Uncertainty Estimation of Turbulence Model Predictions in SU2

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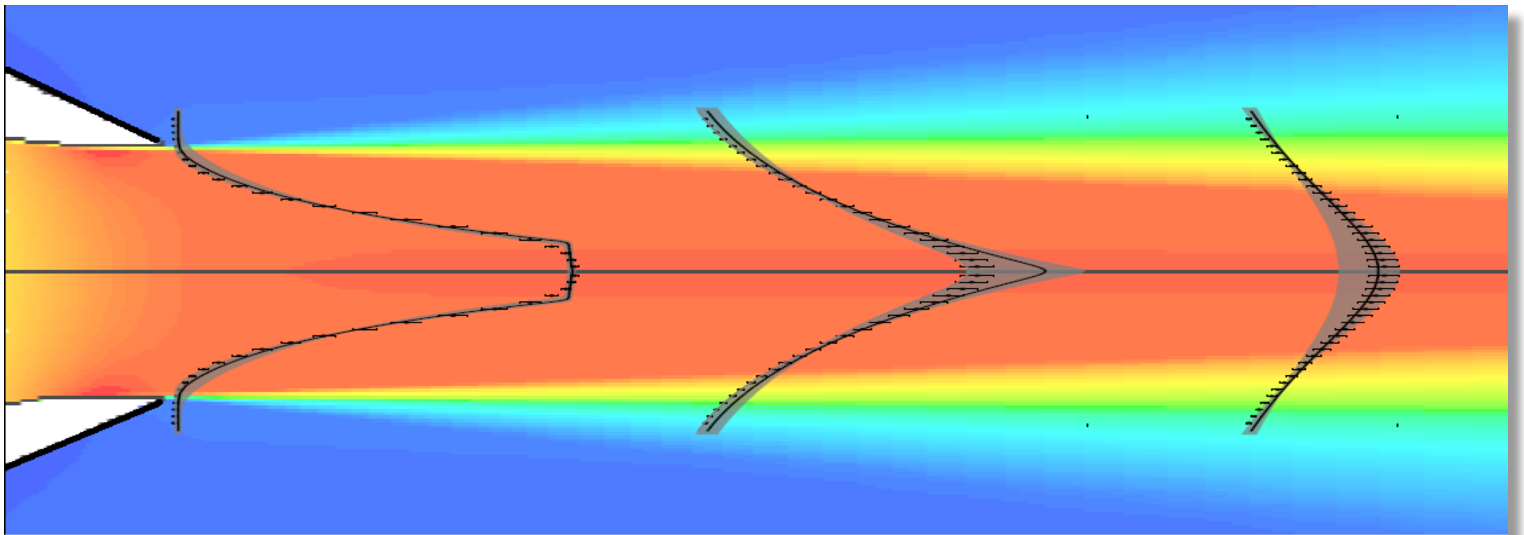

2nd Annual SU2 Developers Meeting
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December 18, 2017

SU2
The Open-Source CFD Code

Stanford University

Outline

I. *Overview of turbulence modeling & challenges*

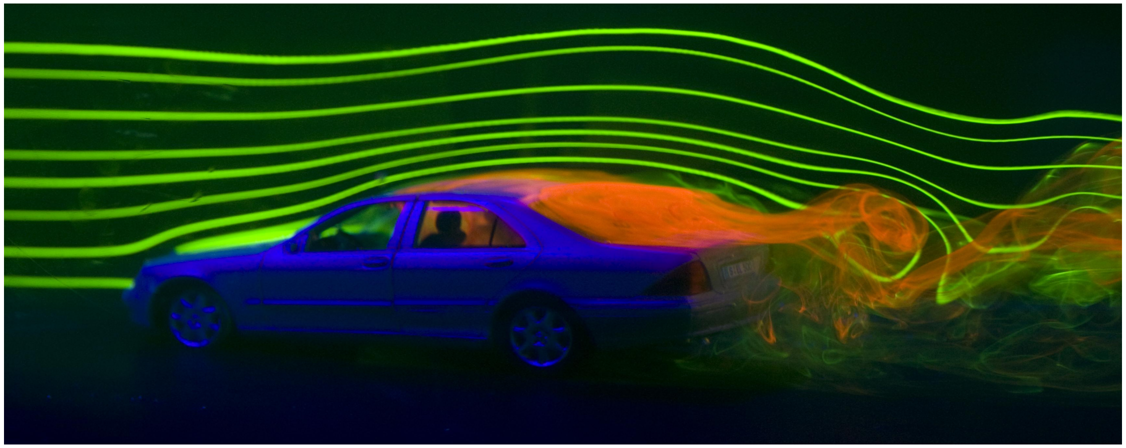
II. *Motivation & Objectives*

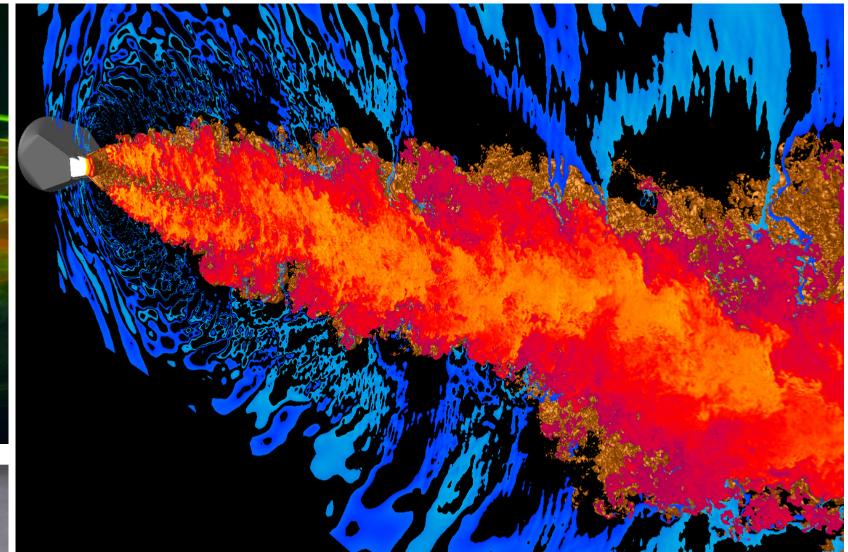
III. *Mathematical and computational details*

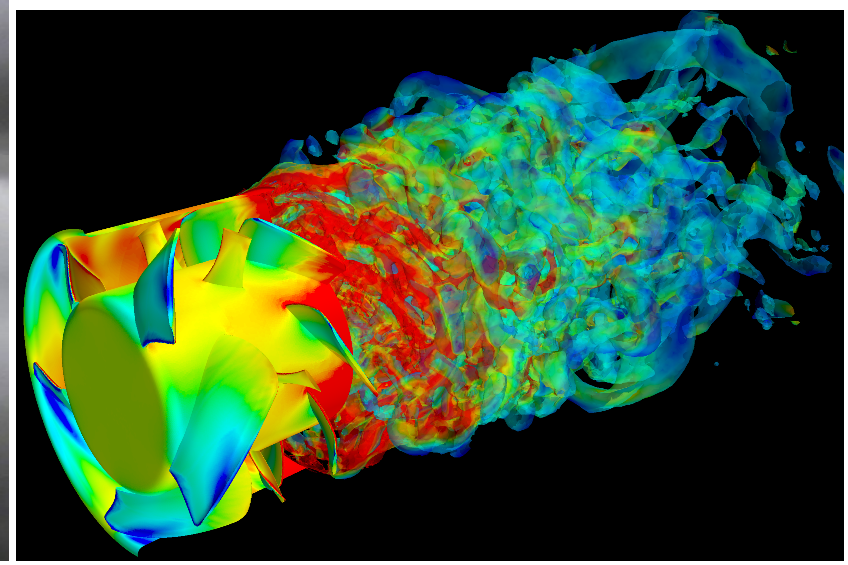
IV. *Testing and verification*

V. *Summary & Conclusions*

Turbulent Flows



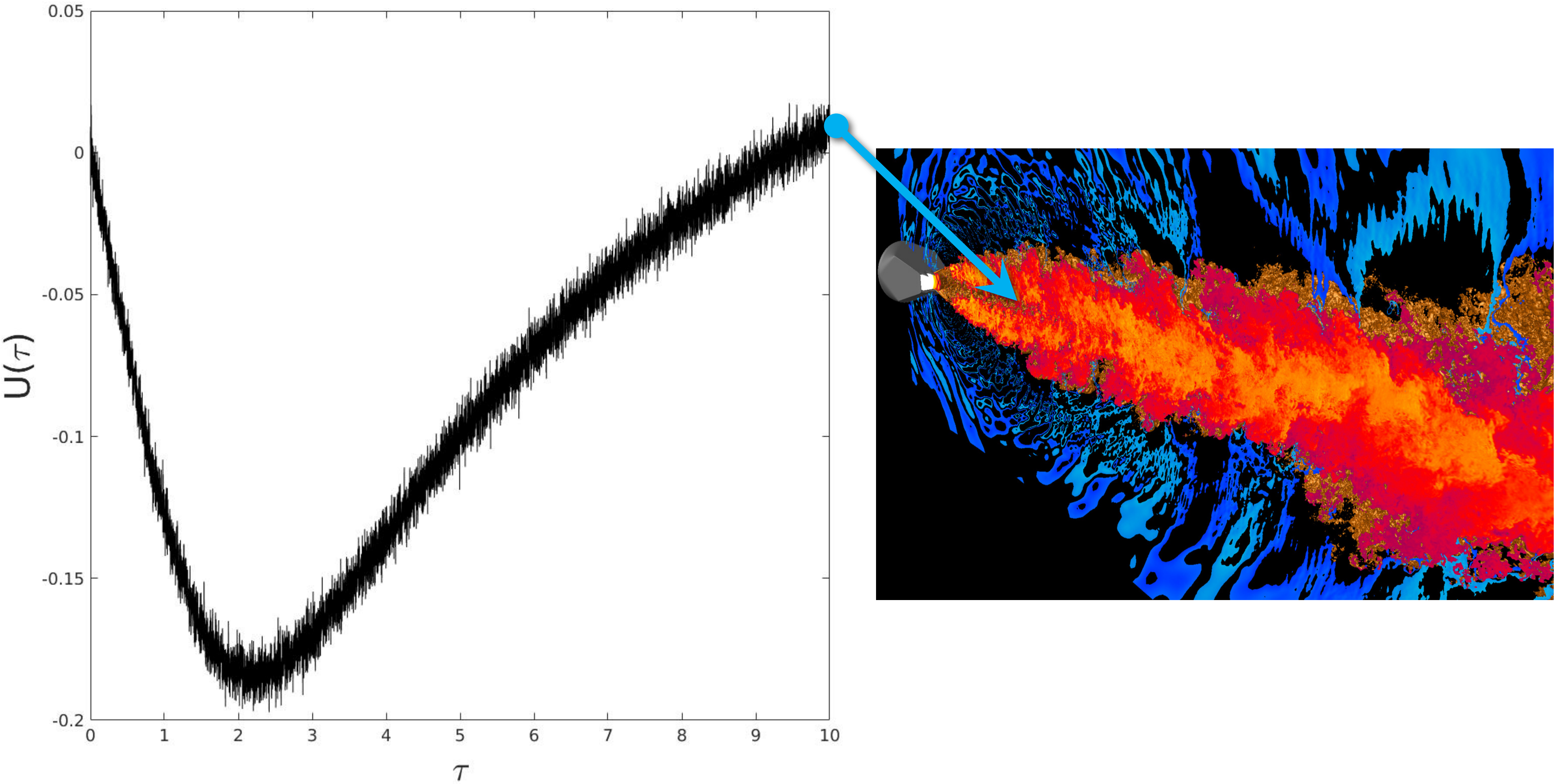




"Turbulence is the rule, not the exception, in complex engineering systems"

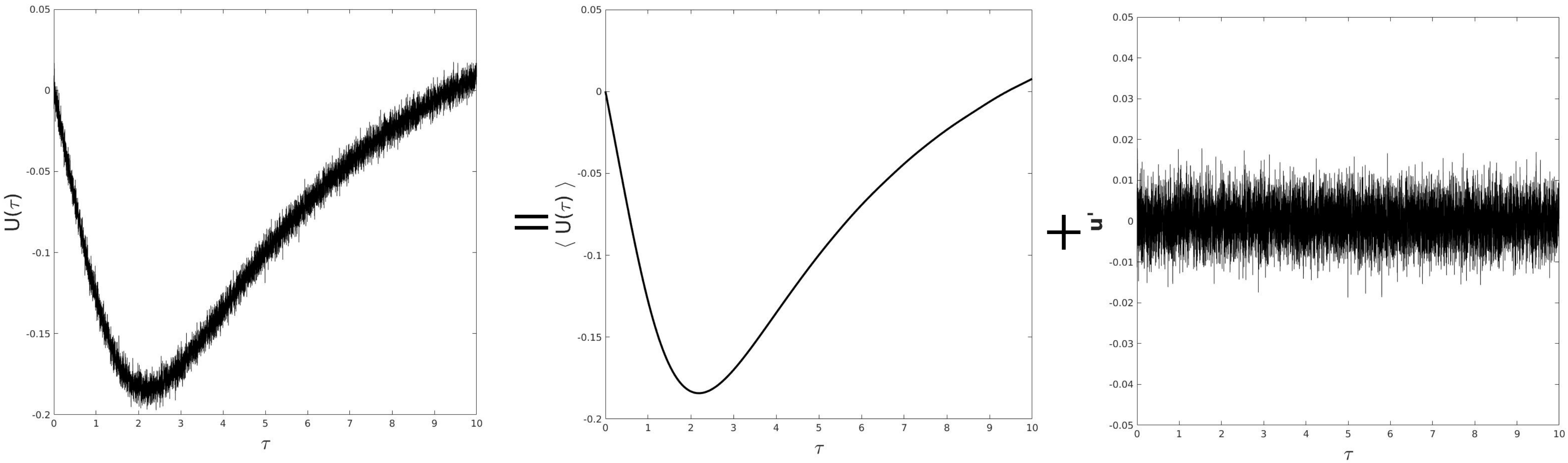
P. Moin, Scientific American (1997)

Turbulent Flows



- Irregular, small scale fluctuations in velocity and pressure.
- Increased dissipation, diffusivity, mixing of momentum, species.
- Increased drag, reduced lift.
- Loss of predictability.

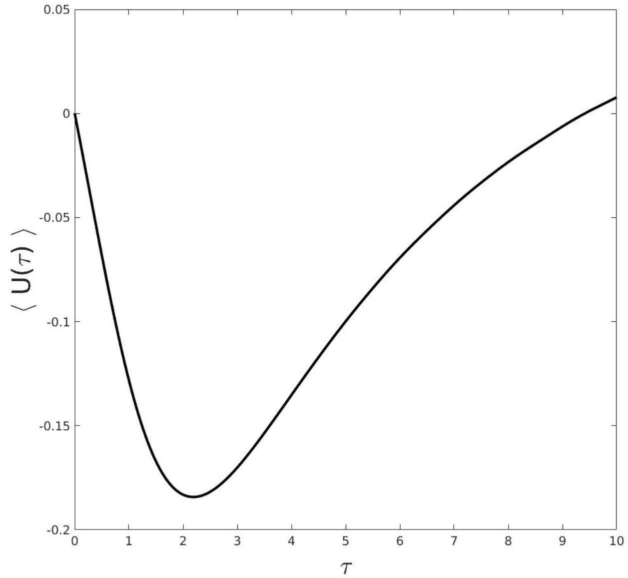
Mathematical Approach: Reynolds's Decomposition



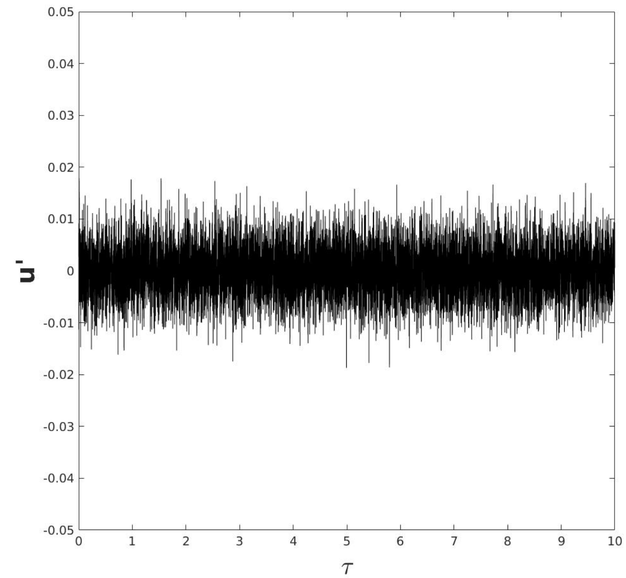
Instantaneous velocity = Mean velocity + Fluctuating velocity

Average over many repetitions of the experiment.
For design, at the zeroth level, we need this Mean quantity.

Mathematical Approach: Reynolds's Decomposition



Mean velocity



Fluctuating velocity

$$\frac{D\langle U_j\rangle}{Dt} = \nu \nabla^2 \langle U_j\rangle - \frac{1}{\rho}\frac{\partial\langle P\rangle}{\partial x_j} - \boxed{\frac{\partial\langle u_i u_j\rangle}{\partial x_i}}$$

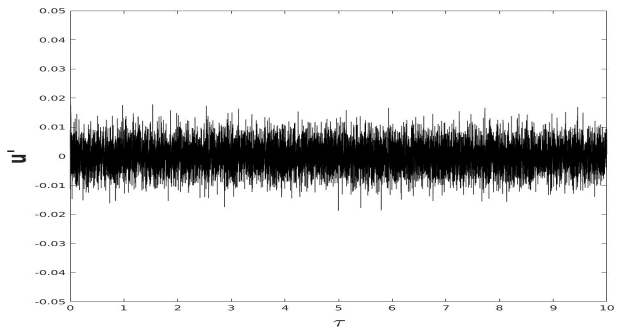
To solve for the mean, we need the covariance of the fluctuations

$$R_{ij} = \begin{bmatrix} \langle u_1 u_1\rangle & \langle u_1 u_2\rangle & \langle u_1 u_3\rangle \\ \langle u_2 u_1\rangle & \langle u_2 u_2\rangle & \langle u_2 u_3\rangle \\ \langle u_3 u_1\rangle & \langle u_3 u_2\rangle & \langle u_3 u_3\rangle \end{bmatrix}$$

Covariance of the fluctuations, Reynolds stresses

Stanford University

Mathematical Approach: Reynolds's Decomposition



Fluctuating velocity

$$R_{ij} = \begin{bmatrix} \langle u_1 u_1 \rangle & \langle u_1 u_2 \rangle & \langle u_1 u_3 \rangle \\ \langle u_2 u_1 \rangle & \langle u_2 u_2 \rangle & \langle u_2 u_3 \rangle \\ \langle u_3 u_1 \rangle & \langle u_3 u_2 \rangle & \langle u_3 u_3 \rangle \end{bmatrix}$$

$$\partial_t R_{ij} + U_k \frac{\partial R_{ij}}{\partial x_k} = P_{ij} - \frac{\partial T_{ijk}}{\partial x_k} - \epsilon_{ij} + \pi_{ij},$$

where,

$$P_{ij} = -R_{kj}\frac{\partial U_i}{\partial x_k} - R_{ki}\frac{\partial U_j}{\partial x_k},$$

$$T_{kij} = \boxed{\langle u_i u_j u_k \rangle} - \nu \frac{\partial R_{ij}}{\partial x_k} + \boxed{\delta_{jk}\left\langle u_i \frac{p}{\rho} \right\rangle + \delta_{ik}\left\langle u_j \frac{p}{\rho}\right\rangle,}$$

$$\epsilon_{ij} = -2\nu \boxed{\left\langle \frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}\right\rangle}, \qquad \boxed{\pi_{ij} = \left\langle \frac{p}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right\rangle}$$

Computationally expensive
Unclosed
Nonlinearity
&
Nonlocality

Eddy Viscosity Based Models

- Simpler eddy viscosity based models represent the workhorse of industrial investigations into turbulence. $(\mathrm{k}-\varepsilon, \mathrm{k}-\omega, \ldots\ldots)$

- Simplifications and Assumptions used in formulation.

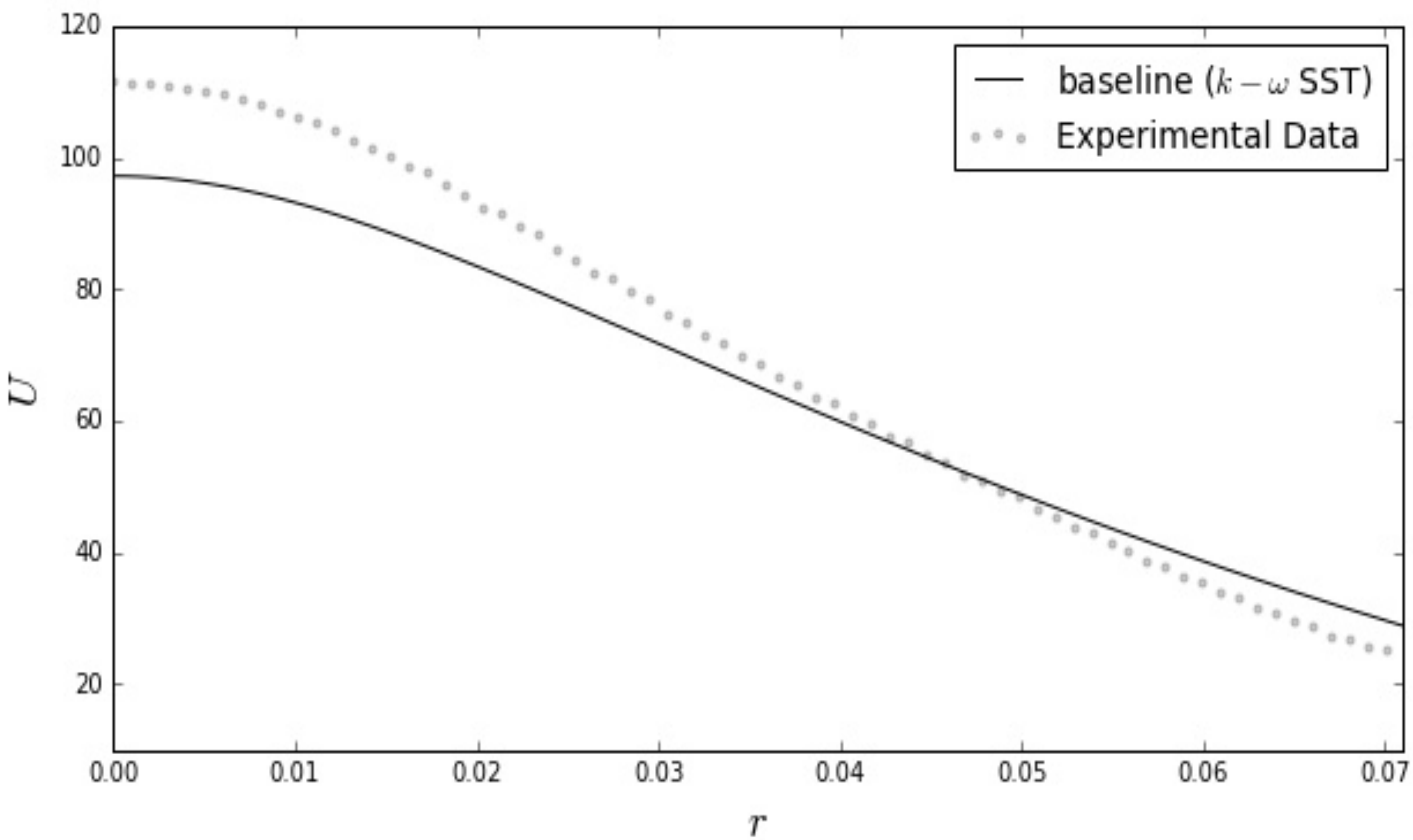
  Eddy viscosity hypothesis: $R_{ij} = \frac{2}{3} k \delta_{ij} - 2\nu_T S_{ij}$

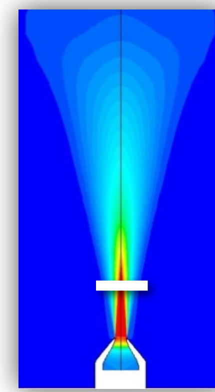
  Gradient Diffusion hypothesis: $T_i = -\frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial x_i}$

  …………………

- Limit the features of turbulence these models can replicate and the fidelity with which they can replicate these features.

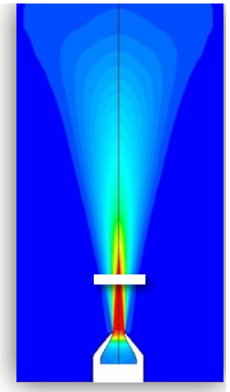
Eddy Viscosity Based Models: Limitations

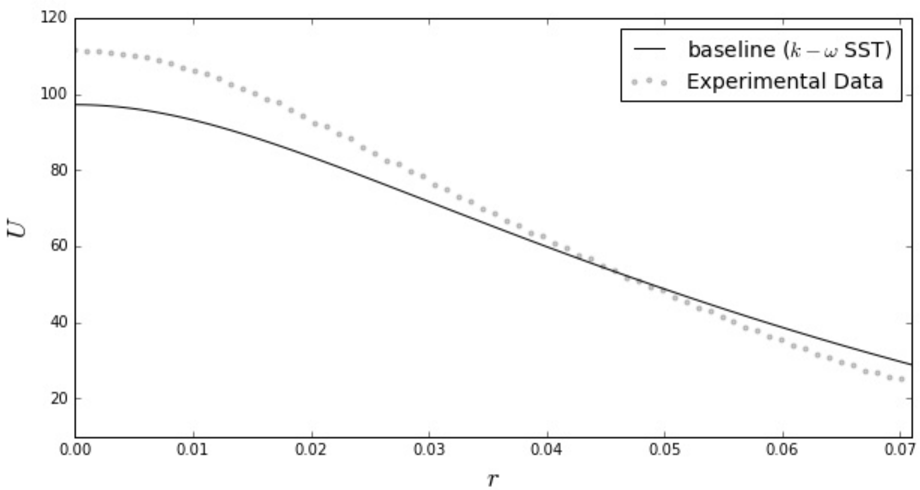




Significant discrepancy in RANS predictions,
Uncertainty in design.

Main Idea:
From Point Predictions to Interval Predictions

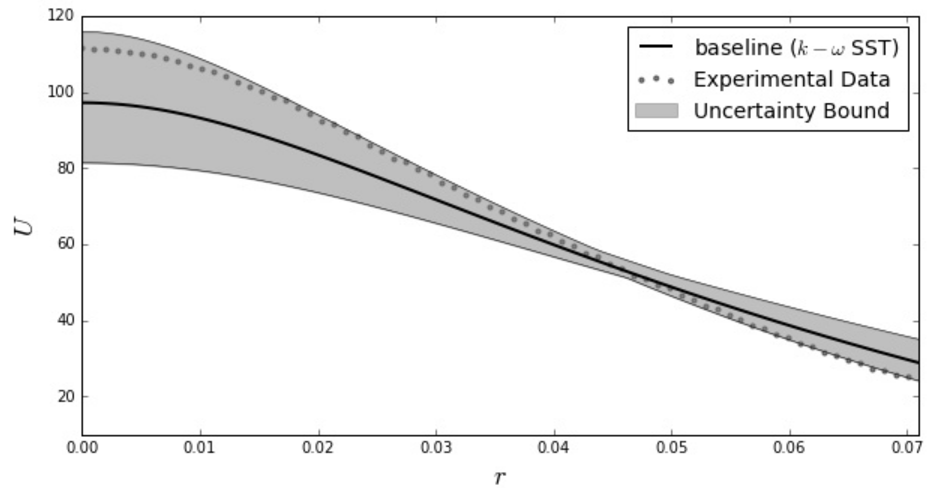




Point predictions

Dubious accuracy

Uncertain discrepancy



Interval predictions

Explicit quantification of uncertainty

Aid decisions under uncertainty

Motivation & Objectives

- Simulations via RANS models represent the workhorse for turbulent flows in industry.

- To establish RANS closures as engineering tools ☞ explicit and reliable estimates of the uncertainty in predictions.

- Over 250 CFD software packages available. None offer internal modules for UQ.

- External packages (NESSUS, COSSAN..) available for aleatoric uncertainty estimation.

- No reliable, built-in modules for epistemic uncertainties, especially focusing on RANS models.

- Development and validation of a reliable RANS-UQ module for the SU2 CFD suite.

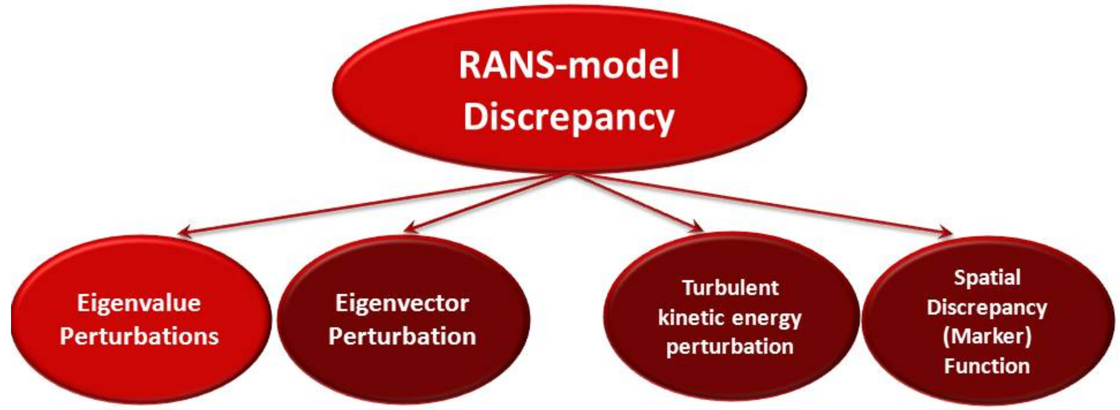
Intended Features

- *Versatility*: cater to the needs and abilities of the neophyte and the expert.
- *Rigorous theoretical foundations.*
- *Reliability*: Tested and validated across flows of disparate types.
- *Computationally inexpensive.*
- *Computationally pliable*: Parallelized and sequential execution.
- *Ancillary*: open source; part of a widely used suite.

Eigenspace Perturbation Framework

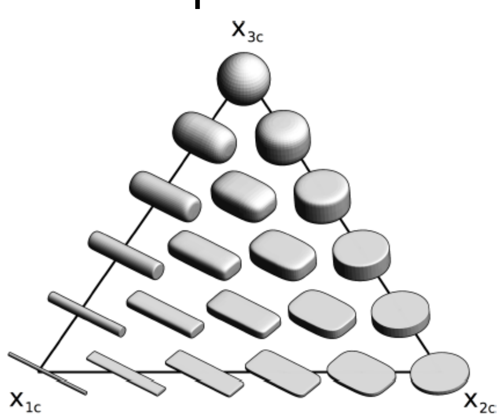
- Introducing perturbations directly into the modeled Reynolds stress:

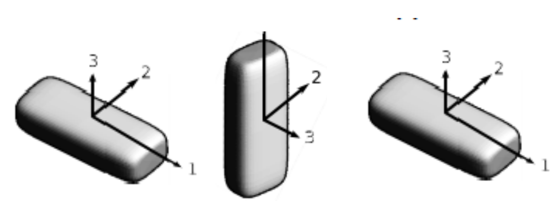
$$R_{ij}^* = 2k^*(\frac{\delta_{ij}}{3} + v_{in}^* \Lambda_{nl}^* v_{lj}^*)$$



- *Theoretical underpinnings*:
  Eigenvalue perturbations → Extremal states of componentiality,
  Eigenvector perturbations→ Extremal states of turbulence production.

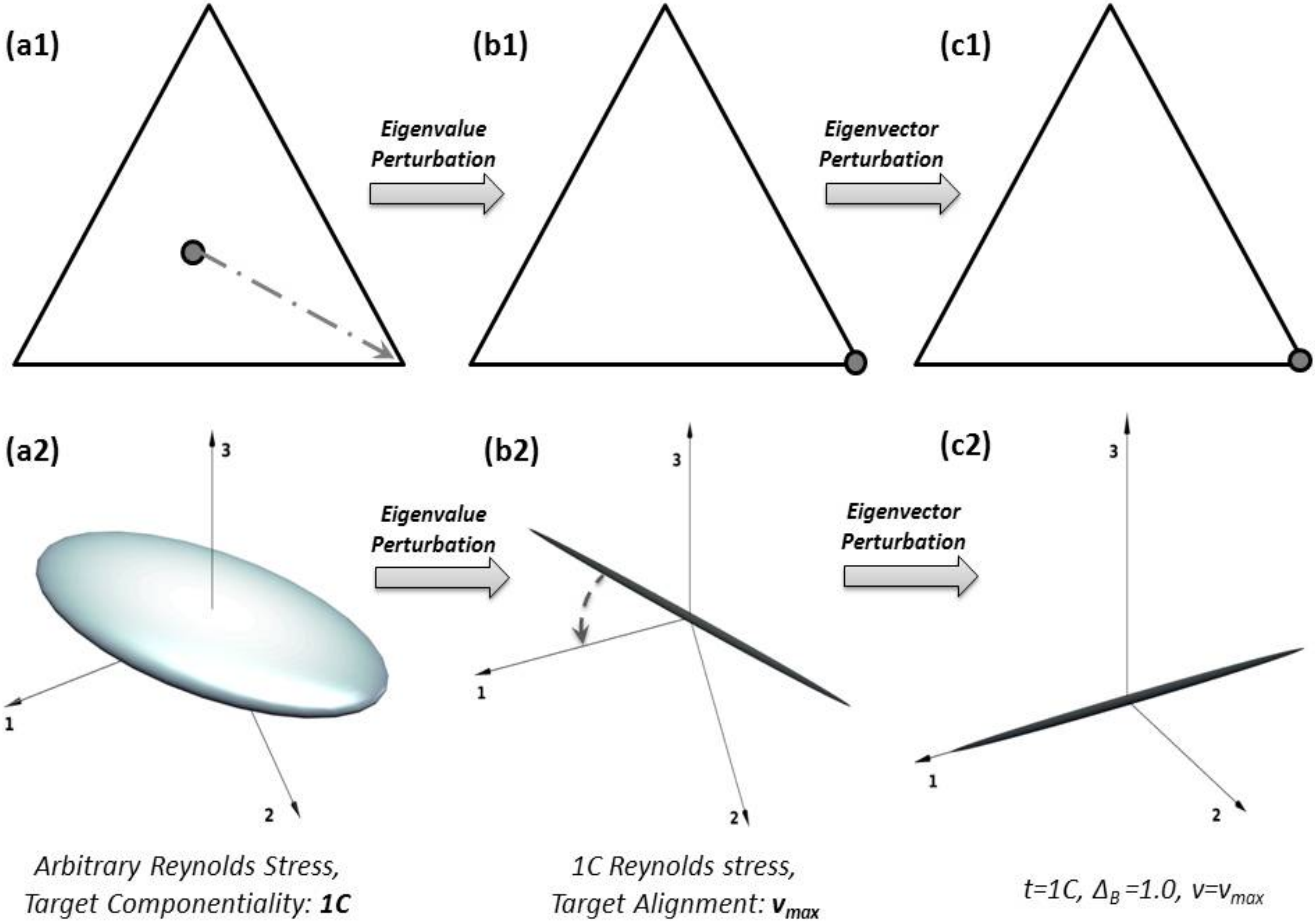
- *Functional utility:*
  Eigenvalue perturbations → Shape of Reynolds stress ellipsoid,
  Eigenvector perturbations→ Alignment of Reynolds stress ellipsoid





Iaccarino, Mishra & Ghili, “Eigenspace perturbations for uncertainty estimation of single-point turbulence closures”, Physical Review Fluids (2017)

Eigenspace Perturbation Framework: Visualization



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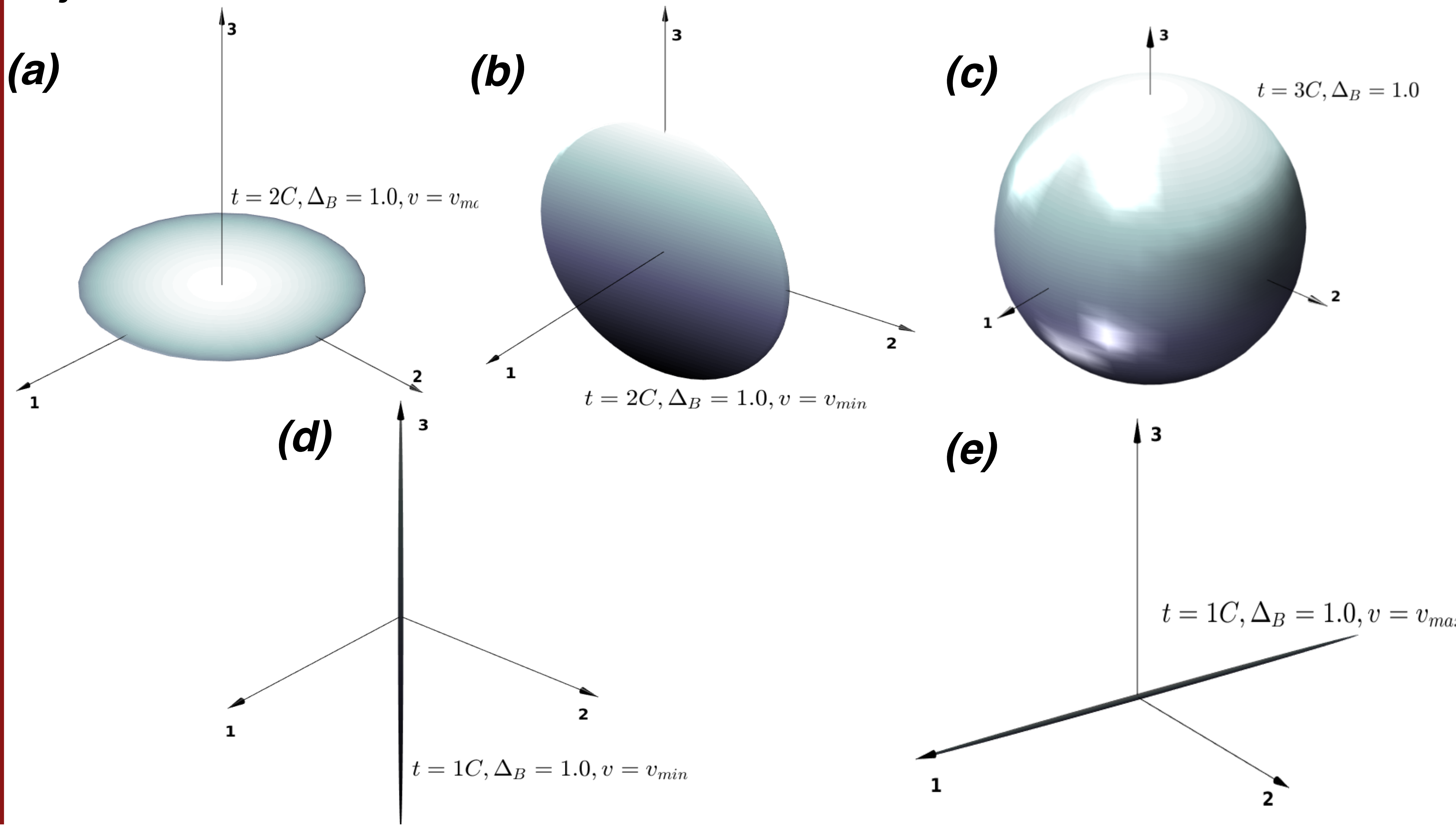
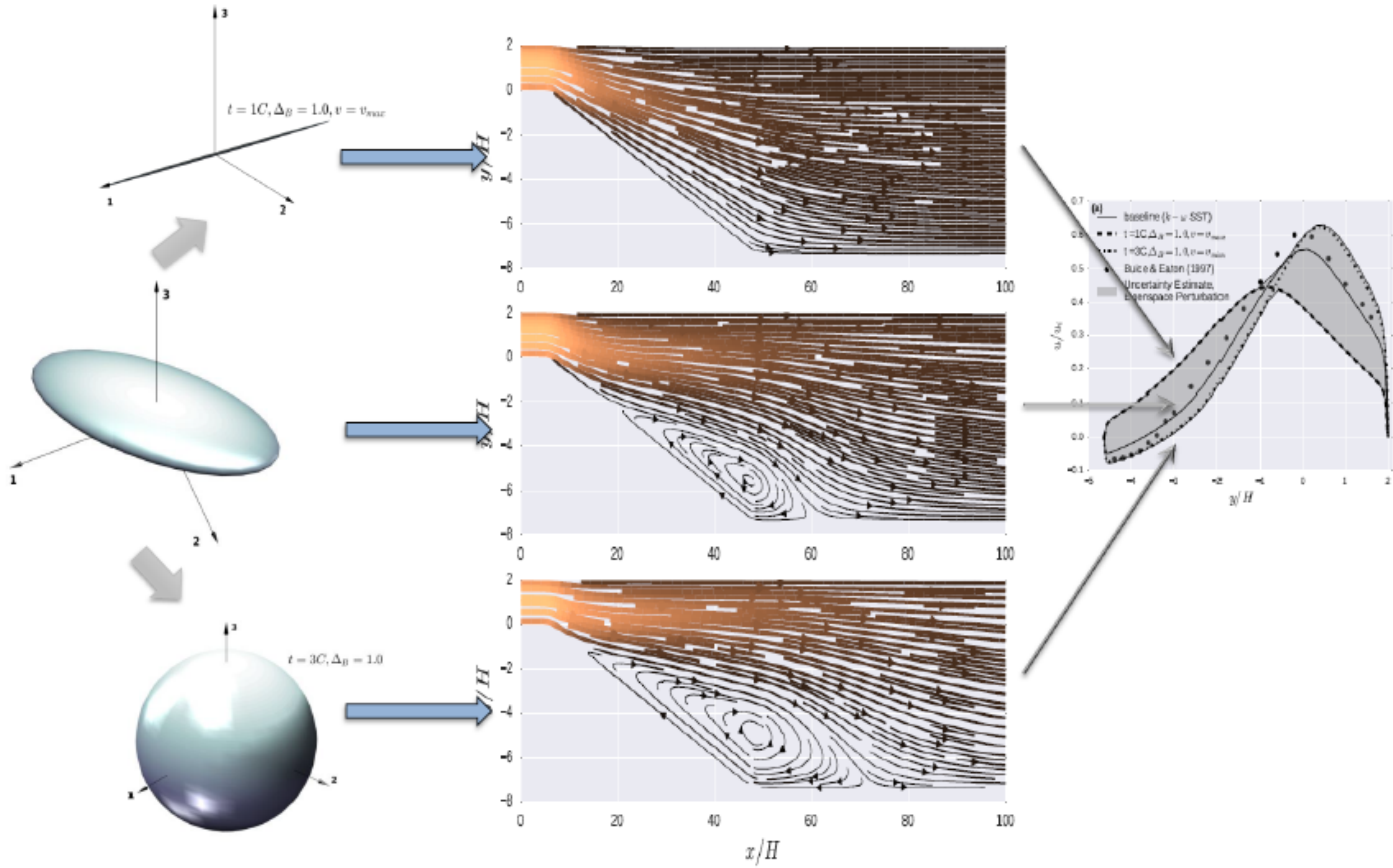
Eigenspace Perturbation Framework: Extremal States

- **3** limiting states of componentiality, **2** extremal eigenvector alignments= **5** RANS simulations for uncertainty bounds.
- Computationally inexpensive: Bounds of engineering utility with just *5 simulations*.



Visual Overview of the Methodology



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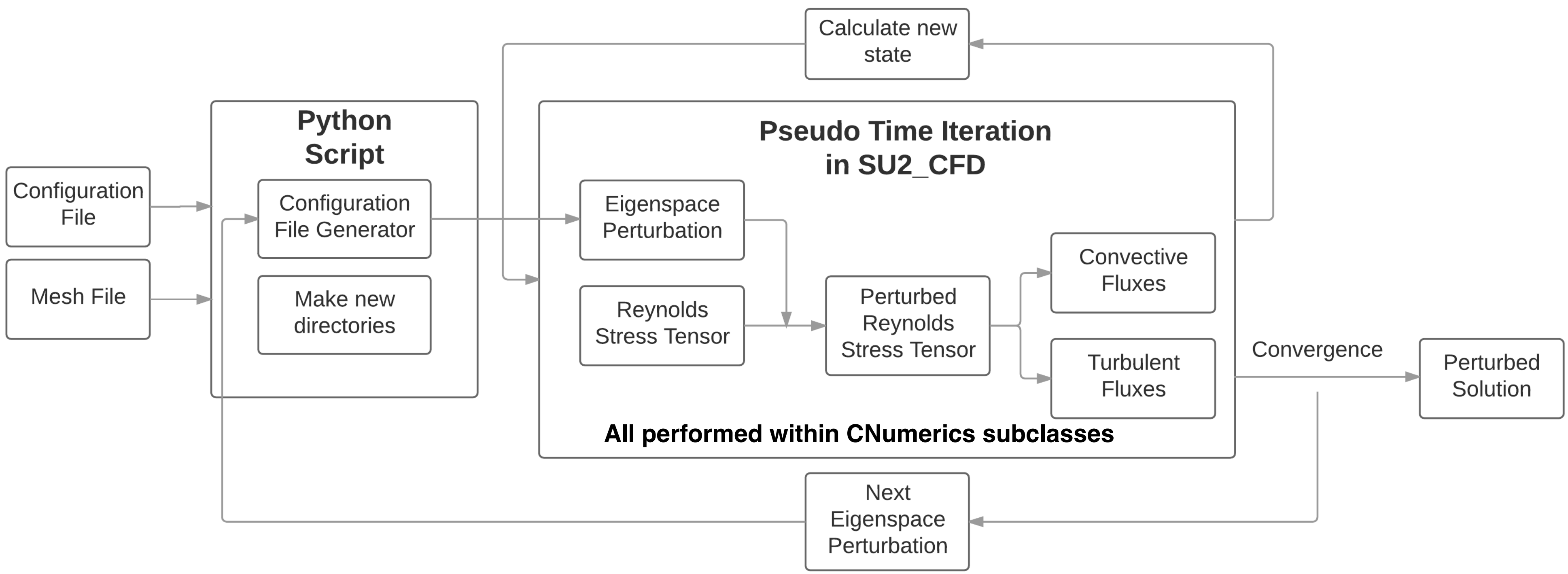
- Mishra & Iaccarino,"RANS predictions for high-speed flows using enveloping models”, *CTR Annual Research Briefs* (2016)

SU2 Implementation

- **Python Script:** Sequentially specifies perturbation to be performed; generates corresponding configuration files and subdirectories for solution files
- **C++ code:** Perturbations are performed during the viscous, and turbulent flux calculations in numerics_direct_mean.cpp and numerics_direct_turbulent.cpp
- For best results, need to have converged the baseline solution with SU2. This same configuration file and mesh file can then be used with the python script

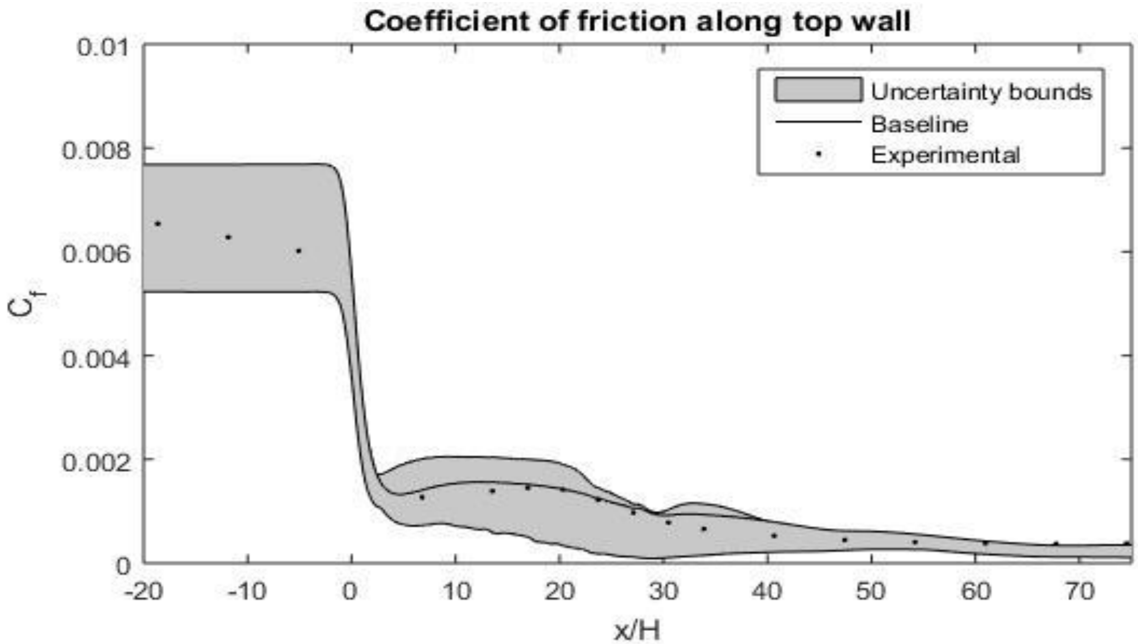


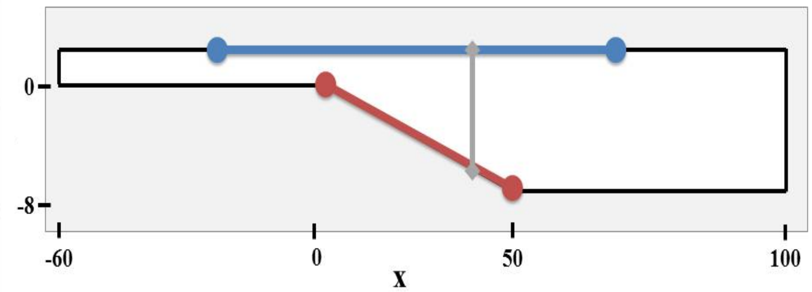
Testing & Validation Cases

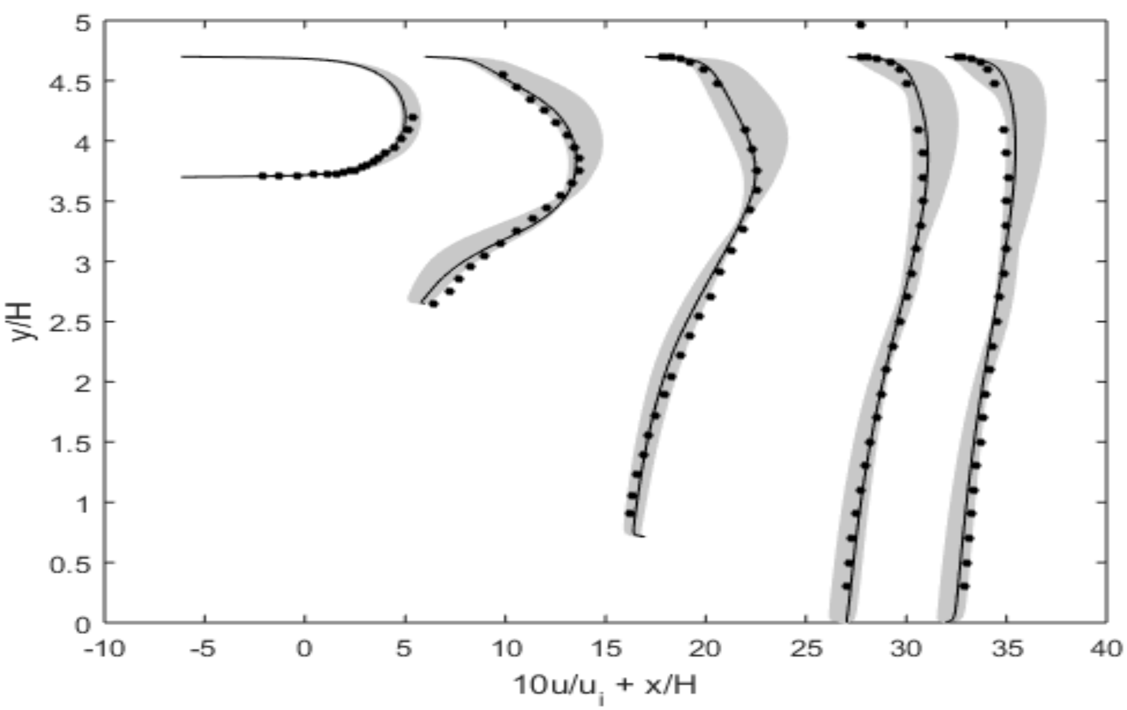
	Case	Rationale	Notes
I.	Turbulent Flow over a backward-facing step	Benchmark flow	2D Steady Simulation
II.	Flow through an asymmetric diffuser	Benchmark flow	2D Steady Simulation
III.	Jet efflux of the NASA Acoustic Response Nozzle	Engineering case	3D subsonic flow
IV.	Heated jet efflux via a convergent divergent Seiner nozzle	Engineering case	3D supersonic flow
V.	NACA 0012 airfoil at different angles of attack	Engineering case	Range of 3D simulations with separation & stall.
VI.	30P30N, Multi-element Airfoil	Engineering case	3D, subsonic, compressible simulation.

- Default settings of parameters adopted for results.
- k-ω SST turbulence model used for all simulations.

Flow in an Asymmetric Diffuser

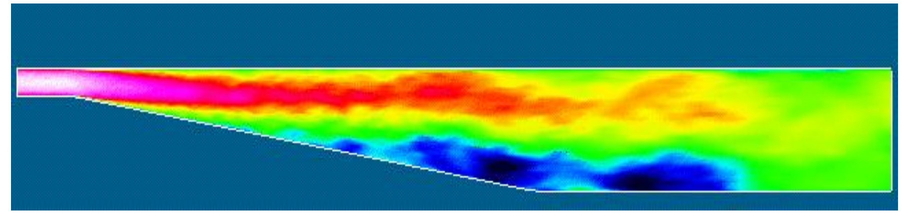


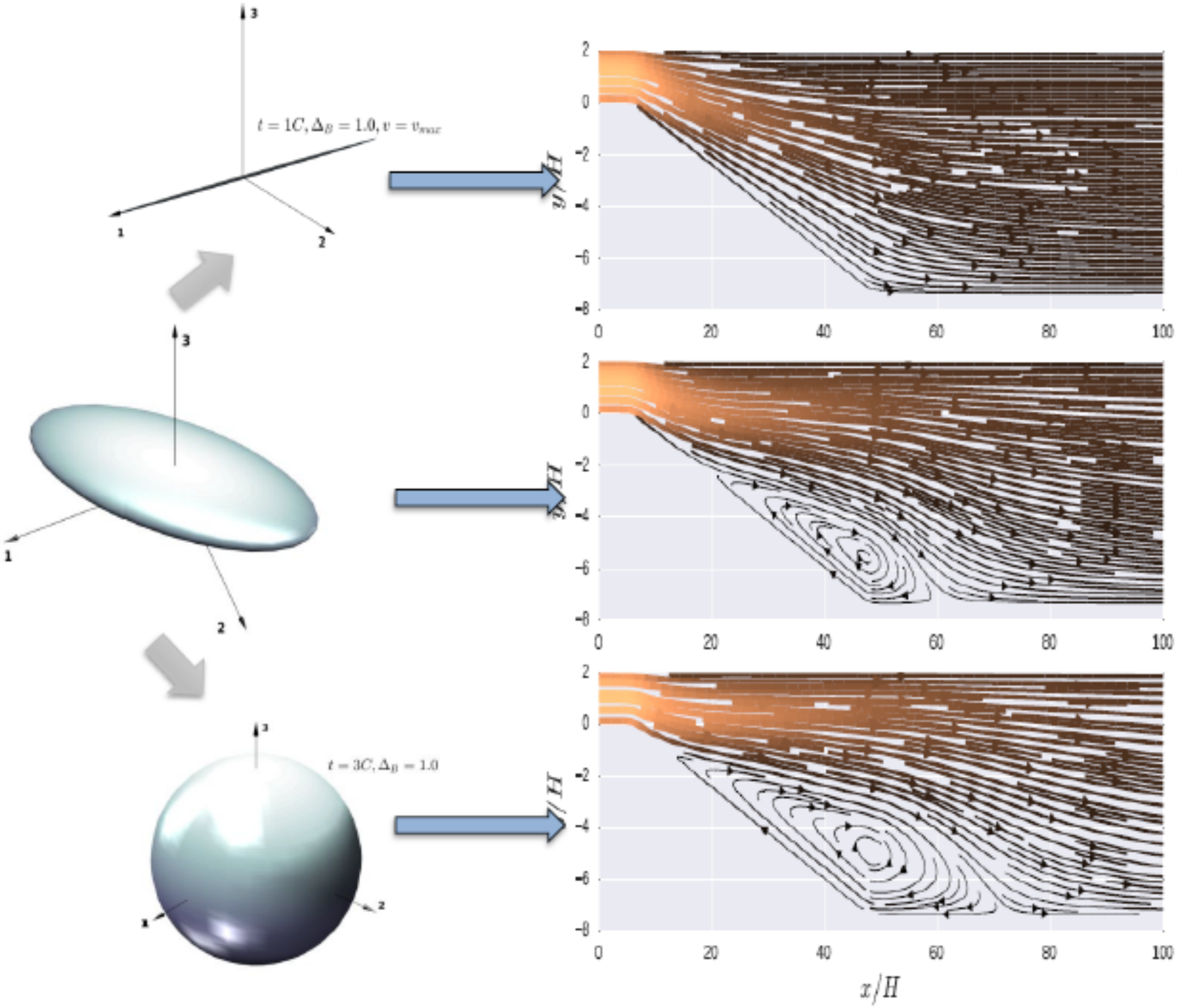




Take Home:
Uncertainty bounds account for RANS discrepancy, Experimental measurements enveloped by bounds.

Flow in an Asymmetric Diffuser: Visualization



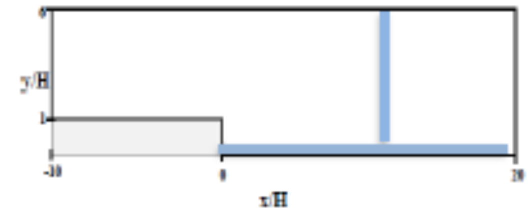


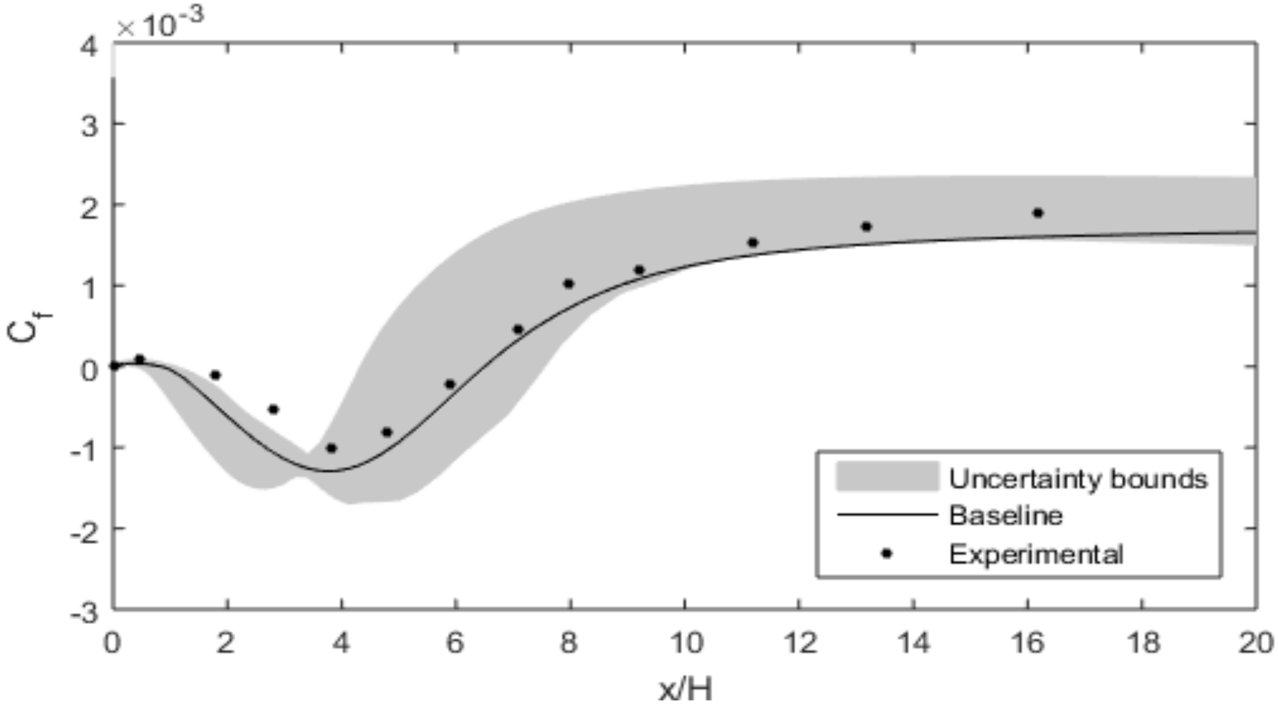
Perturbations correlate to physics

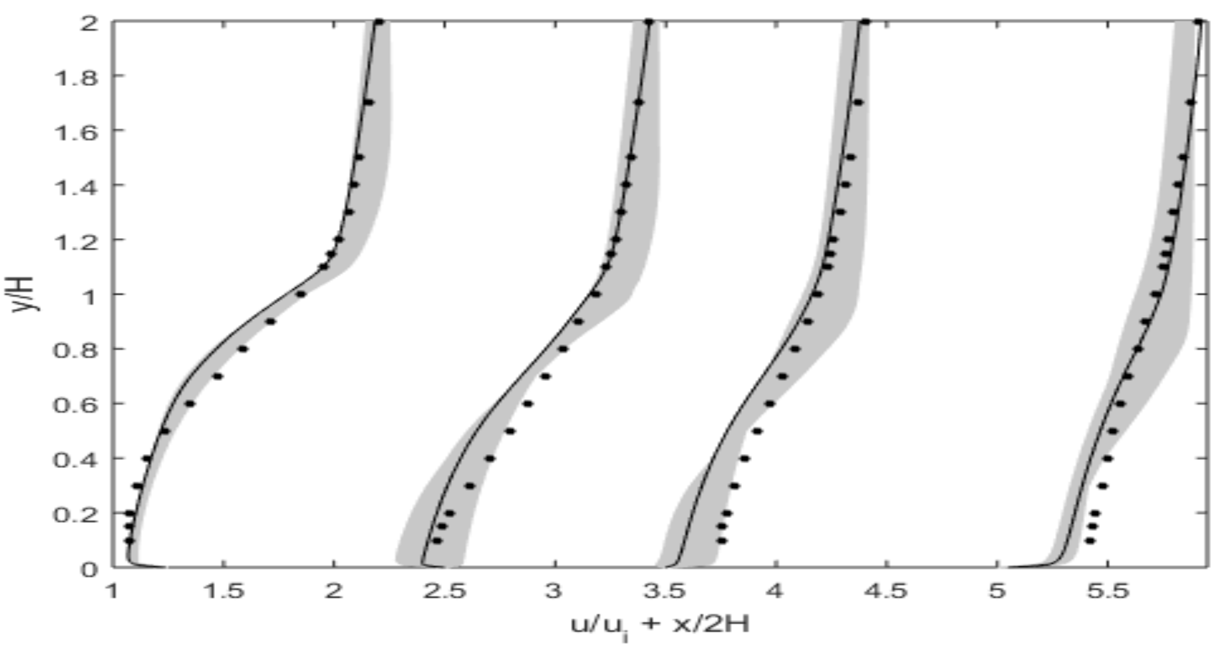
Maximize turbulence production:
Suppress flow separation

Minimize turbulence production:
Increase flow separation

Flow over a Backward-Facing Step



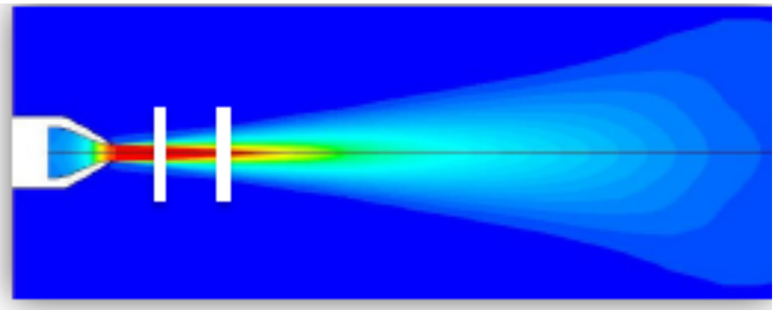


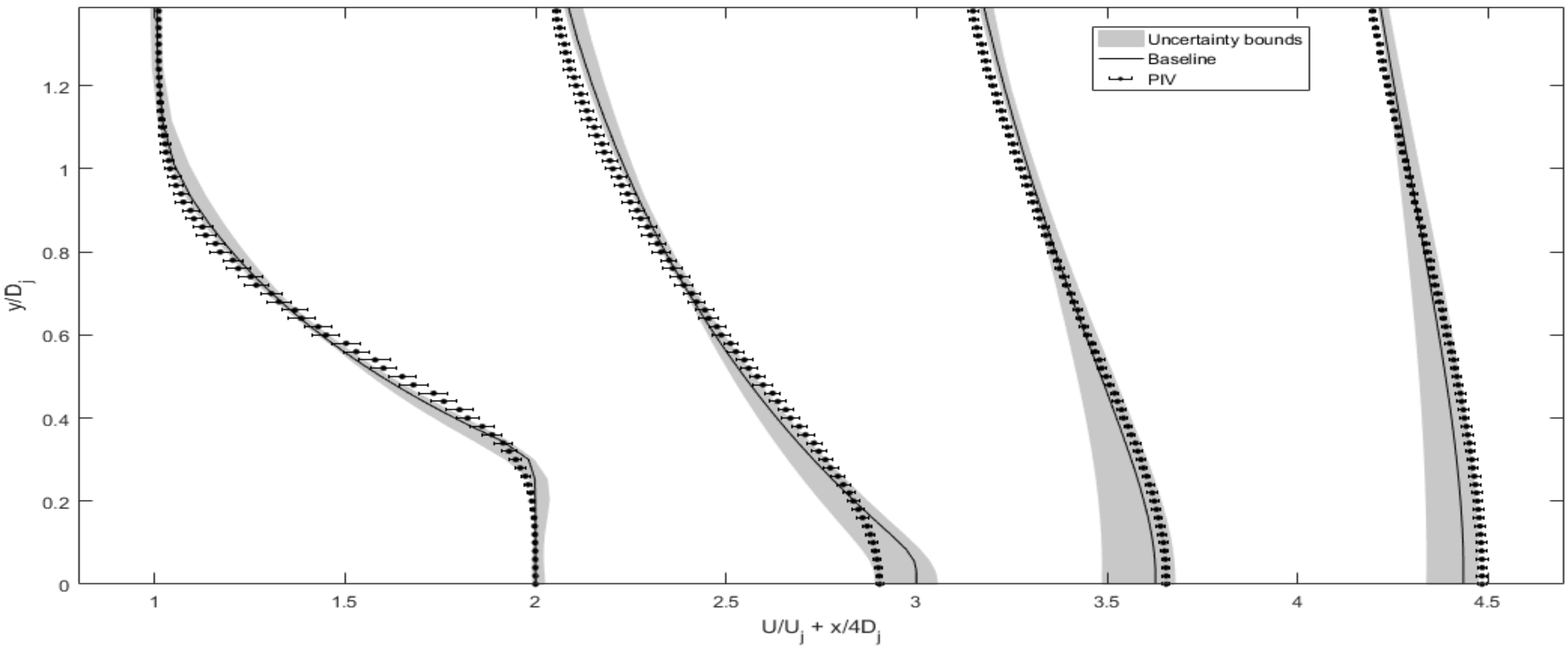


Take-home message:
Uncertainty bounds account for significant proportion of RANS discrepancy

Most Experimental measurements enveloped by bounds.

Jet Efflux of the NASA ARN



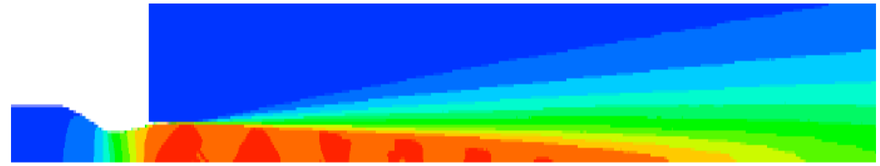


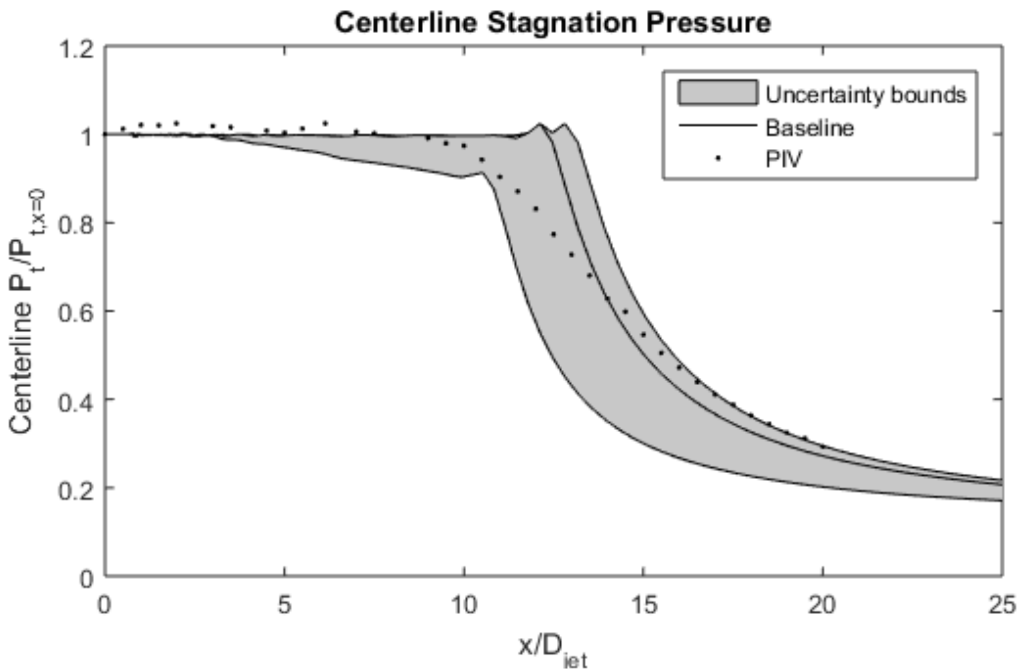
Take-home message:

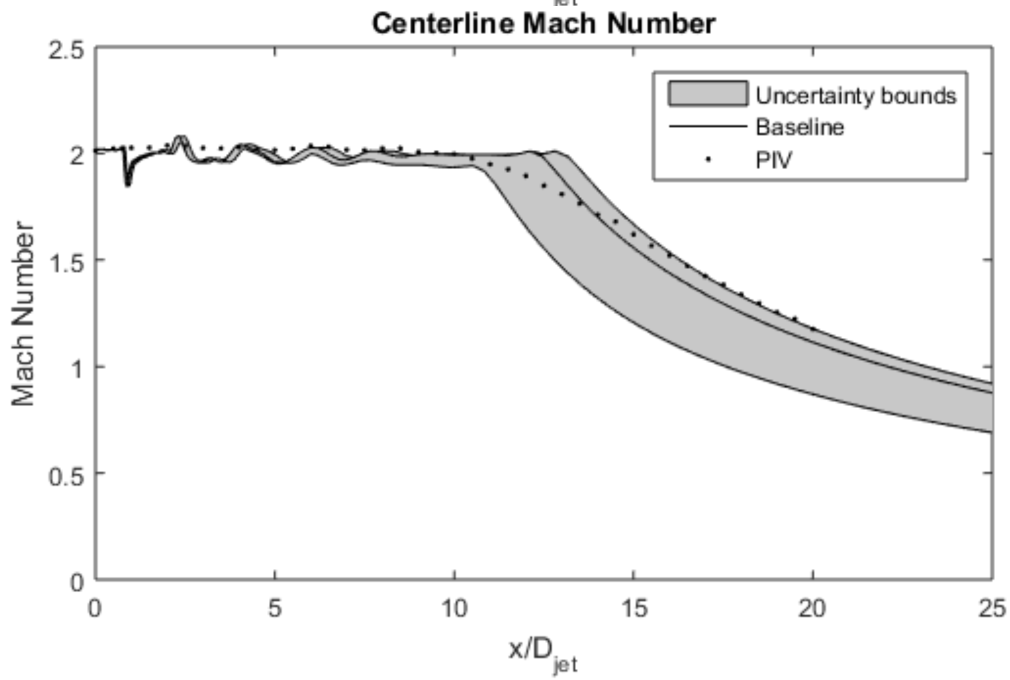
Uncertainty Bounds mimic discrepancy between PIV data and RANS predictions. Methodology may account for missing physics.

- Mishra & Iaccarino,"Uncertainty Estimation for Reynolds-Averaged Navier–Stokes Predictions of High-Speed Aircraft Nozzle Jets." *AIAA Journal* (2017)

Jet Efflux of the Seiner Supersonic Nozzle

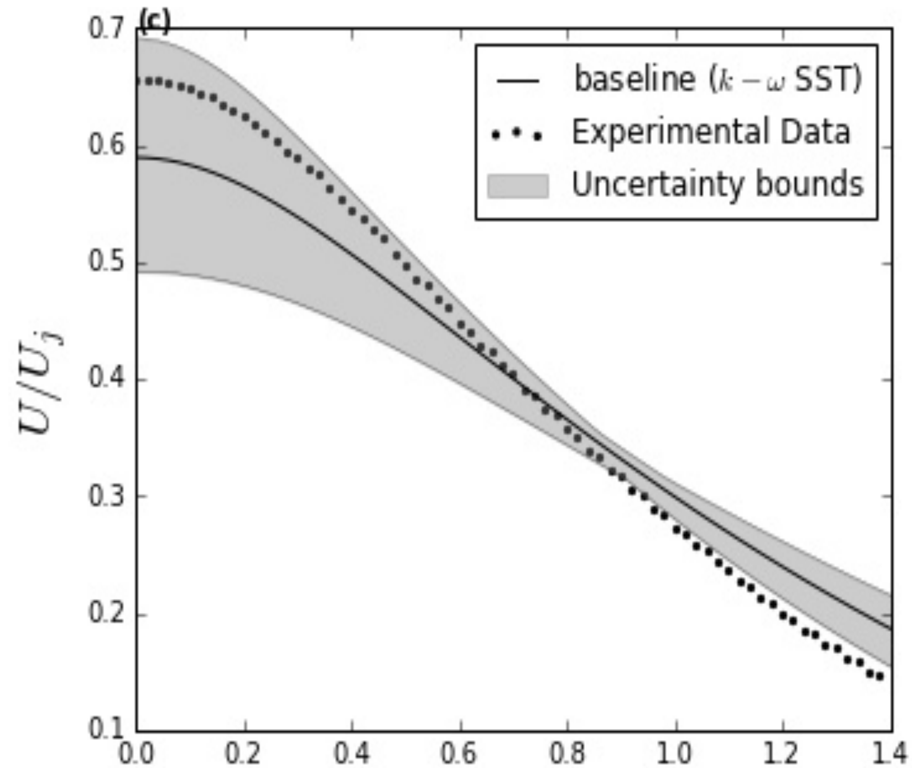




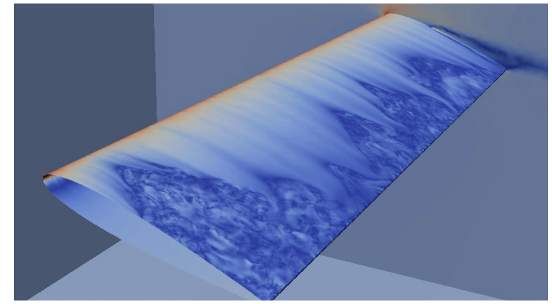


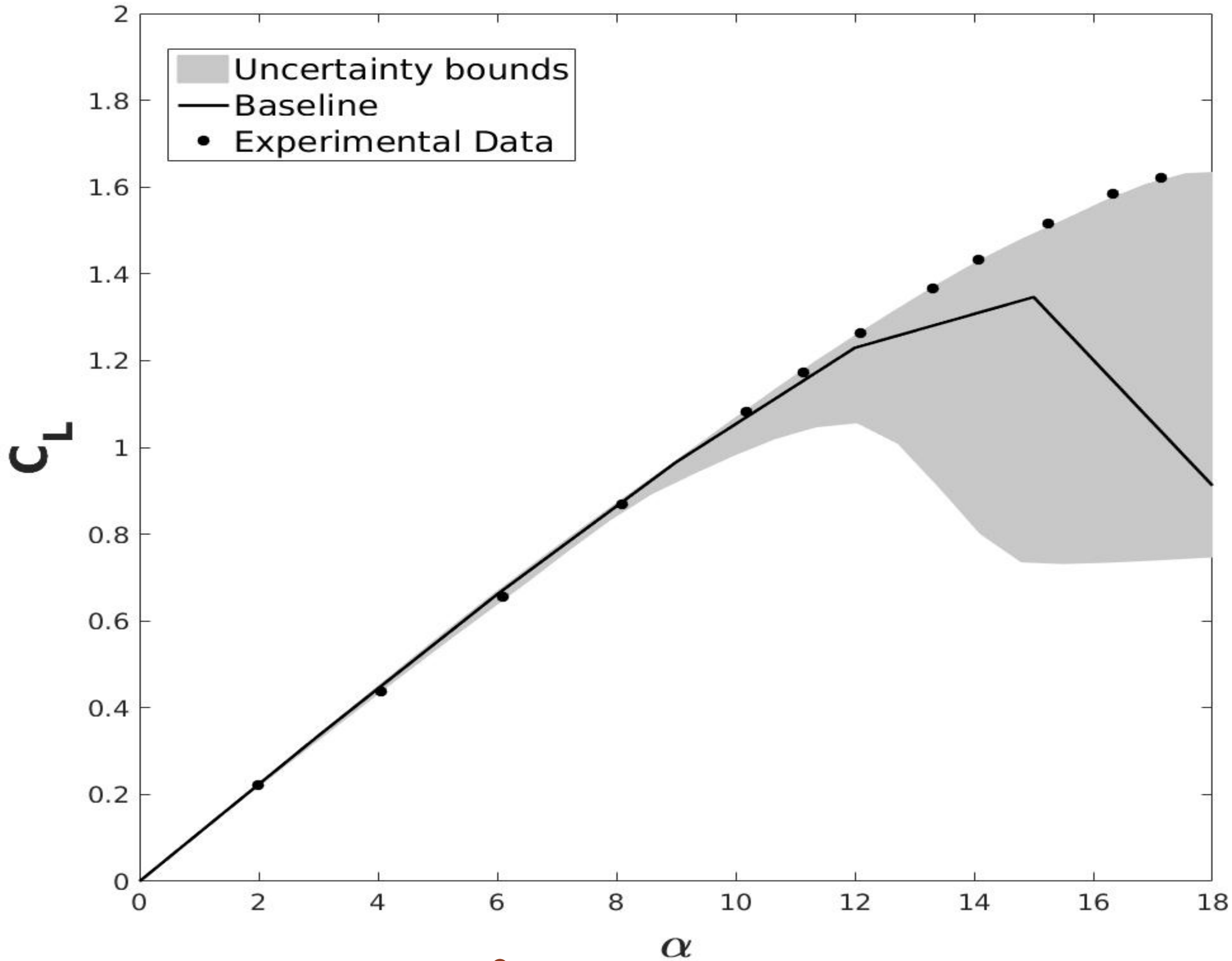
Take-home message:
Uncertainty bounds account for RANS discrepancy in Velocity and Pressure

Experimental measurements enveloped by bounds.



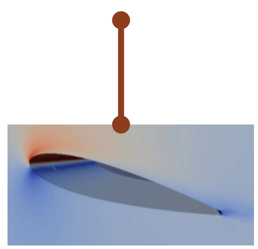
Flow over a NACA 0012 Airfoil

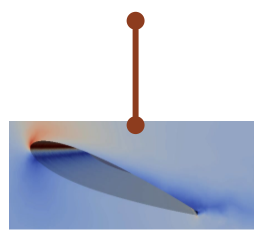


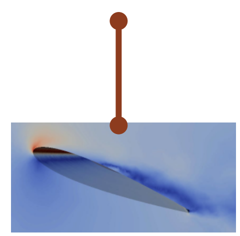


Take-home message:
Uncertainty bounds account for RANS discrepancy, especially near stall

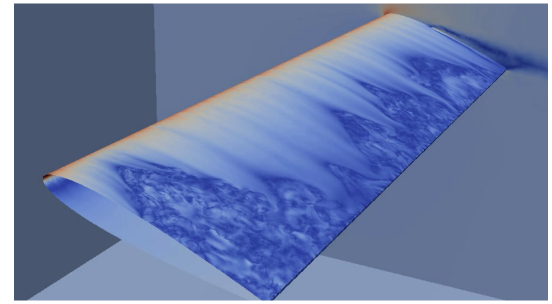
Experimental measurements enveloped by bounds.

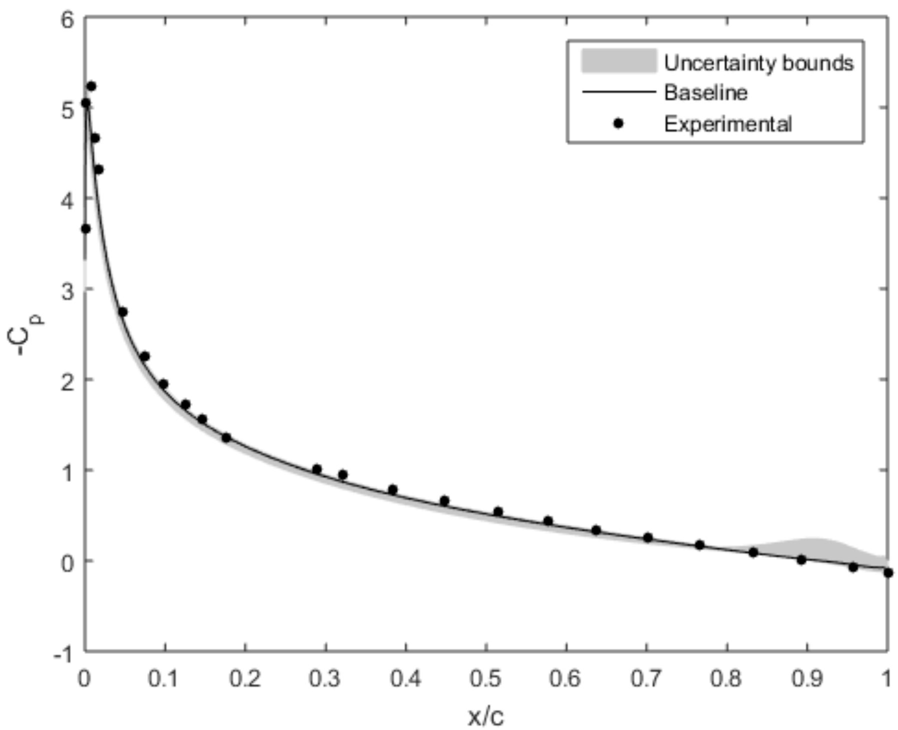


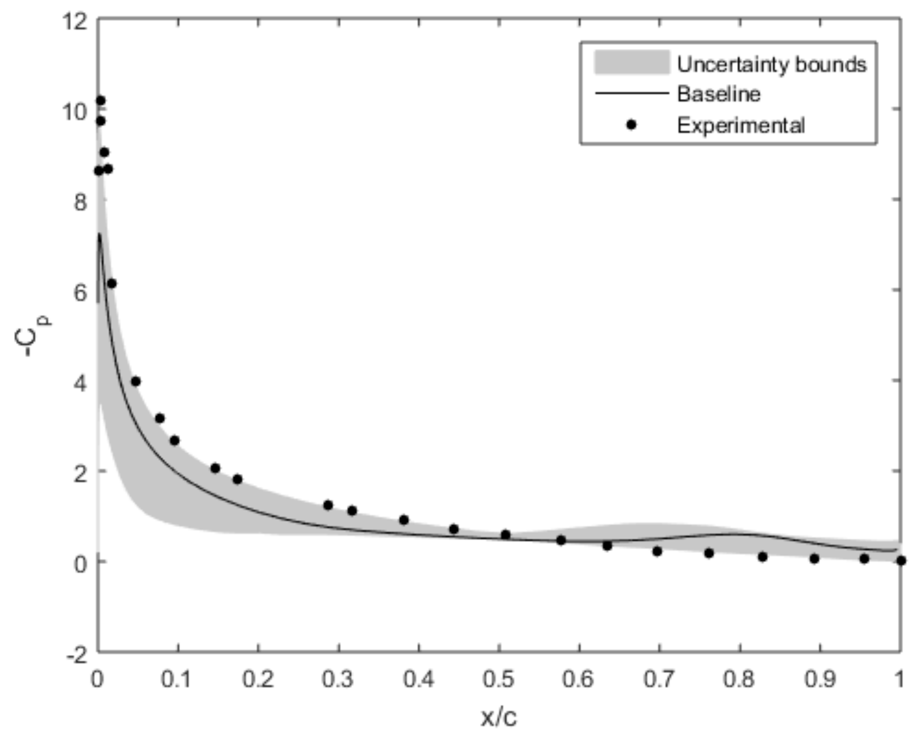




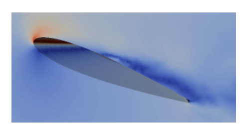
Flow over a NACA 0012 Airfoil





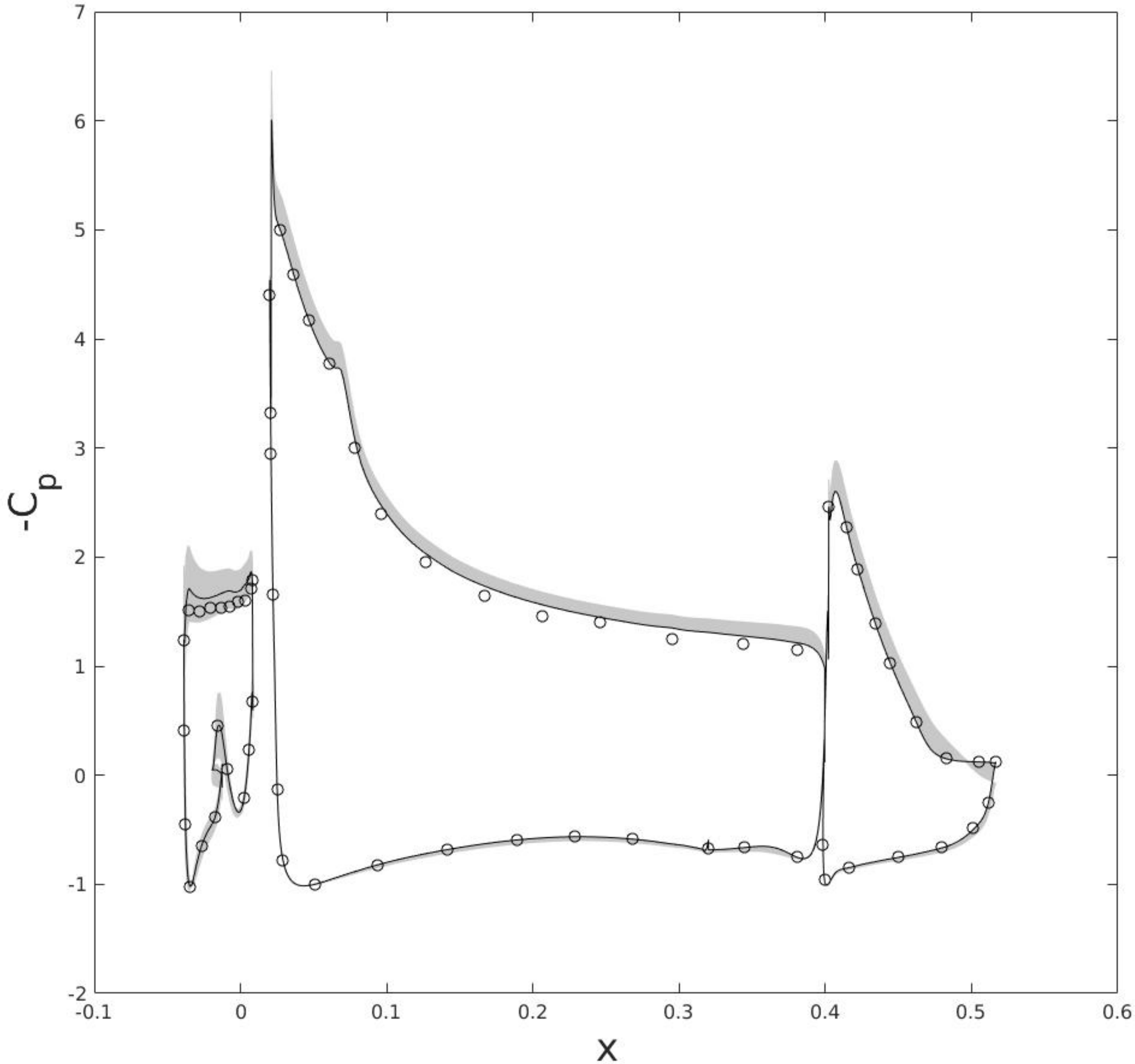


Angle of Attack: 10
Low discrepancy
Negligible uncertainty bounds



Angle of Attack: 15
Significant discrepancy
Substantial uncertainty bounds

Flow over a Multi-Element Airfoil



Test for false positives:
If RANS predictions are accurate, then Uncertainty bounds should ideally be negligible.

Summary & Next Steps

- Epistemic uncertainty quantification module for SU2 focusing on uncertainties from turbulence models.
- Usable by both experts and non-experts.
- Based on rigorous mathematical theory. Extensively tested. Reliable.
- Computationally inexpensive and parallelized.
- EQUiPS production branch release: early 2018

Acknowledgement: This research was funded by DARPA under the EQUiPS project (technical monitor: Dr Fariba Faroo).

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Questions

Questions & requests for pre-print of the SU2 UQ module article:

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