < 0$$





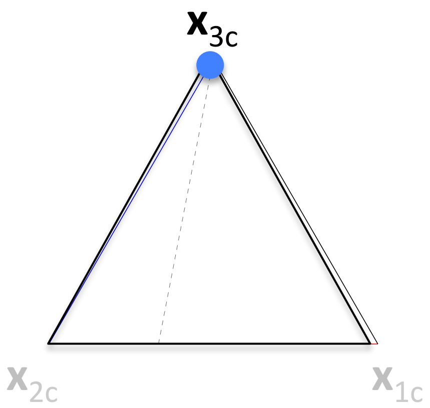
Reynolds stress glyph

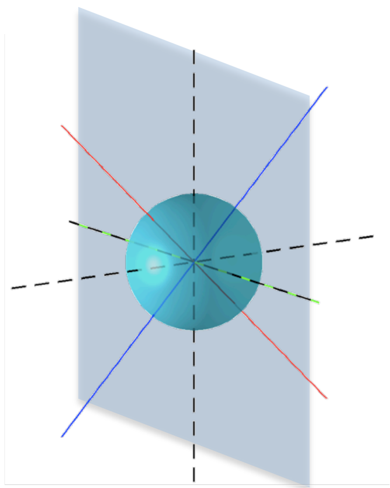




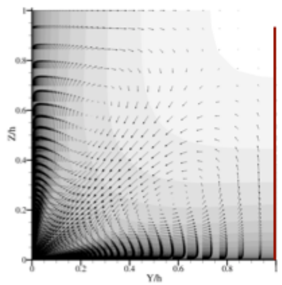
Why envelopes?

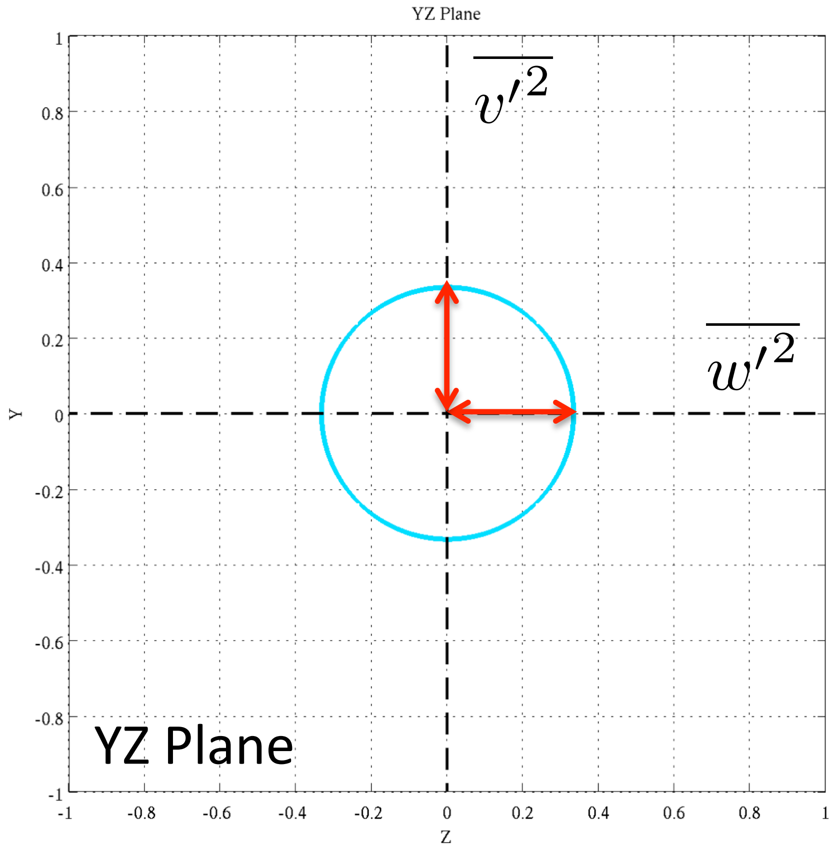
$$\overline{v'^2} - \overline{w'^2} = 0$$





Reynolds stress glyph



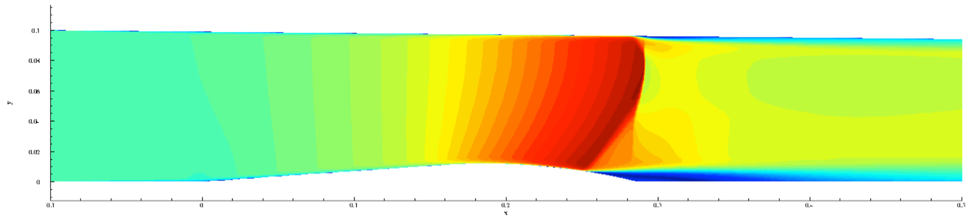


Shock/Turbulent BL Interaction

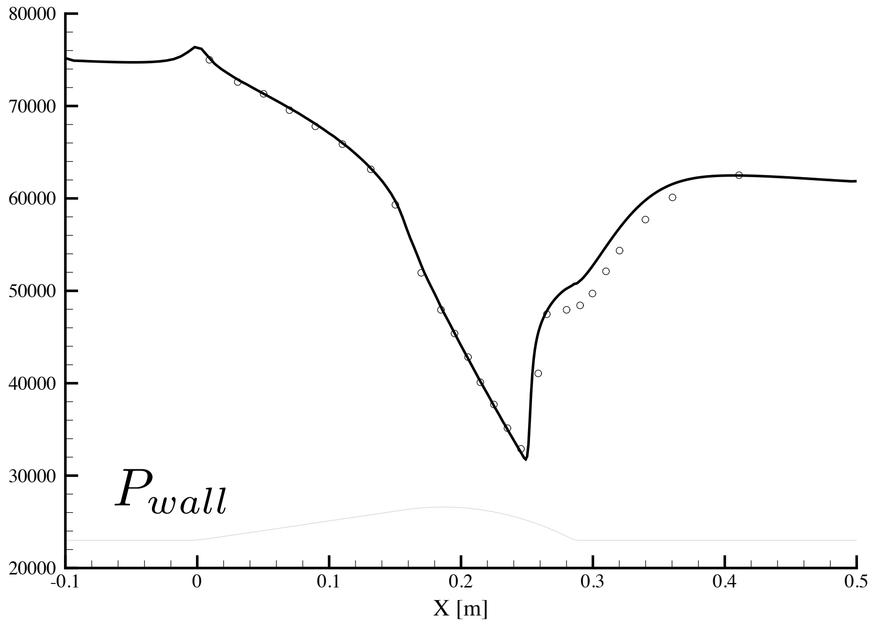
$y_1^+ \approx 1$

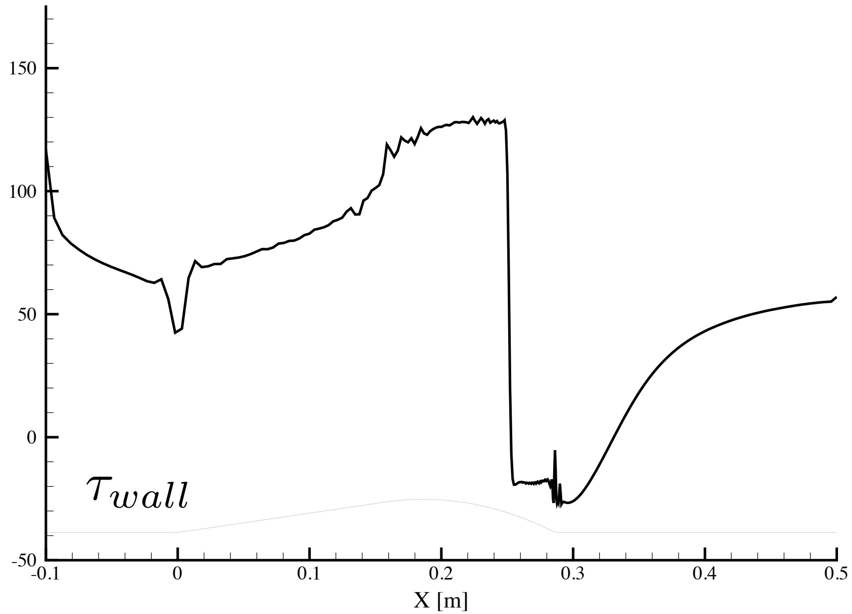
$nx = 280$

$ny = 100$



Mach Number Contours



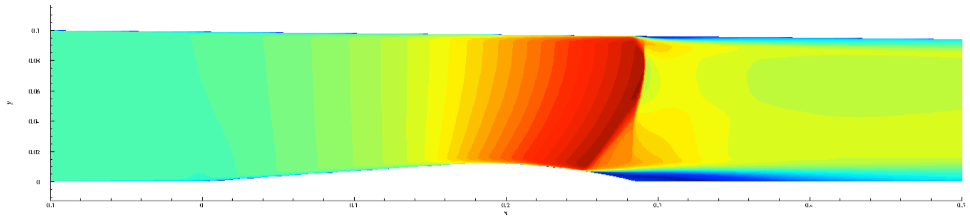


Shock/Turbulent BL Interaction

$y_1^+ \approx 1$

$nx = 280$

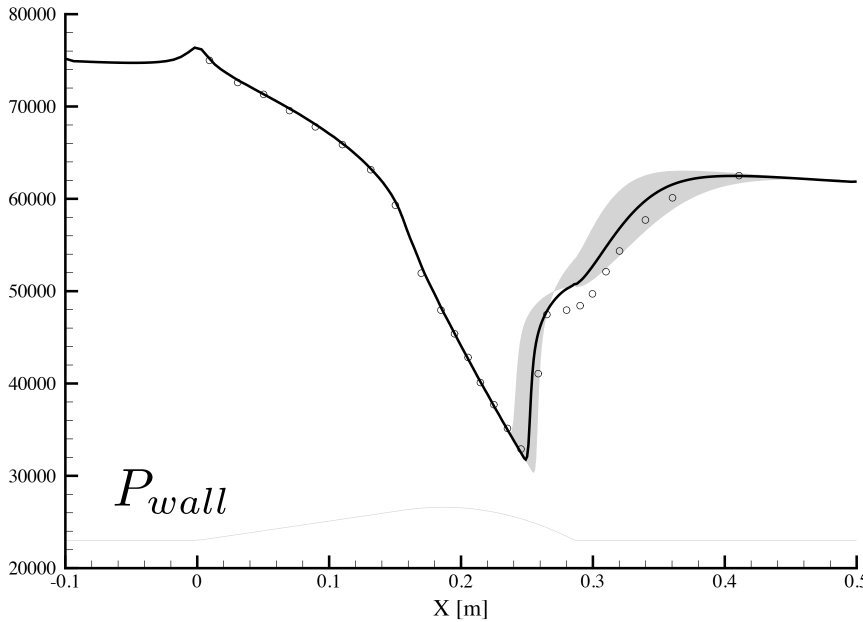
$ny = 100$

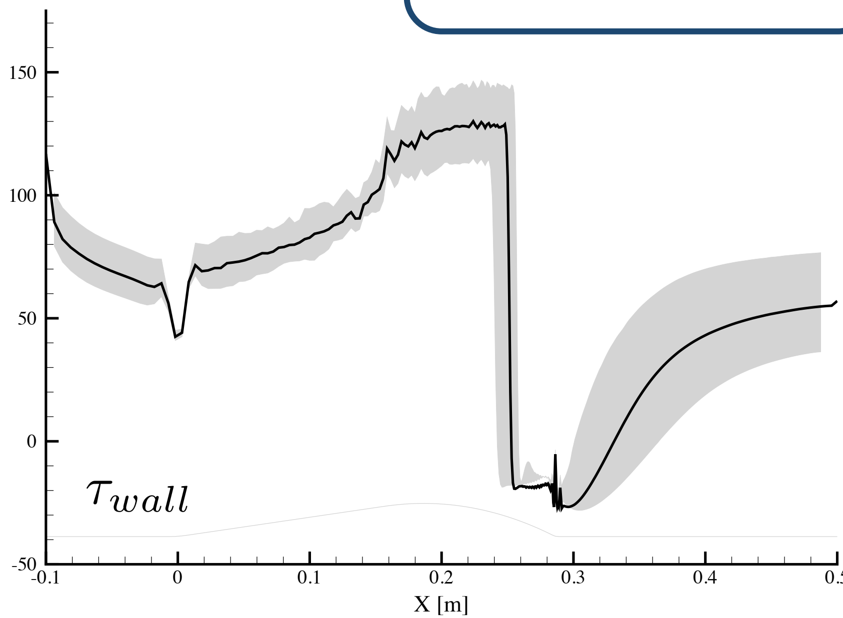


Mach Number Contours

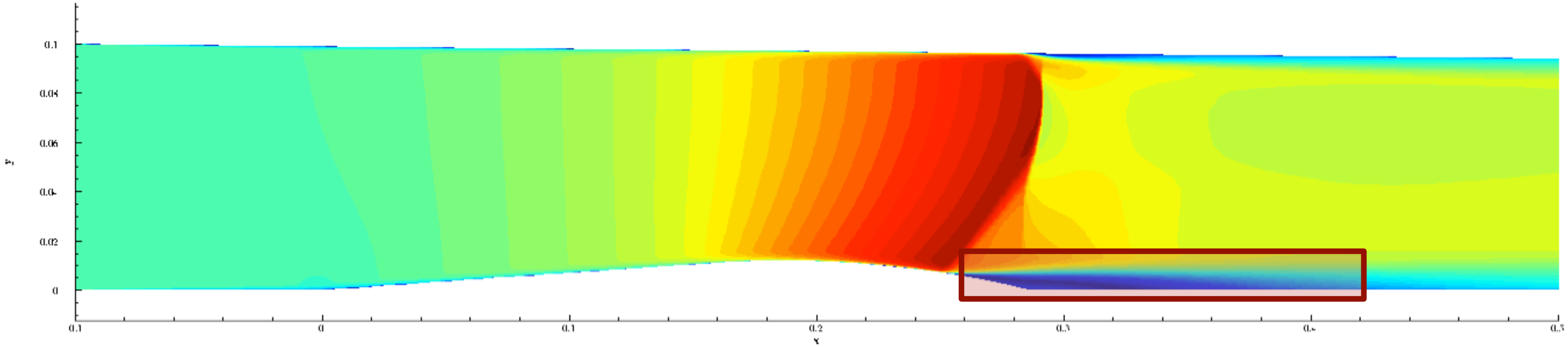
$\Delta_B = 0.5$

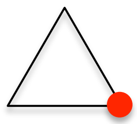
$\mathbf{x}_{1c}$ — $\mathbf{x}_{3c}$





Shock/Turbulent BL Interaction

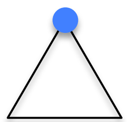




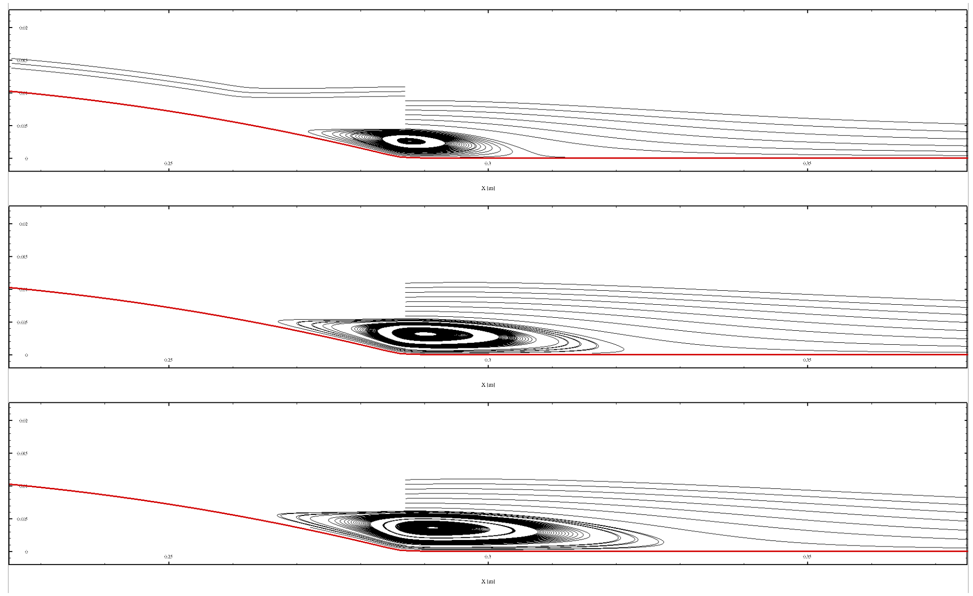
$\mathbf{x}_{1c}$

$$\text{SST } k-\omega$$
$$\Delta_{B,\max} = 0.5$$
$$m_c = 0.001$$

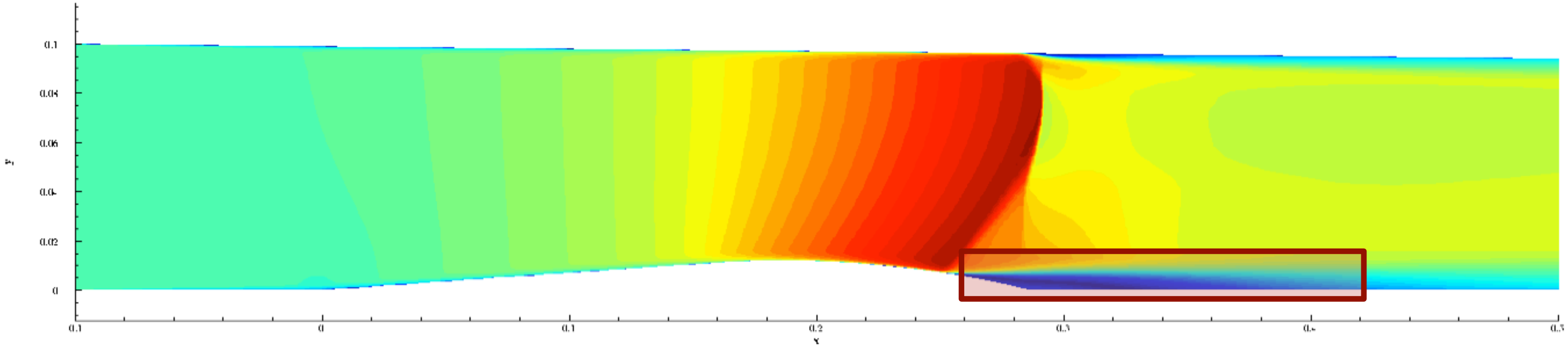
baseline



$\mathbf{x}_{3c}$



Shock/Turbulent BL Interaction



Wilcox $k - \omega$

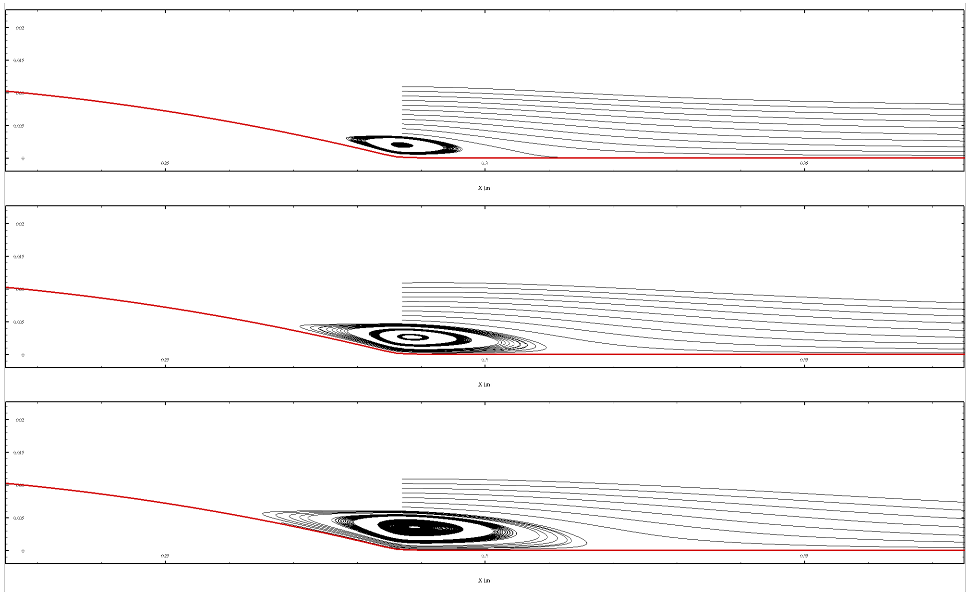
$\Delta_{B,\max} = 0.5$

$m_c = 0.001$

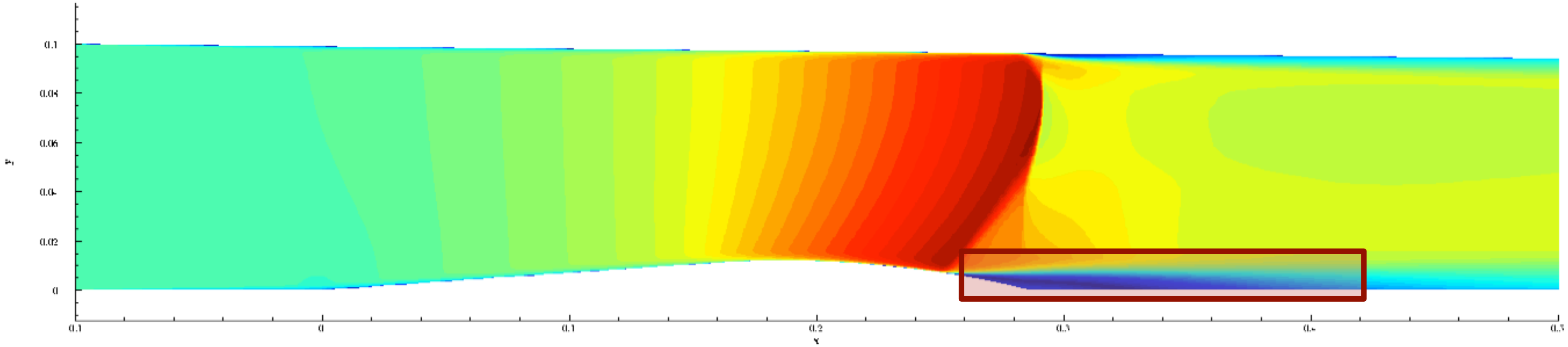
$\mathbf{x}_{1c}$

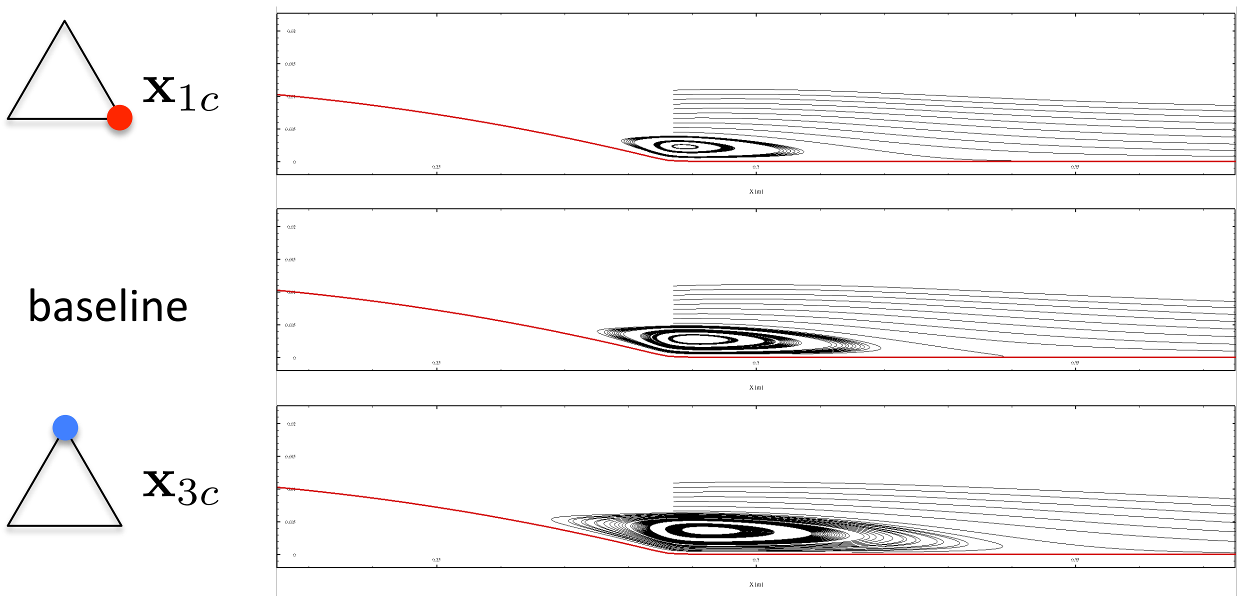
baseline

$\mathbf{x}_{3c}$



Shock/Turbulent BL Interaction





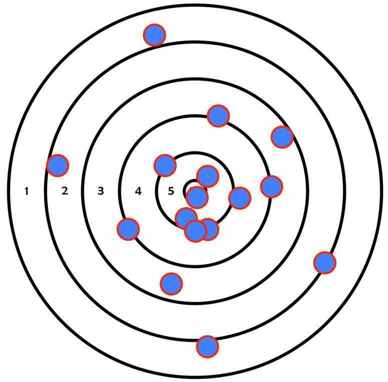
Spalart-Allmaras
$$\Delta_{B,\max} = 0.5$$
$$m_c = 0.001$$

How to Quantify Uncertainties?

Probabilistic approaches are appropriate for uncertainties due to **variability**, e.g. inflow conditions, geometrical tolerances, etc.

- New approaches to accelerate the computations of stastical moments/distributions are required
- Research at frontier of statistics & numerical analysis

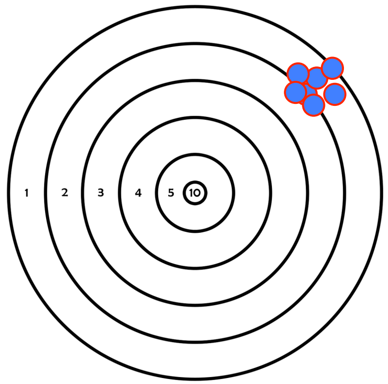
AUQ



Uncertainties related to **physical modeling assumptions** cannot be treated probabilistically

- Methods require the identification and quantification of systematic bias
- Research uses domain specific knowledge (e.g. realizability)

EUQ

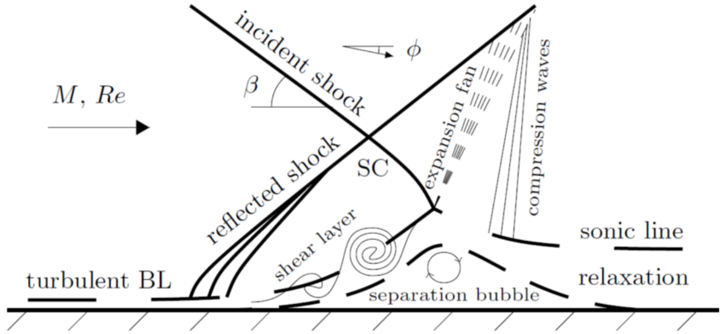


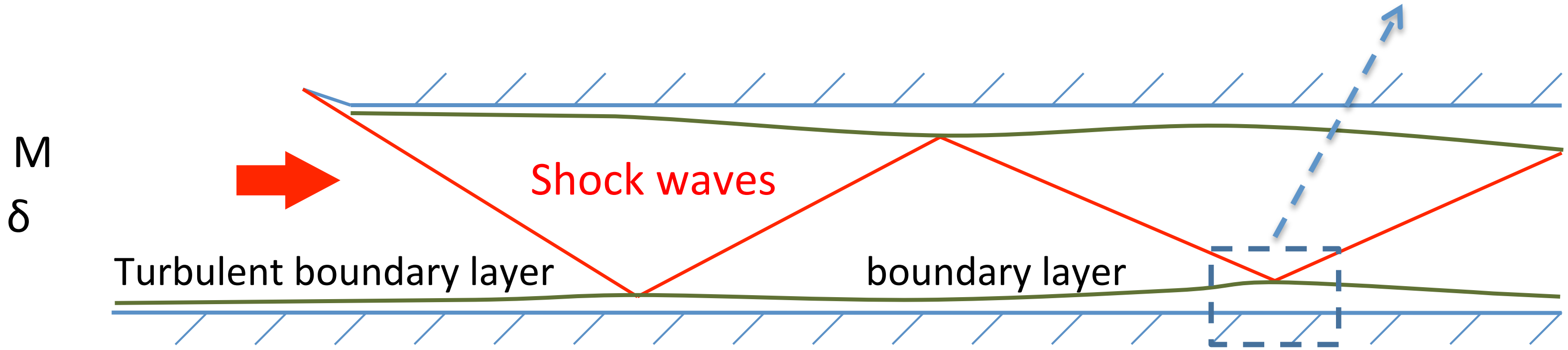
Outline

- Why UQ?
- How to Quantify Uncertainties? AUQ and EUQ
- **The UQ Experiment**
- Conclusions

The UQ Experiment

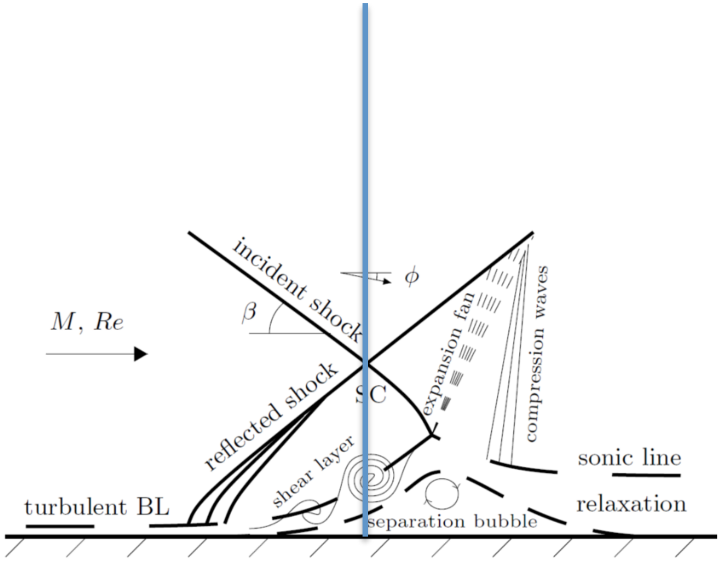
Originated from a conversation with Prof. John Eaton on how to do experiments to "validate" UQ methods

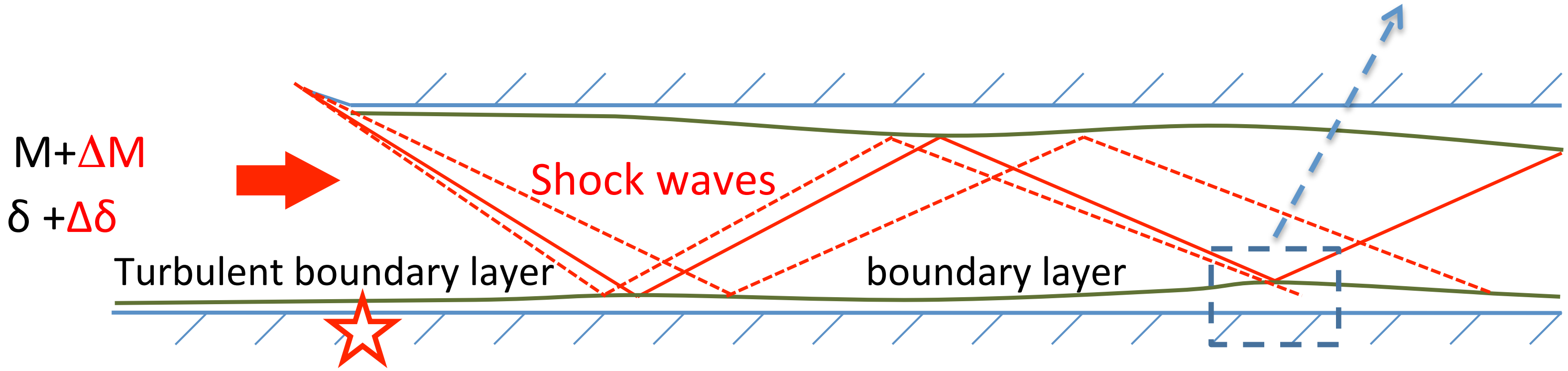




The UQ Experiment

Originated from a conversation with Prof. John Eaton on how to do experiments to "validate" UQ methods

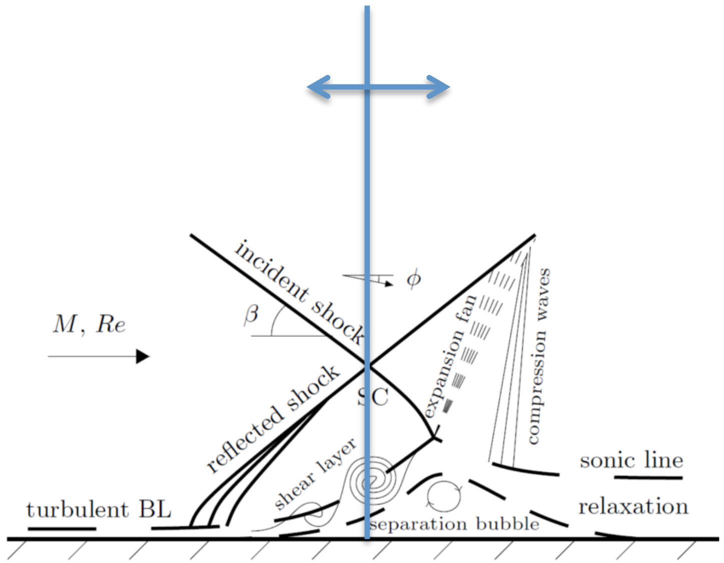


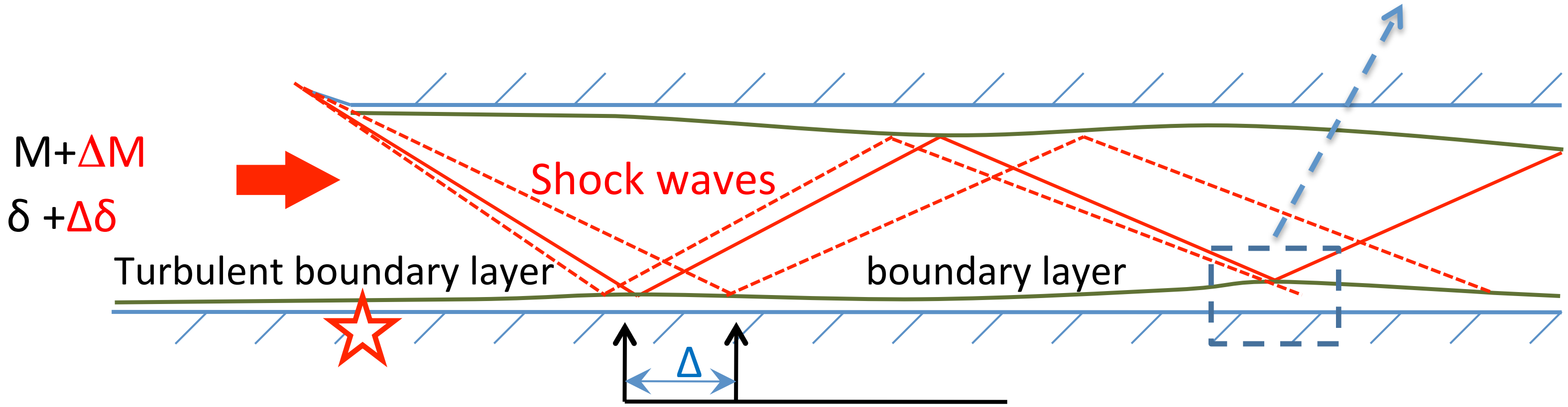


Uncertainties:
Inflow conditions + geometry

The UQ Experiment

Originated from a conversation with Prof. John Eaton on how to do experiments to "validate" UQ methods

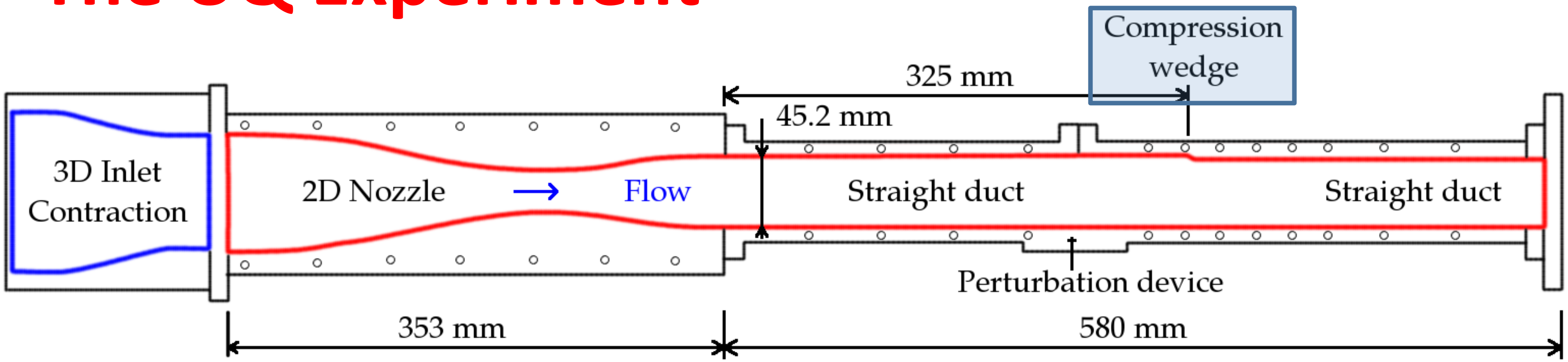




Uncertainties:
Inflow conditions + geometry

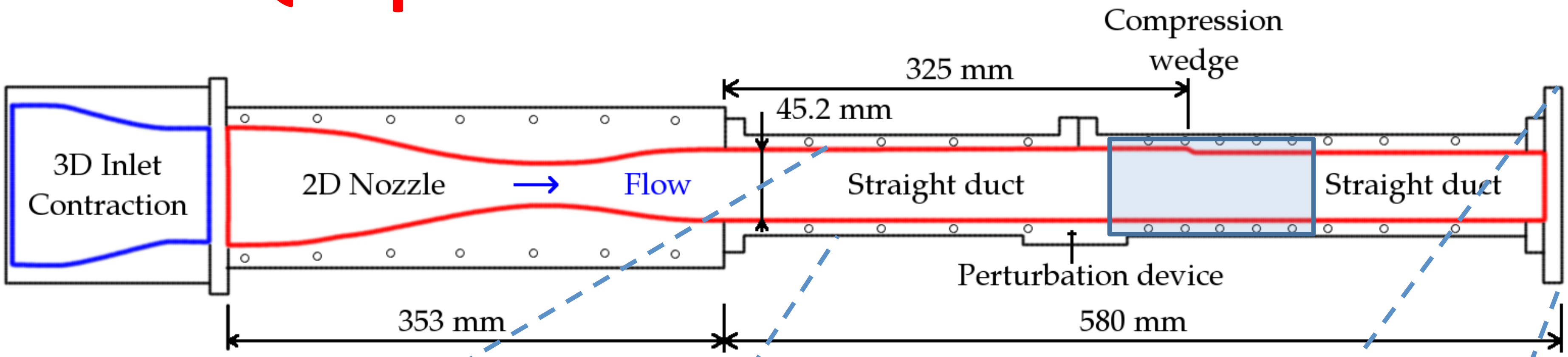
Quantity of Interest (QOI): location of shock-crossing point of first interaction:

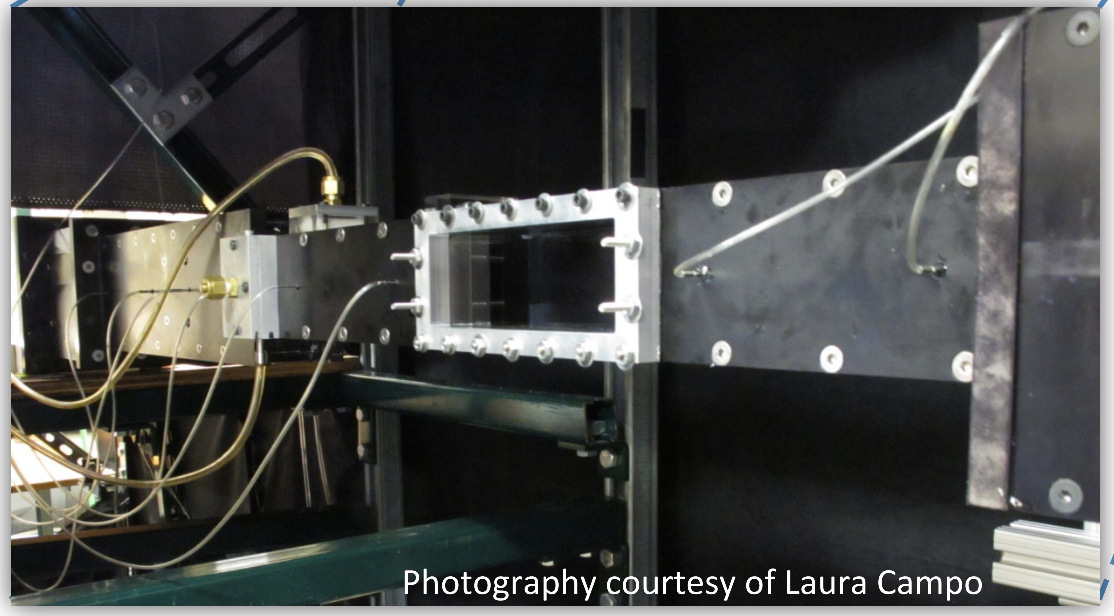
The UQ Experiment



Eaton, Helmer, Campo

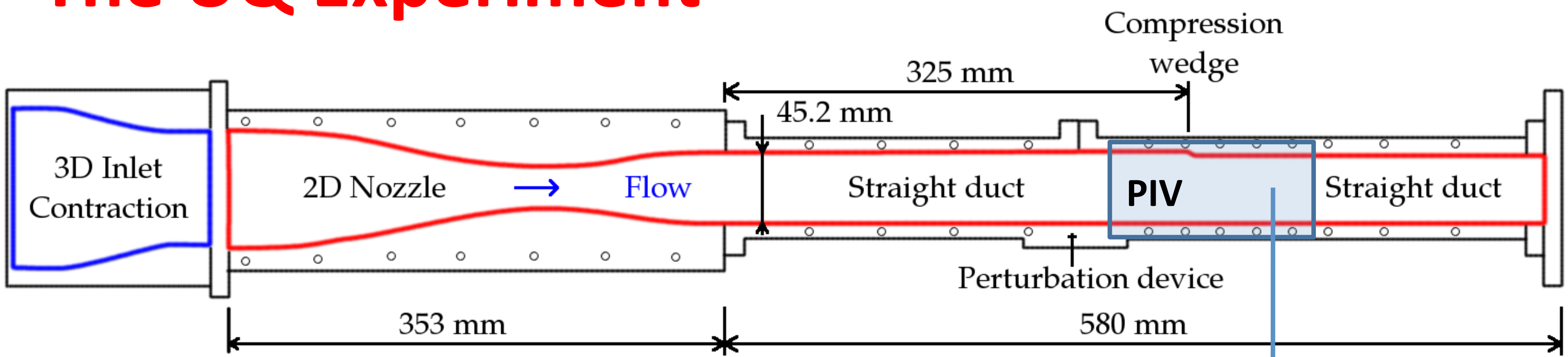
The UQ Experiment



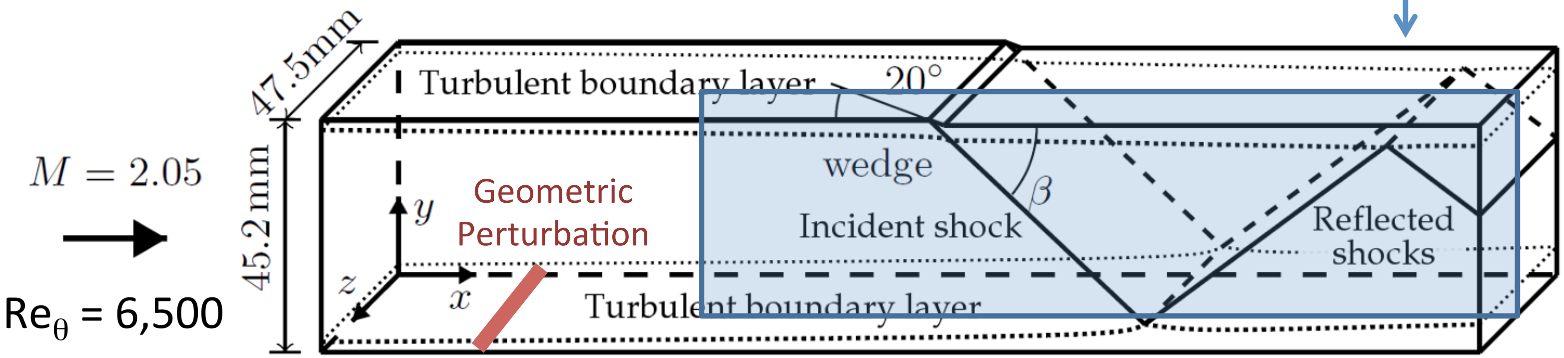


Eaton, Helmer, Campo

The UQ Experiment

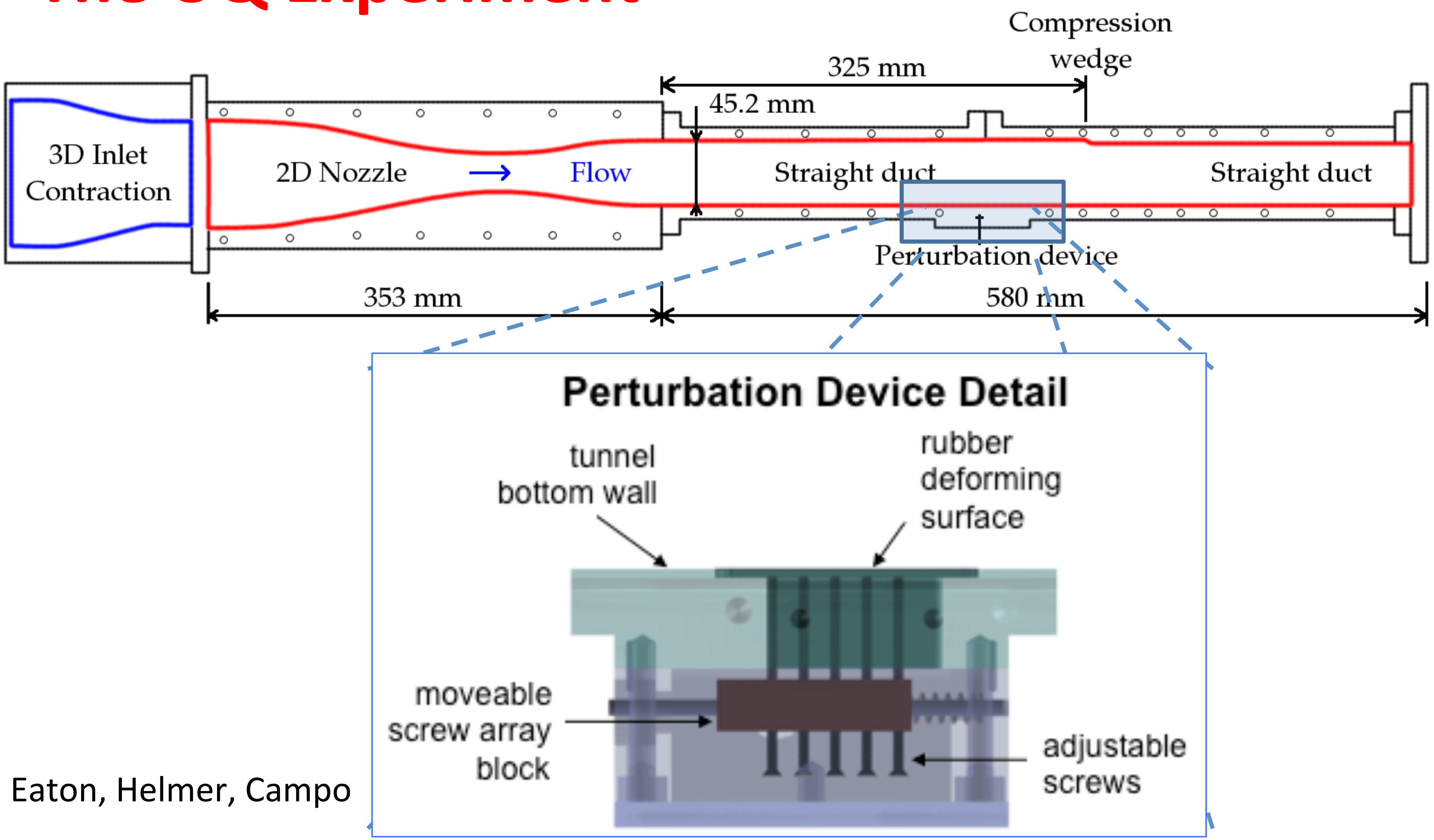


PIV measurements taken at 4 planes (1 near-center, 3 near side-wall)



Eaton, Helmer, Campo

The UQ Experiment

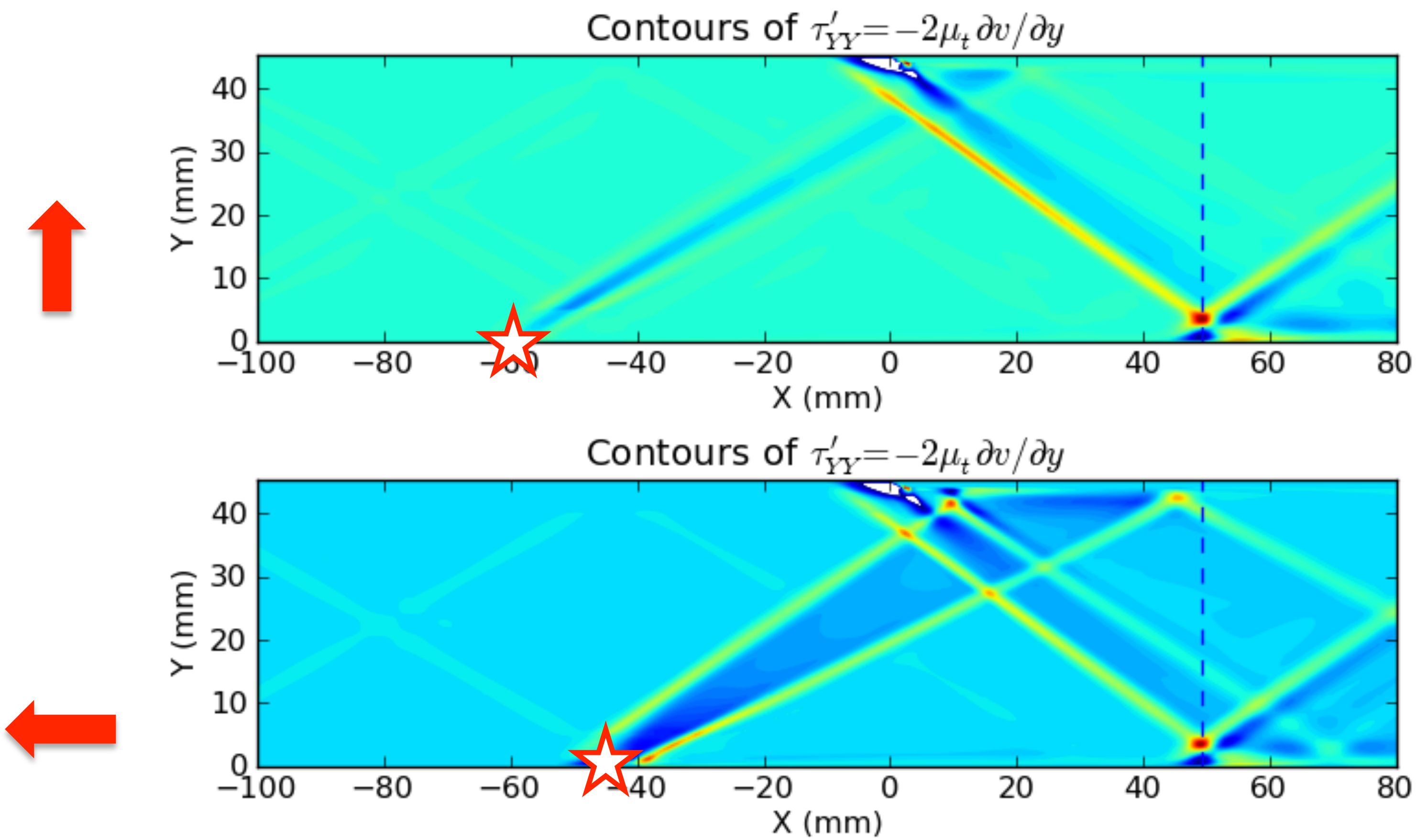


Eaton, Helmer, Campo

The UQ Experiment

RANS Baseline kwSST Simulations

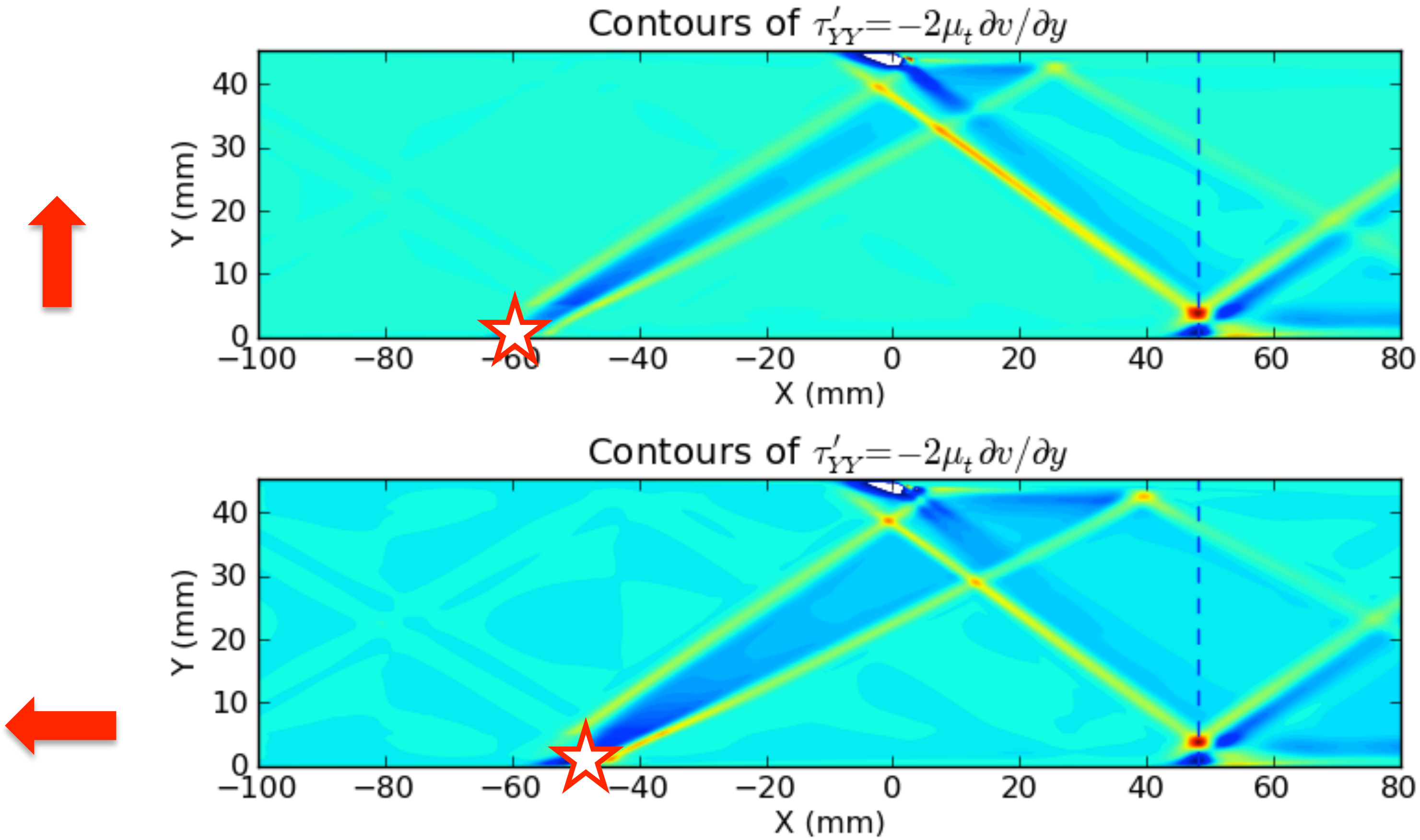
Effect of the "bump" **height** and **location**



The UQ Experiment

RANS Baseline kwSST Simulations

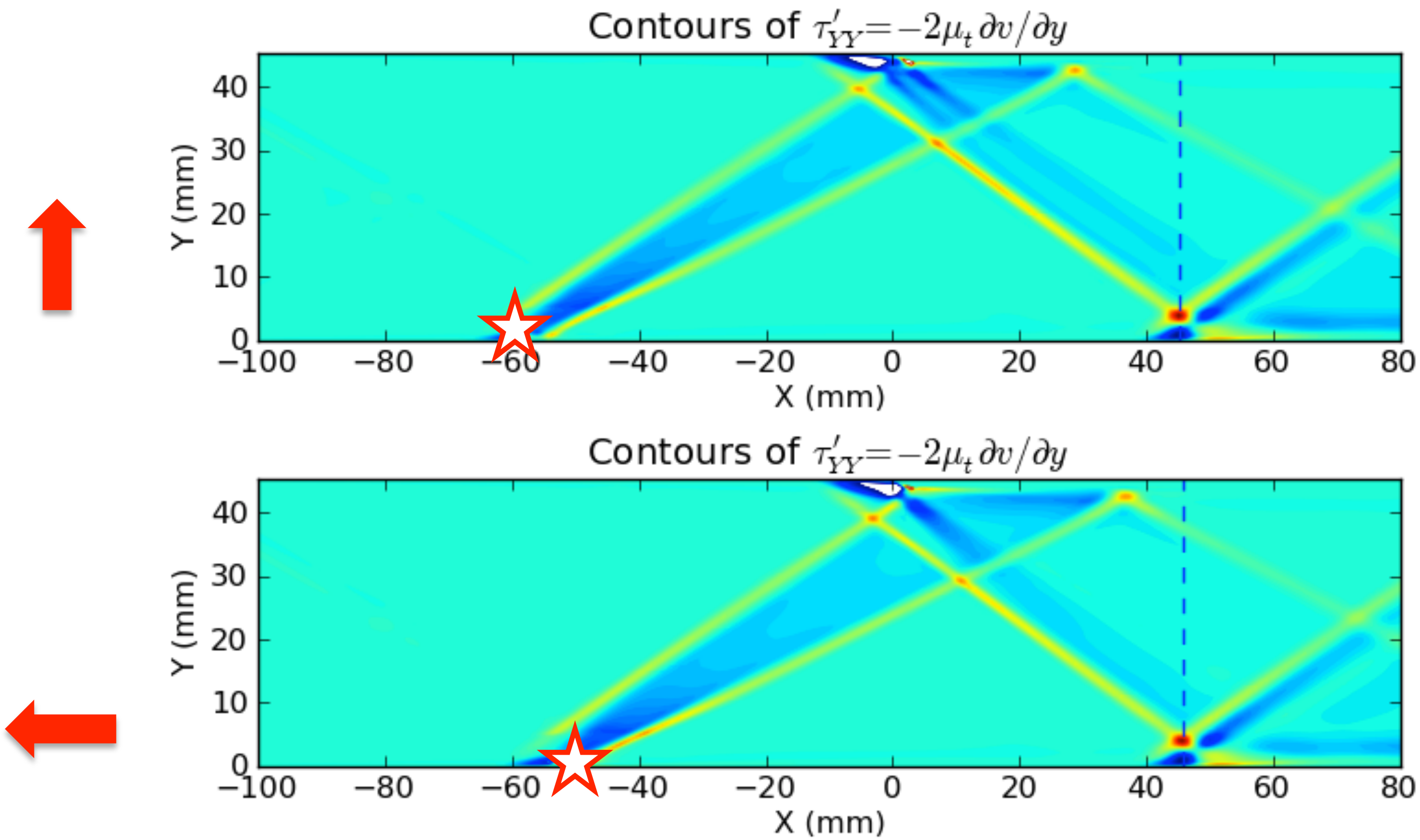
Effect of the "bump" **height** and **location**



The UQ Experiment

RANS Baseline kwSST Simulations

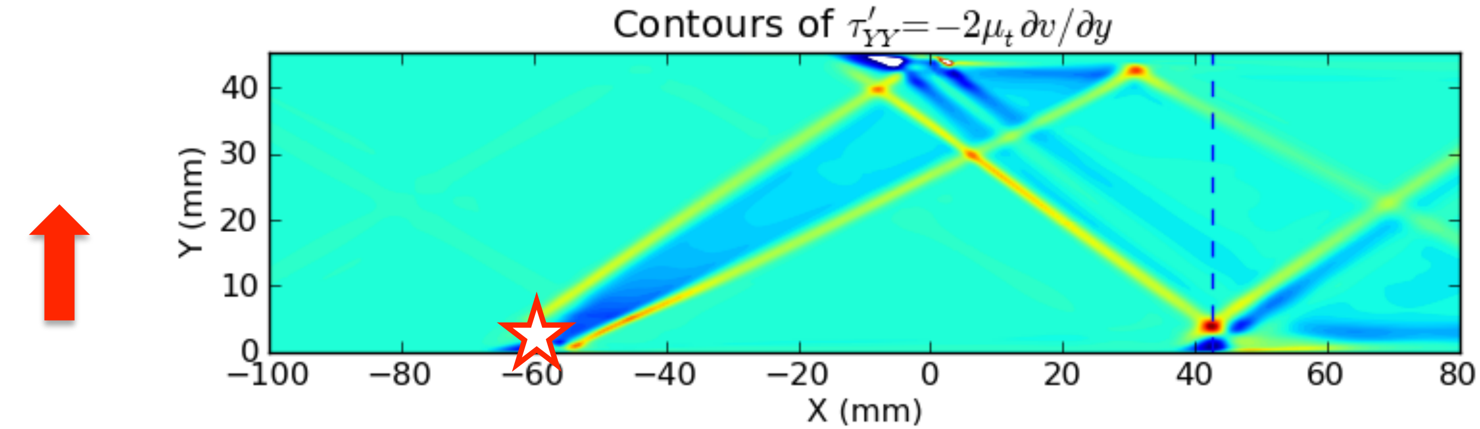
Effect of the “bump” **height** and **location**

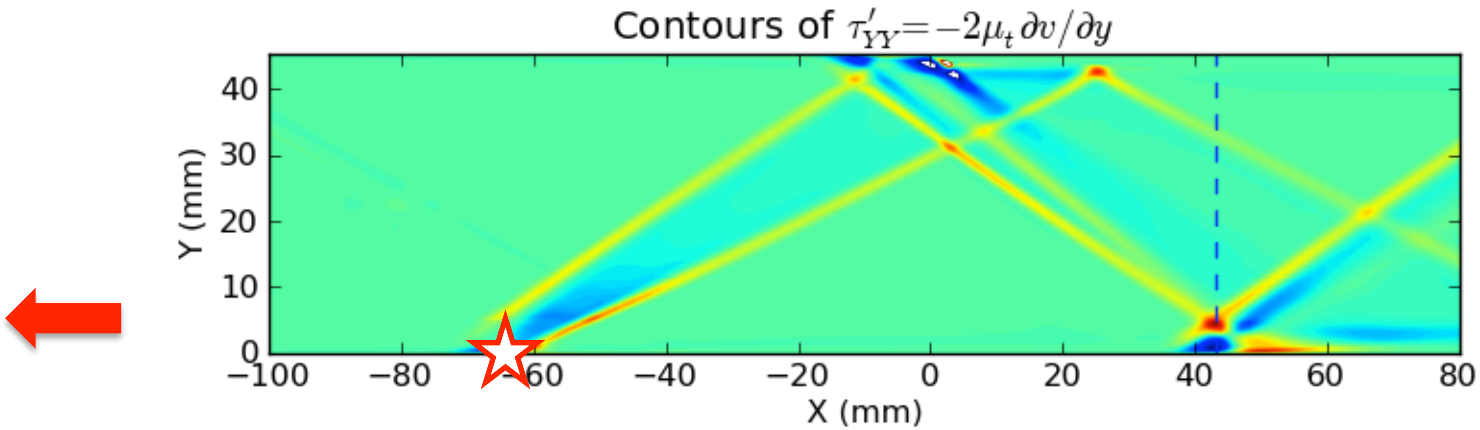


The UQ Experiment

RANS Baseline kwSST Simulations

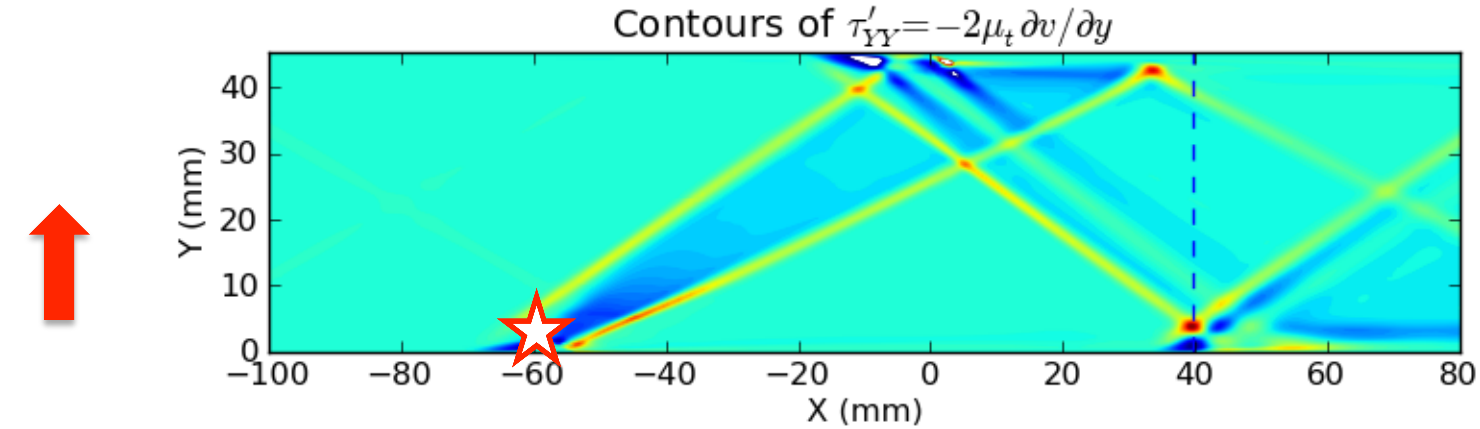
Effect of the "bump" **height** and **location**

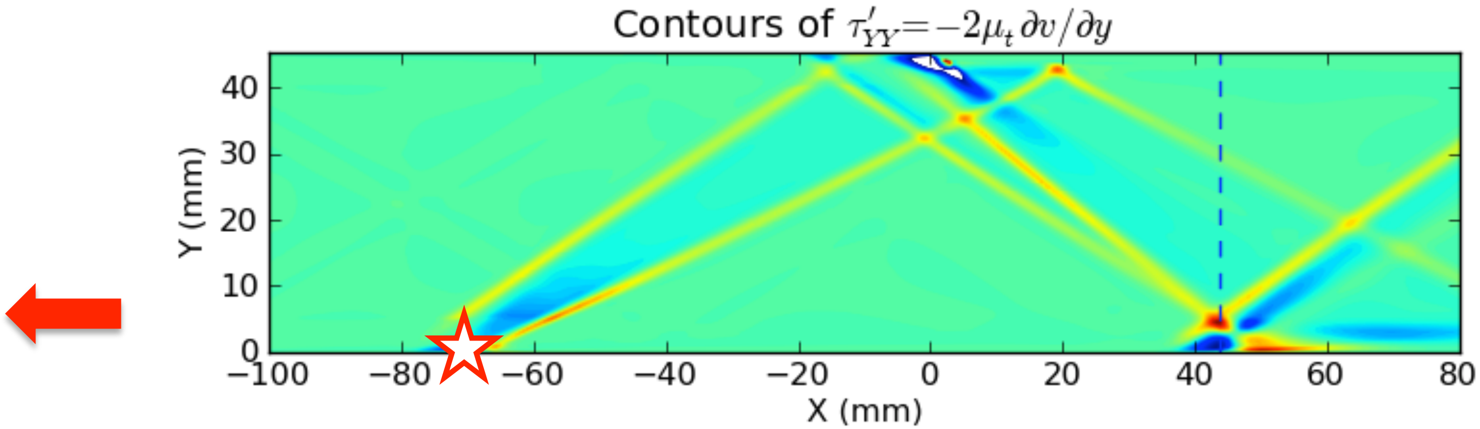




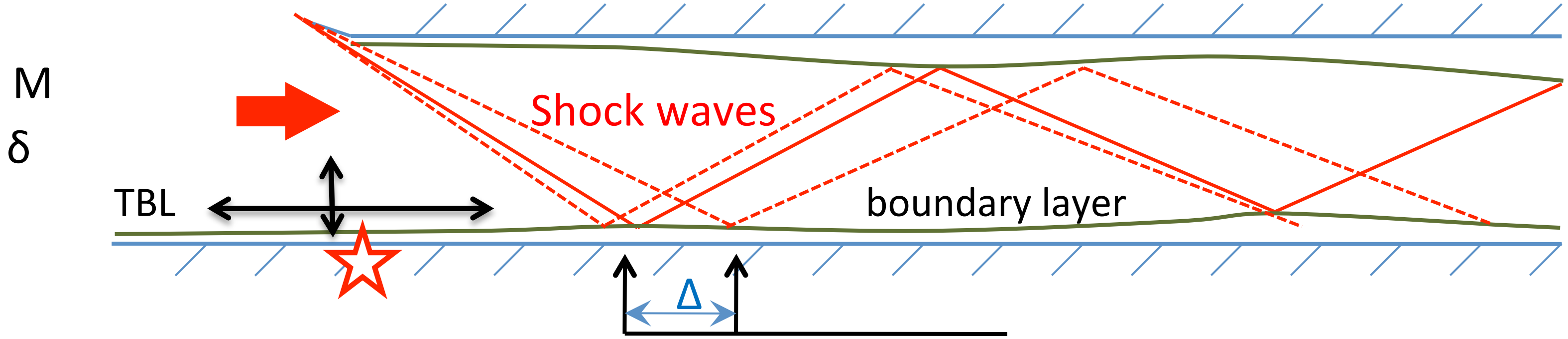
The UQ Experiment

RANS Baseline kwSST Simulations
Effect of the "bump" **height** and **location**



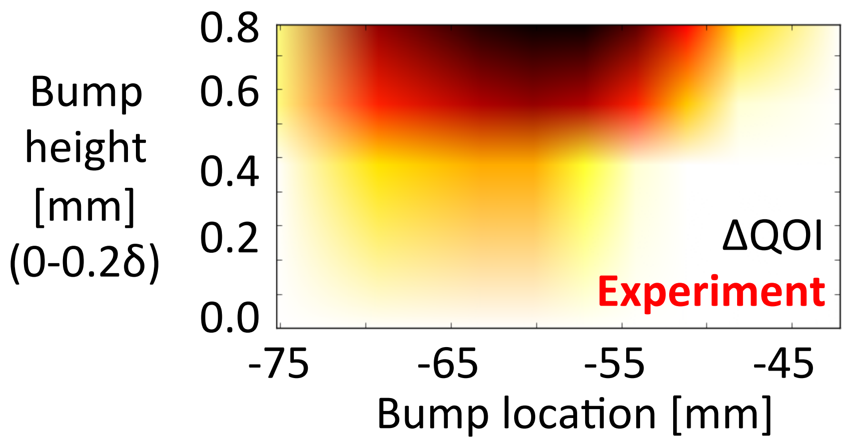


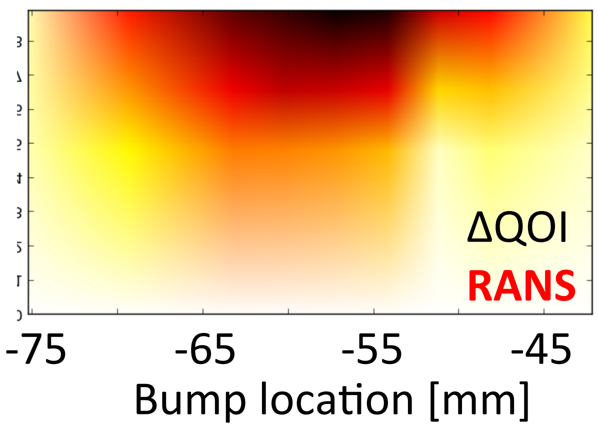
The UQ Experiment



Uncertainties:
Geometry

Quantity of Interest (QOI): location of shock-crossing point of first interaction:

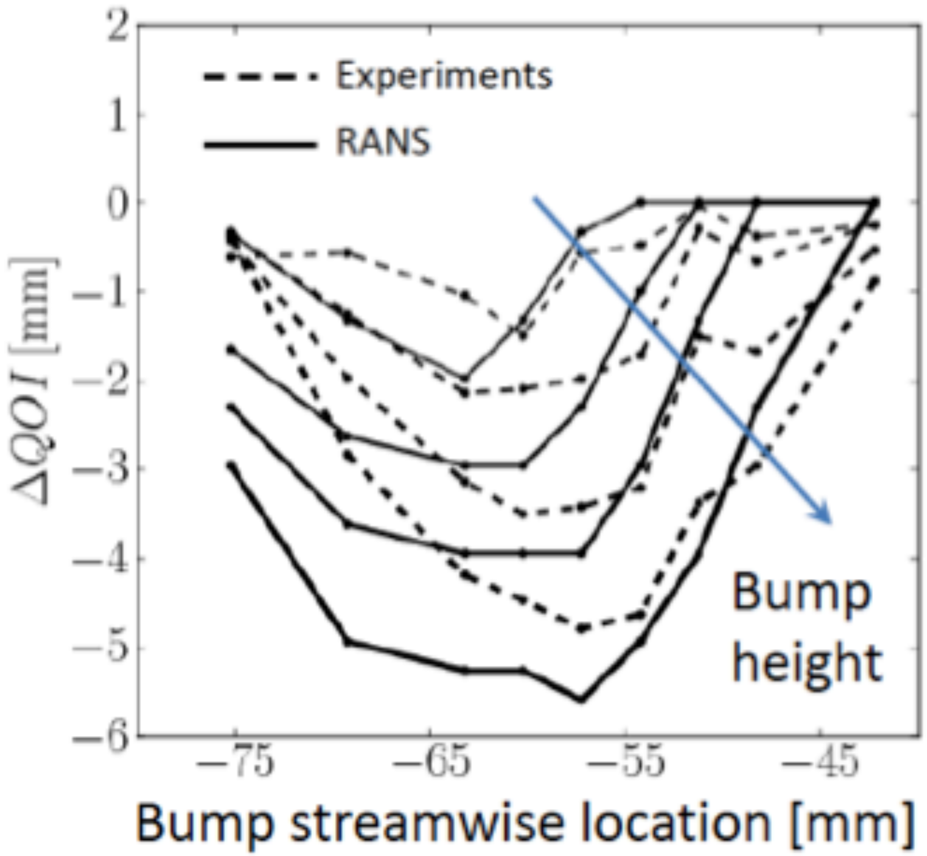




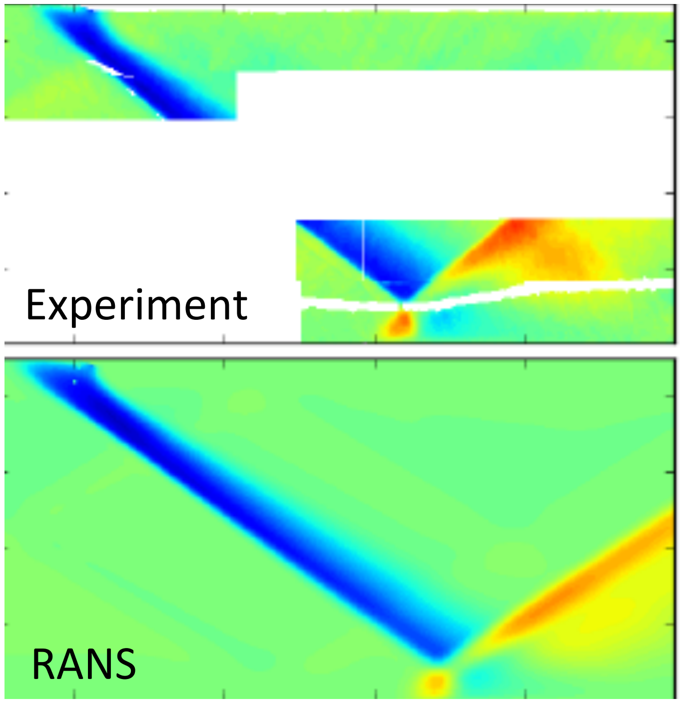
The UQ Experiment

Quantitative comparisons are not satisfactory..

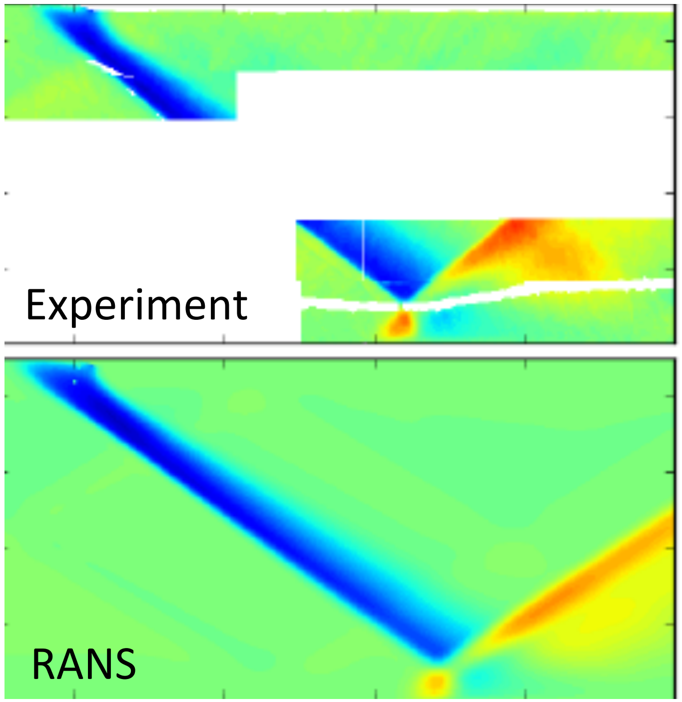
This is AUQ performed using a standard kwSST RANS model, what about the effect of model uncertainty (EUQ)?

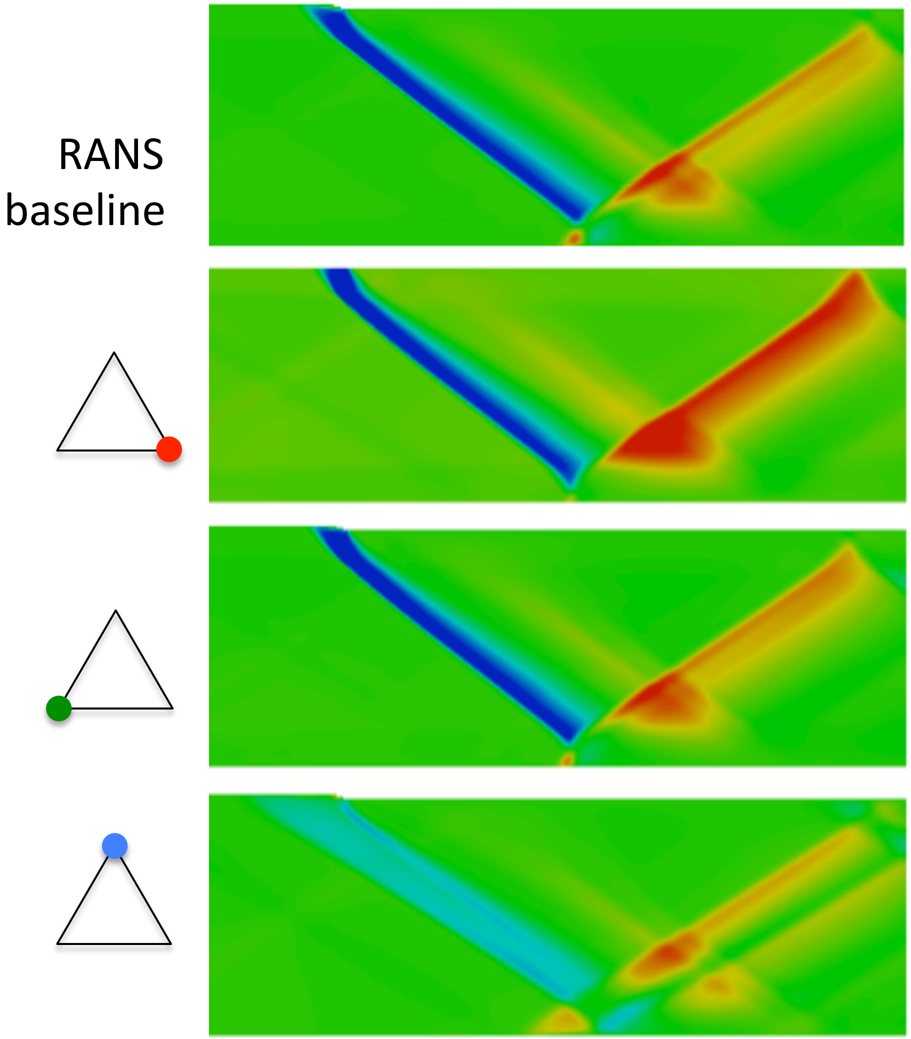


EUQ for the UQ Experiment



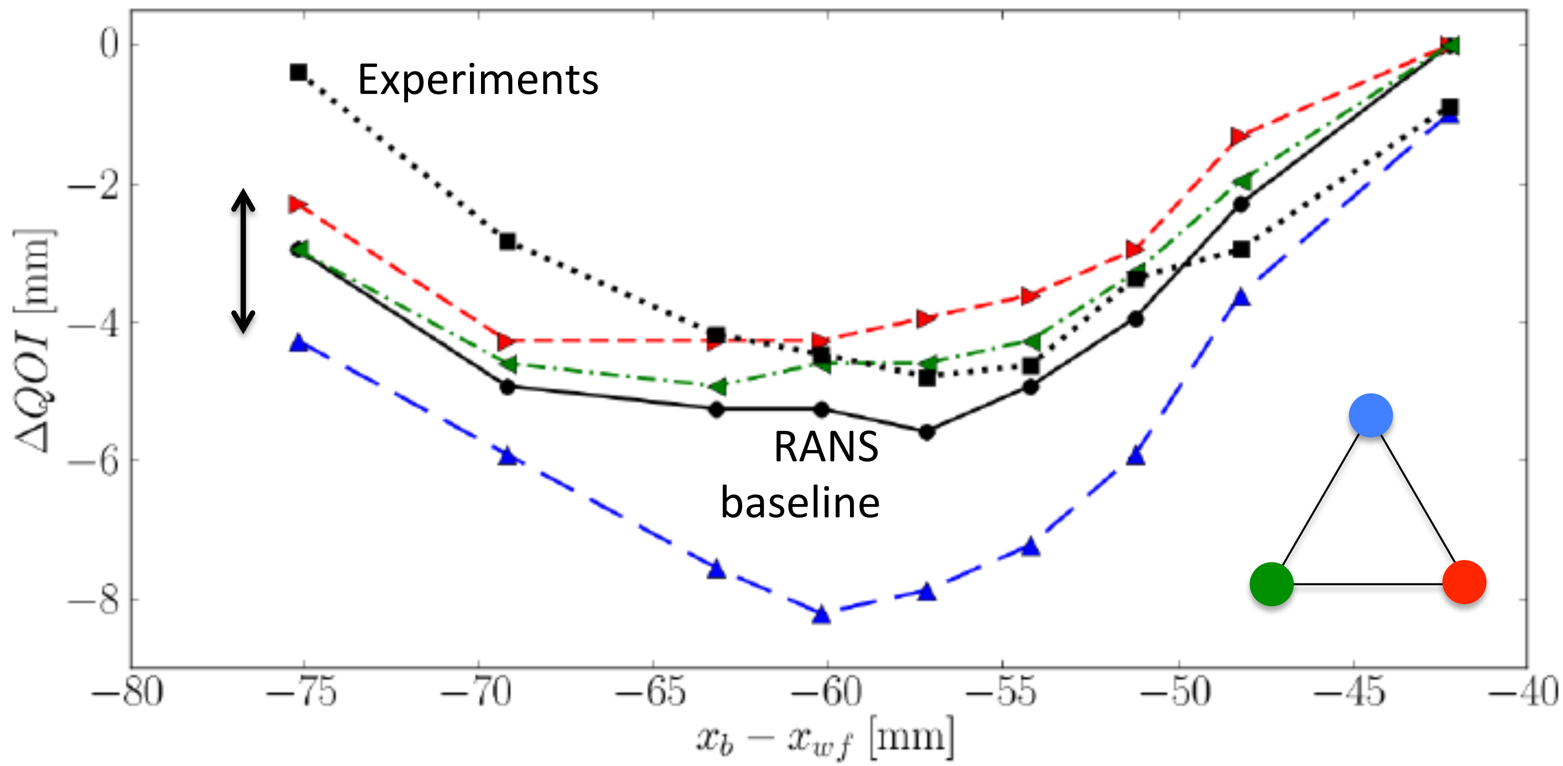
EUQ for the UQ Experiment





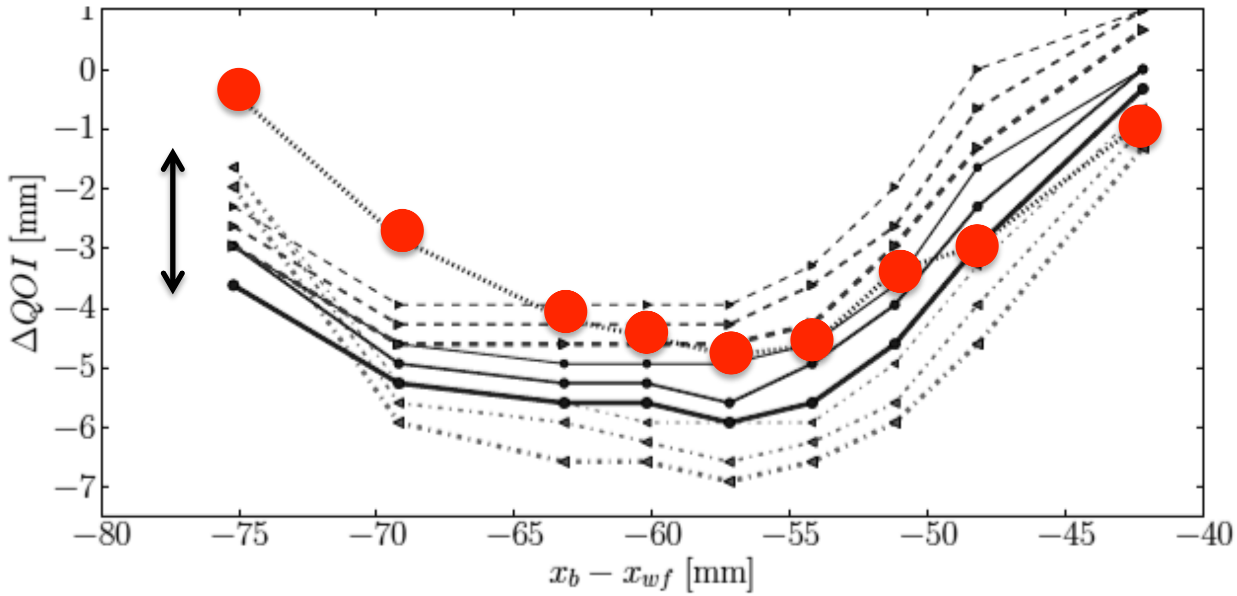
The UQ Experiment

Anisotropy bias is not “sufficient” to bridge the discrepancy between experiments and simulations



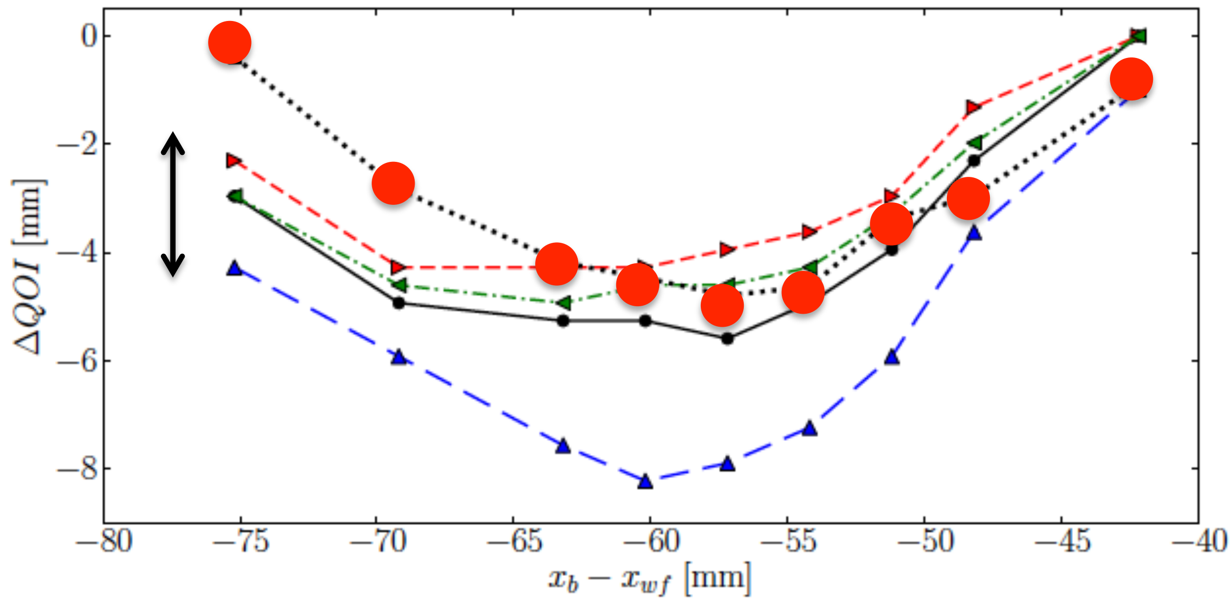
AUQ

Inflow uncertainty in Mach and δ

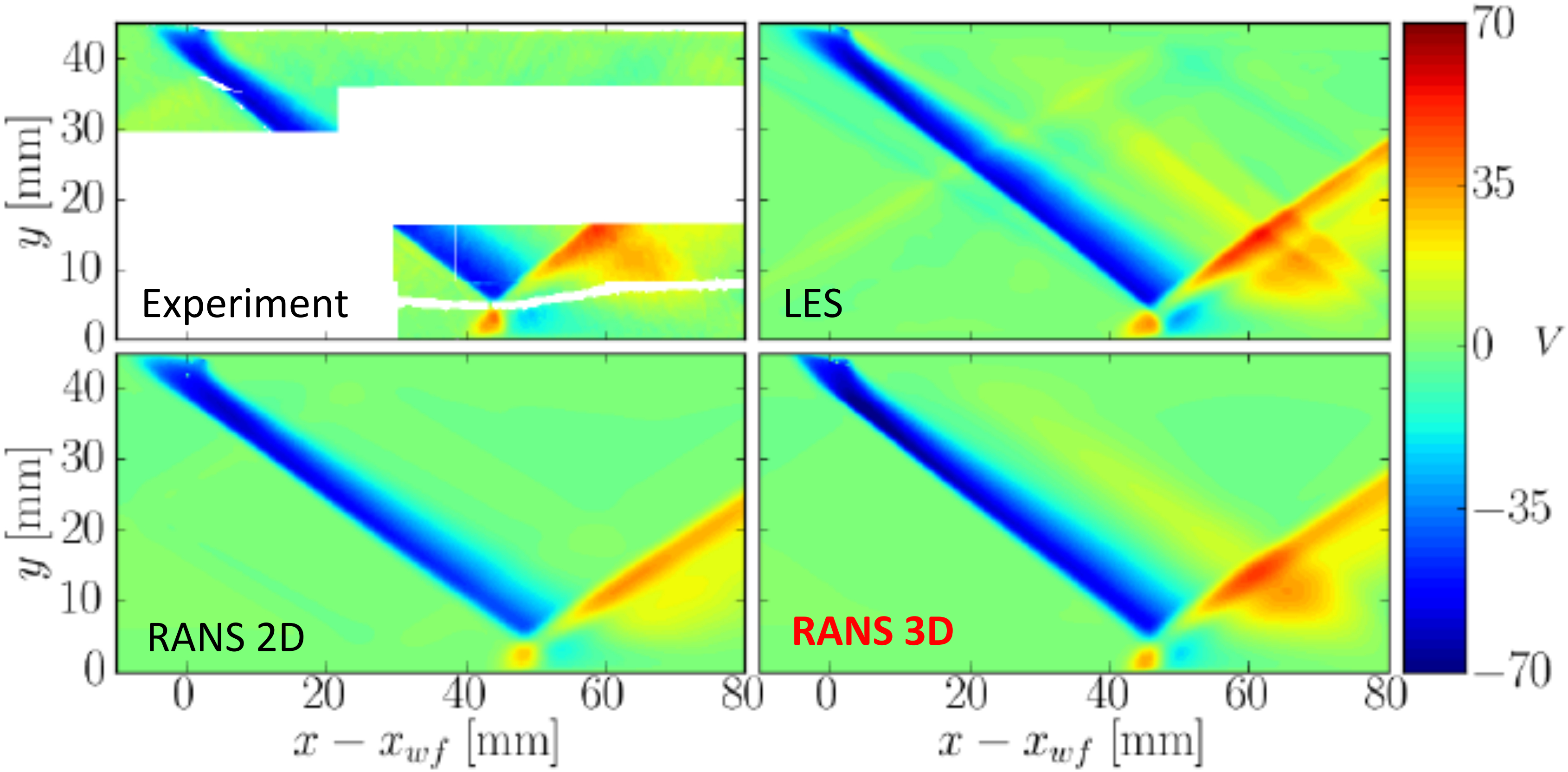


EUQ

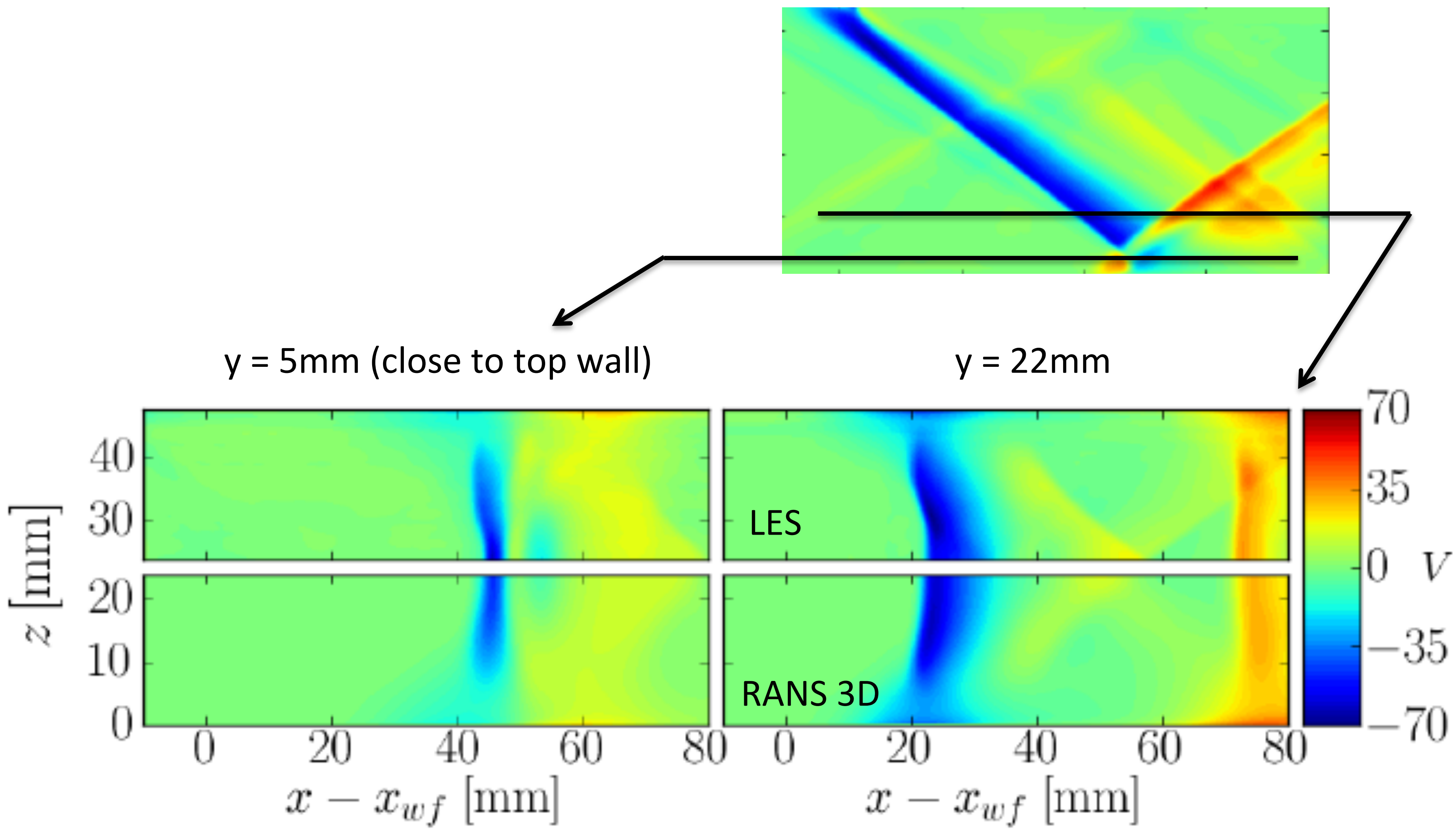
anisotropy bias In RANS

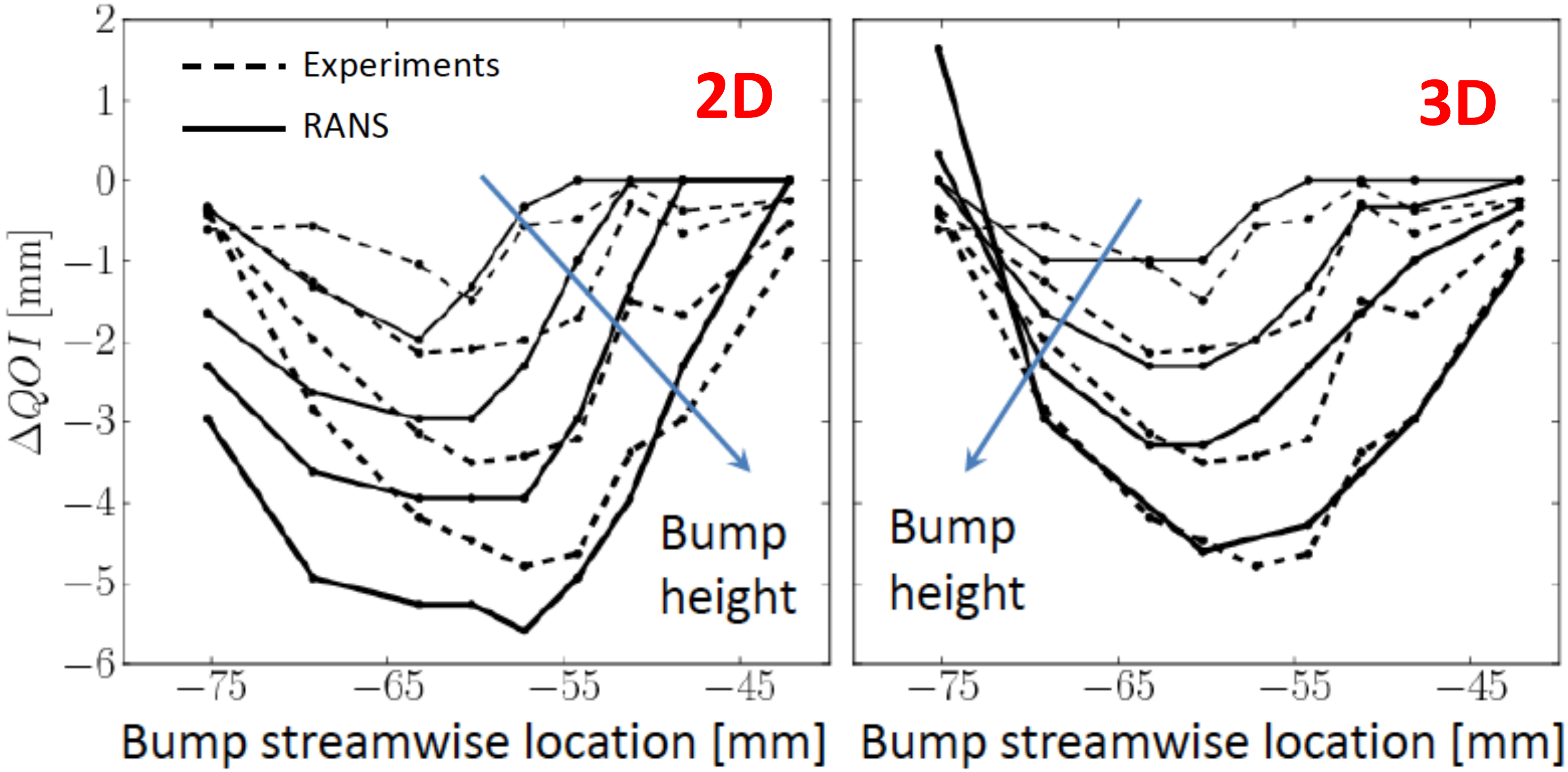


Comparisons between RANS, LES and PIV show good agreement in terms of the interaction – **3D RANS do capture** the interaction accurately…



3D effects are clearly visible (the duct has aspect ratio ~1)





Experiments
RANS
2D
3D
Bump height
Bump height
ΔQOI [mm]
2
1
0
−1
−2
−3
−4
−5
−6
−75
−65
−55
−45
Bump streamwise location [mm]
Bump streamwise location [mm]

Outline

- Why UQ?
- How to Quantify Uncertainties? AUQ and EUQ
- The UQ Experiment
- **Conclusions**

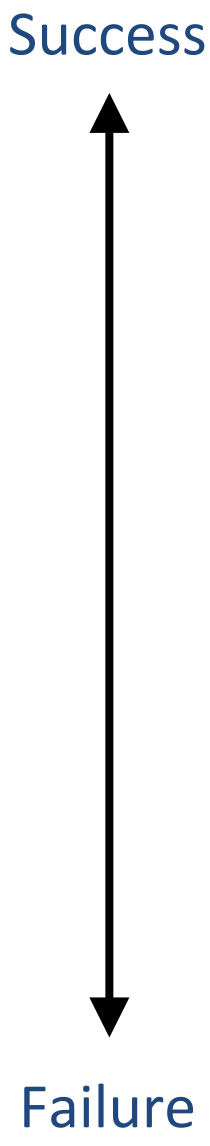
Concluding

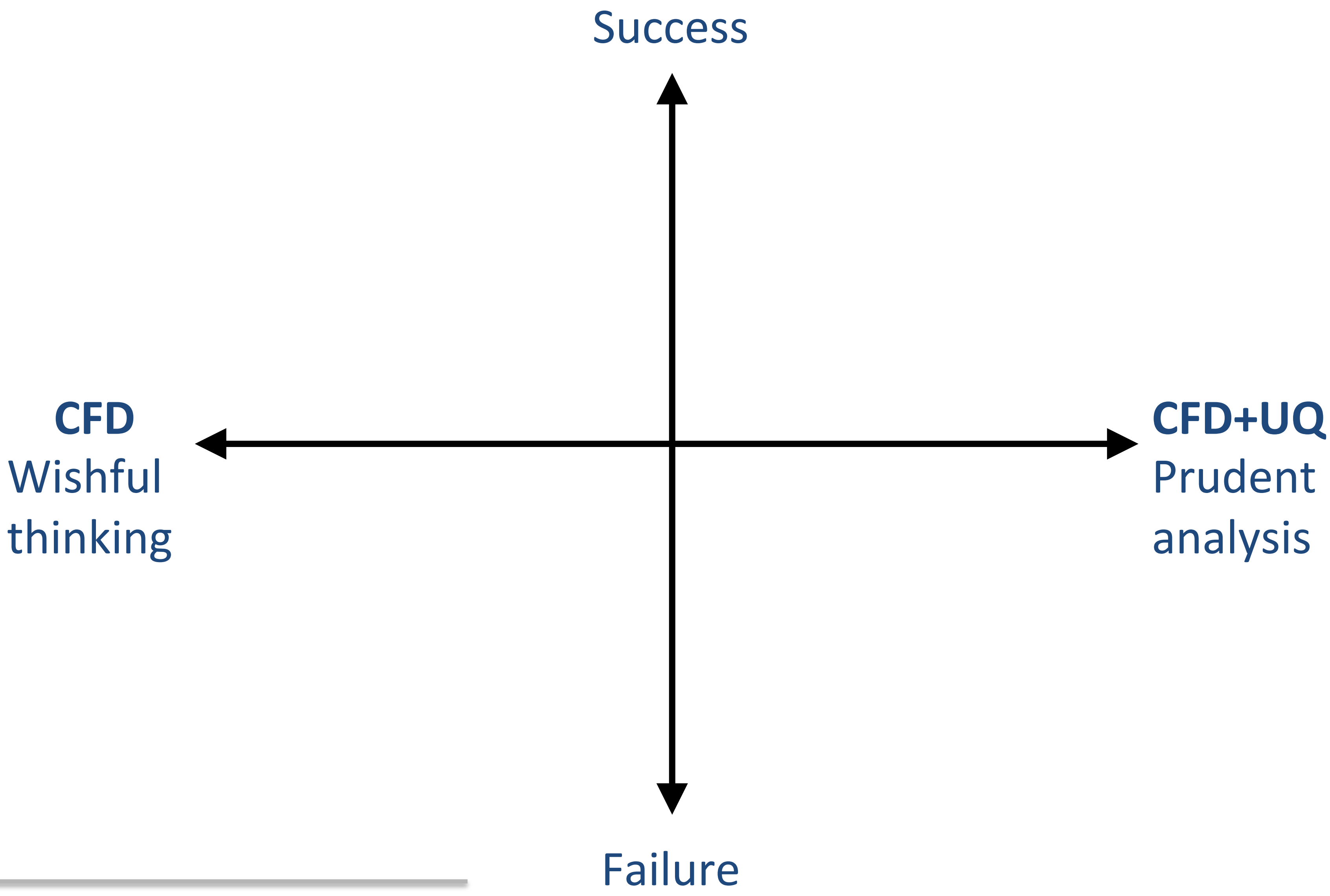
UQ is expensive (requires multiple repetition) so it has to be used wisely and with continuously improved algorithms

It is NOT simply an exercise in math or statistics but require domain-specific knowledge and ideas; especially the EUQ part as it provides measures of bias rather than variability

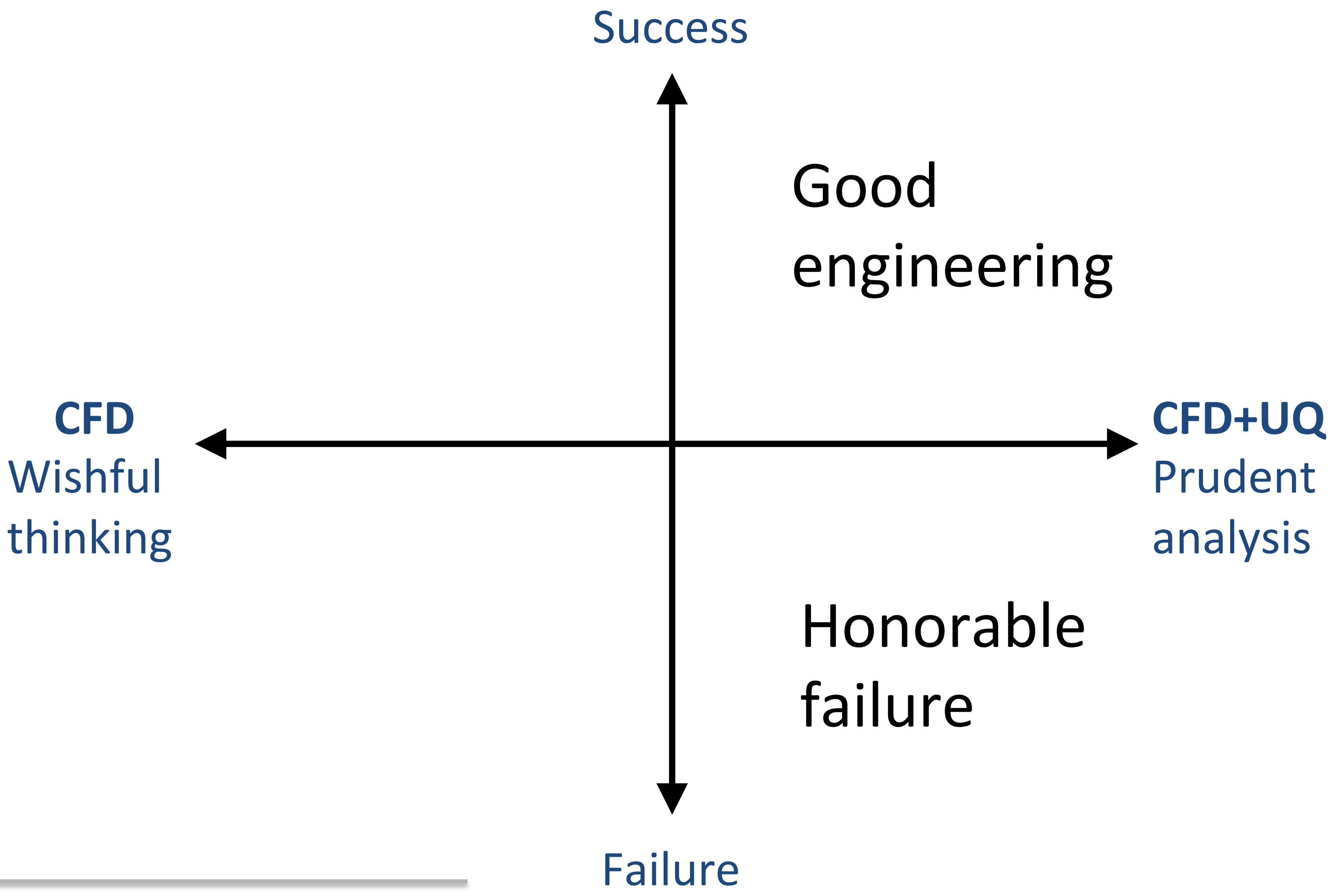
Our present EUQ strategy for RANS modeling provides insights into modeling bias and enables the construction of envelopes

Initial efforts have illustrated both the opportunities and the challenges…much work still ahead!

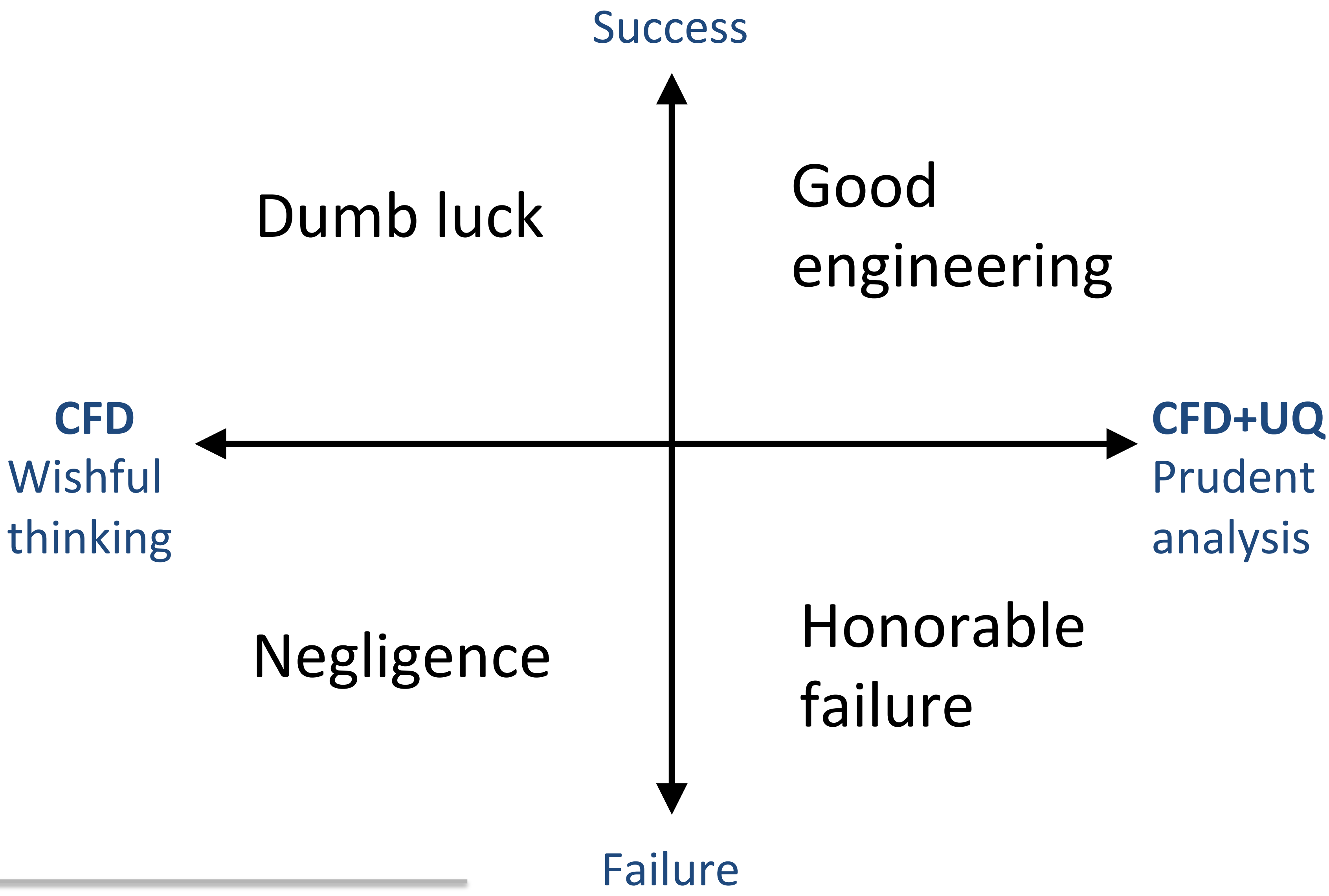

Success
Failure



Scott Ferson, Applied Biomath



Scott Ferson, Applied Biomath



Scott Ferson, Applied Biomath

THANK YOU

Acknowledgements

Collaborators: H. Abdehkakha, I. Bermejo, P. Constantine, A. Doostan, C. Gorle, M. Emory, J. Larsson, J. Witteveen

Funding: DoE, NNSA, Office of Science, NSF, KAUST, Bosch

Special thanks to J.P. Bonnet, R. Friedrich and the TSFP8 organizers

"If a man will begin with certainties, he shall end in doubts; but if he will be content to begin with doubts, he shall end in certainties."
F. Bacon - 1605

http://uq.stanford.edu