Uncertainty Estimation of Turbulence Model Predictions in SU2

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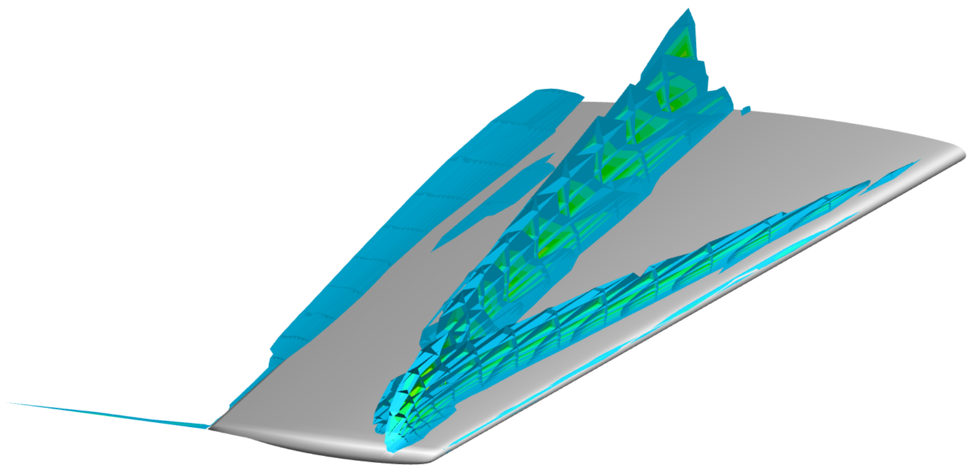


SU2 Developers Meeting 2018
Glasgow, UK
September 14th, 2018

DARPA aerospacedesignlab SU2 The Open-Source CFD Code

Stanford University

Outline

I. *Overview of turbulence modeling & challenges*

II. *Motivation & Objectives*

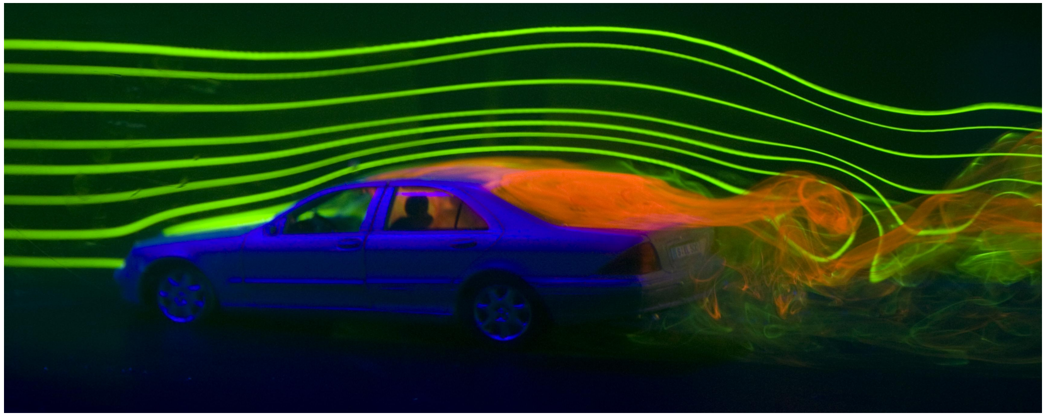
III. *Mathematical and computational details*

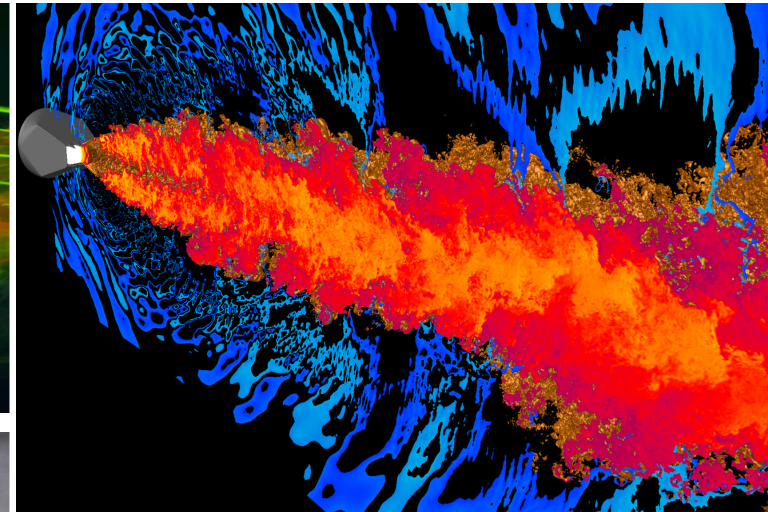
IV. *Implementation in SU2*

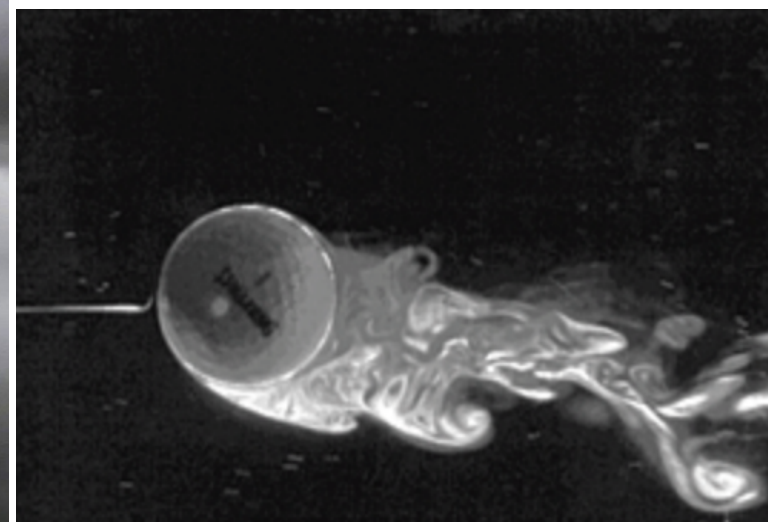
V. *Testing and validation*

VI. *Summary & Conclusions*

Turbulent Flows

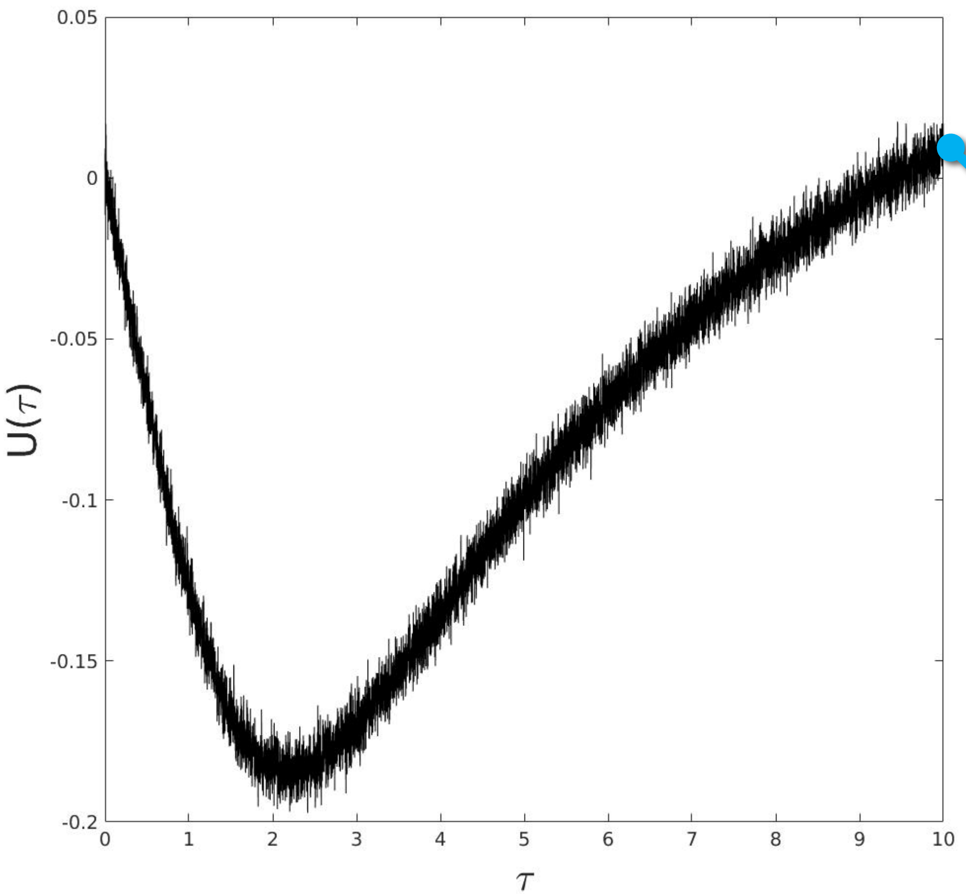


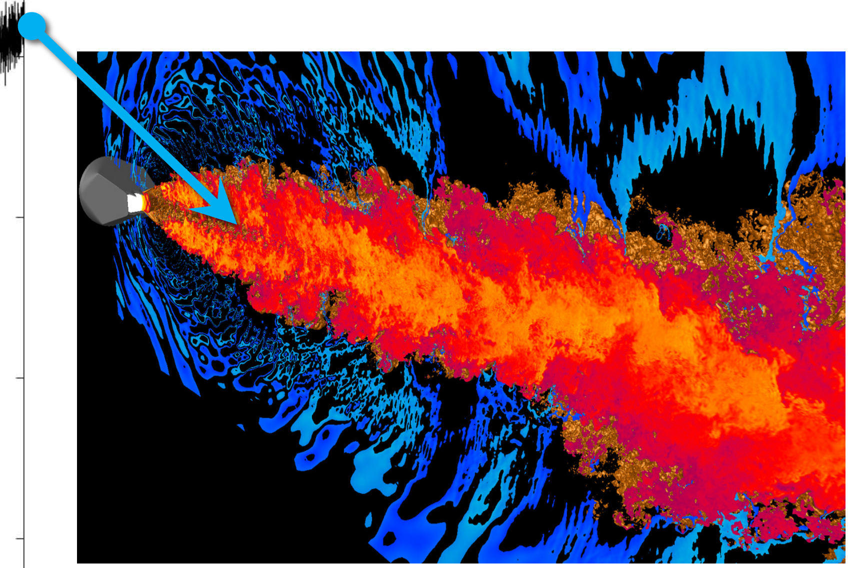




“Turbulence is the rule, not the exception, in complex engineering systems”
P. Moin, Scientific American (1997)

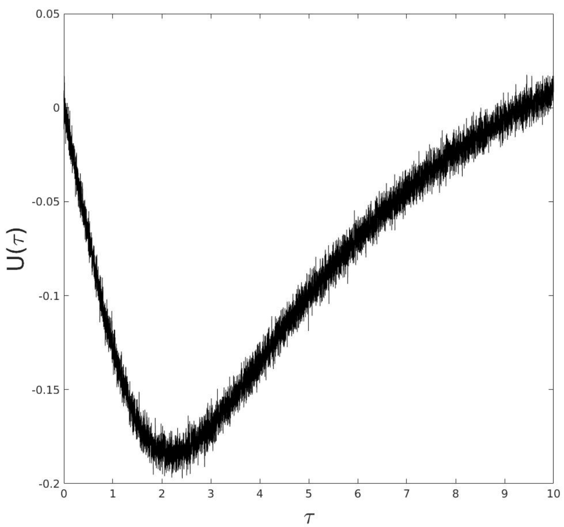
Turbulent Flows

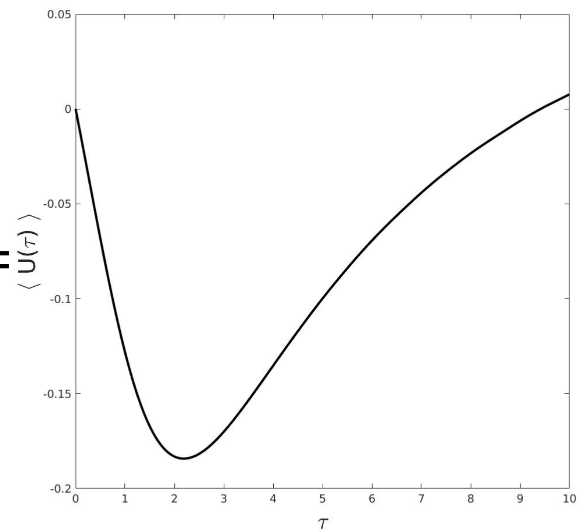


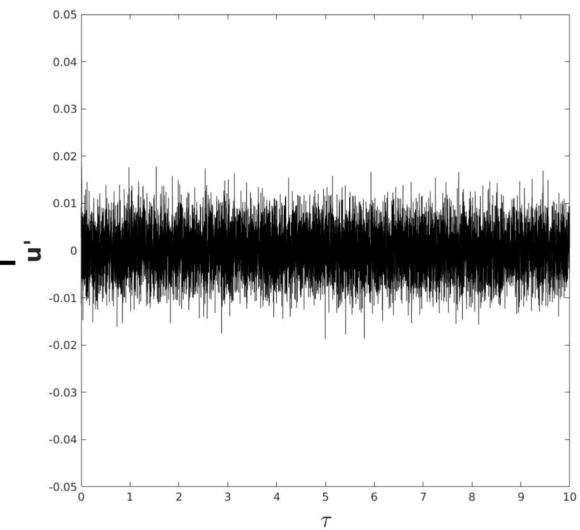


- Irregular, small scale fluctuations in velocity and pressure.
- Increased dissipation, diffusivity, mixing of momentum, species.
- Increased drag, reduced lift.
- Loss of predictability.

Mathematical Approach: Reynolds's Decomposition



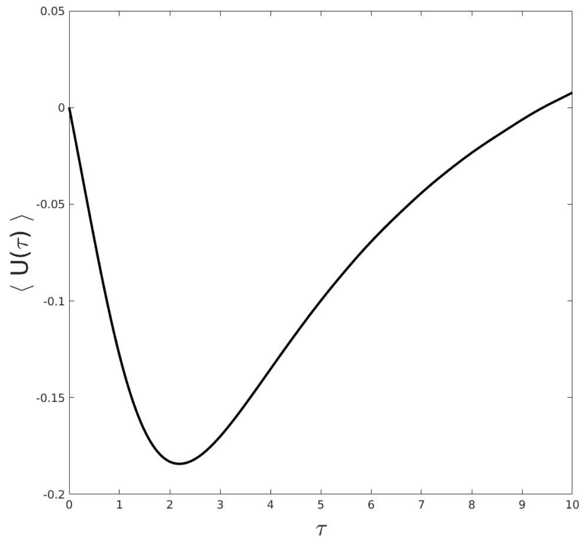




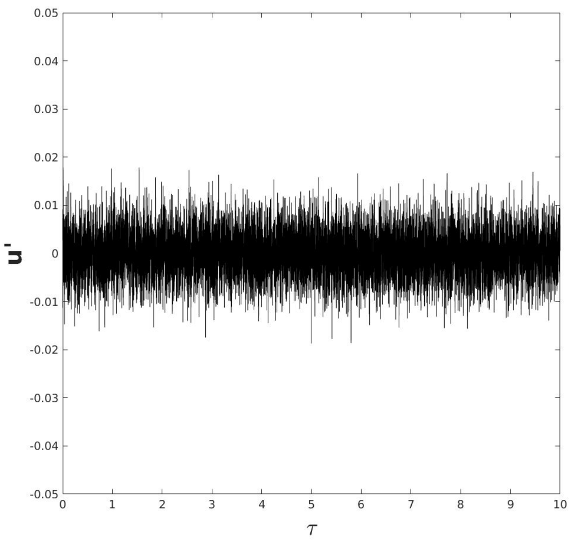
Instantaneous velocity = Mean velocity + Fluctuating velocity

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

$$\frac{\partial}{\partial t}(\rho \bar{u}_j) + \frac{\partial}{\partial x_j}\left(\rho \bar{u}_i \bar{u}_j + p\delta_{ij} - \tau_{ij} + \boxed{\rho \overline{u_i' u_j'}}\right) = 0$$

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

Eddy Viscosity Based Models

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

- Simplifications and assumptions used in formulation.

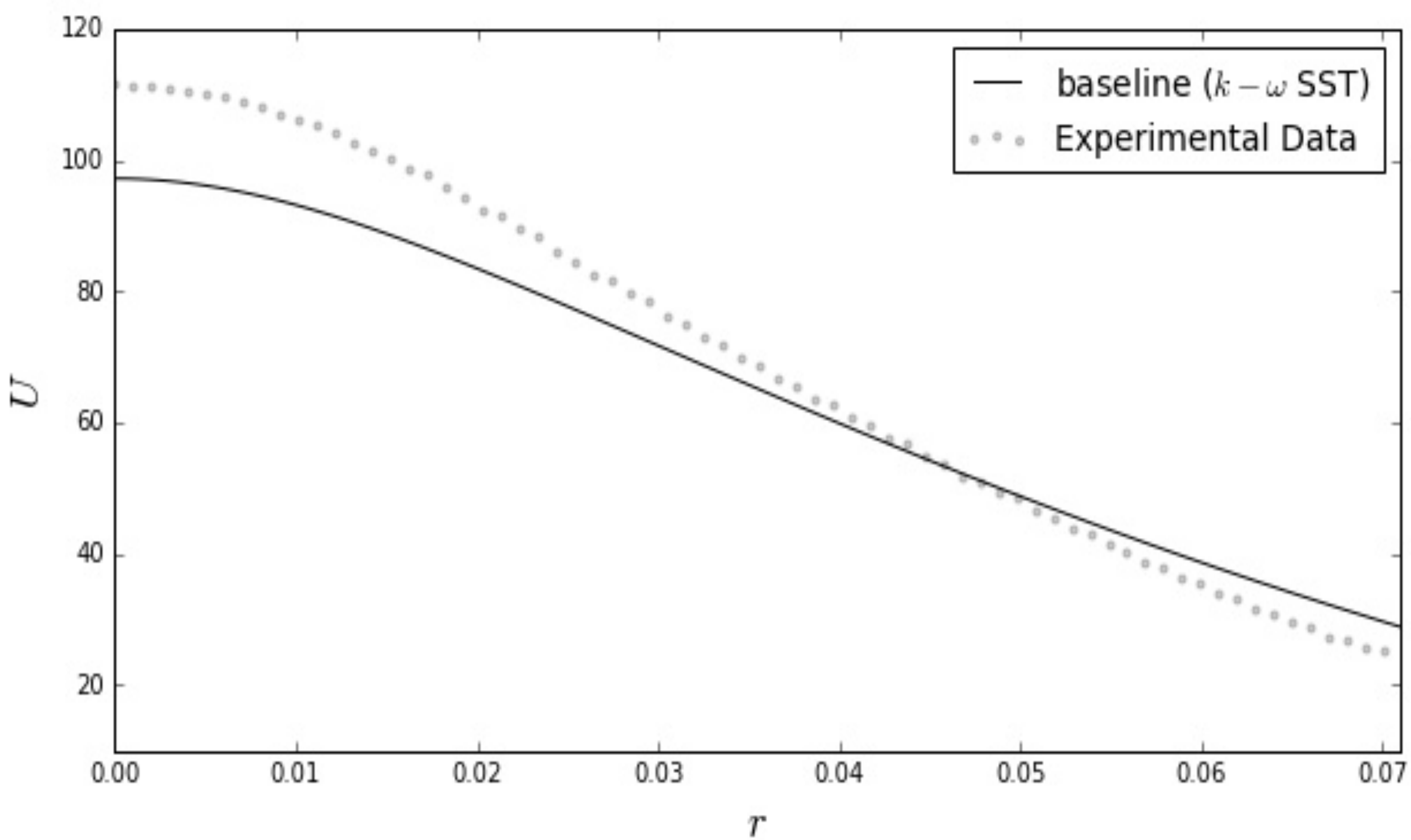
  Eddy viscosity hypothesis: $R_{ij} = \frac{2}{3} k \delta_{ij} - 2\nu_T S_{ij}$

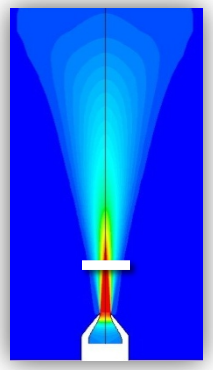
  Gradient Diffusion hypothesis: $T_i = -\frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial x_i}$

  …………………

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

Eddy Viscosity Based Models: Limitations



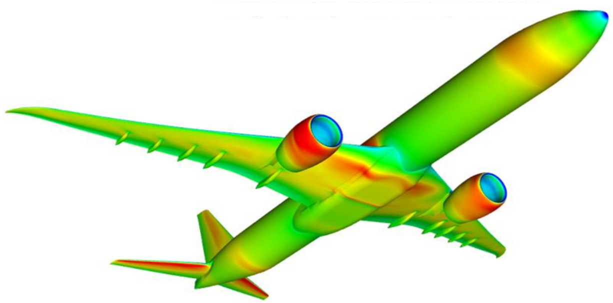


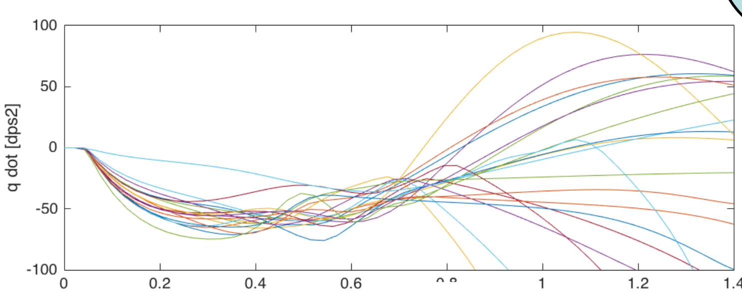
Significant discrepancy in RANS predictions,
Uncertainty in design.

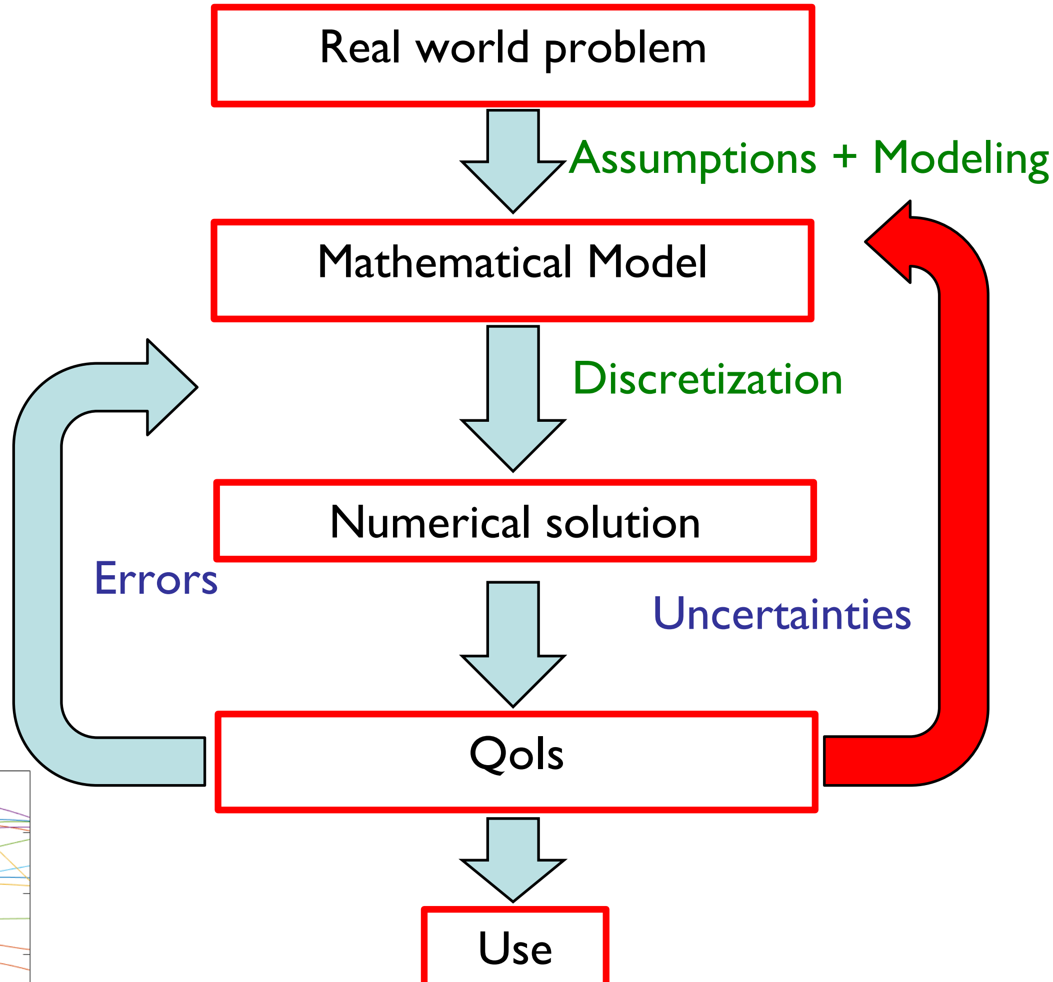
NASA TMR: https://turbmodels.larc.nasa.gov/jetsubsonic_val.html

Predictive Computational Science: V&V and UQ

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla.(\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla.\tau$$



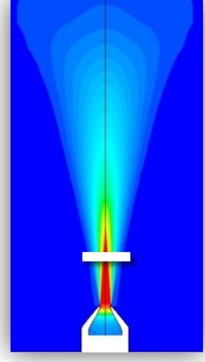


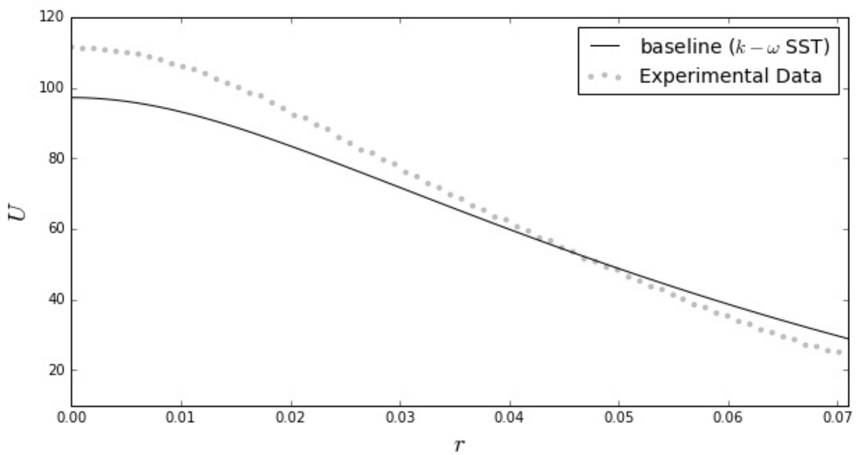


Quantifying discretization errors is a first step to quantify sources of uncertainty.

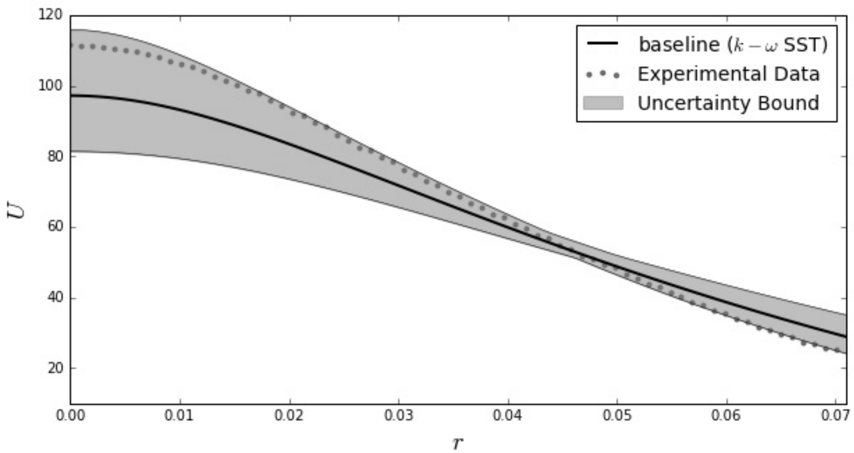
Understanding uncertainties is necessary to achieve certification.

Main Idea:
From Point Predictions to Interval Predictions





Point predictions
Dubious accuracy
Uncertain discrepancy



Interval predictions
Explicit quantification of uncertainty
Aid decisions under uncertainty

Uncertainty intervals must encompass experimental data!

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…until now!

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

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

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

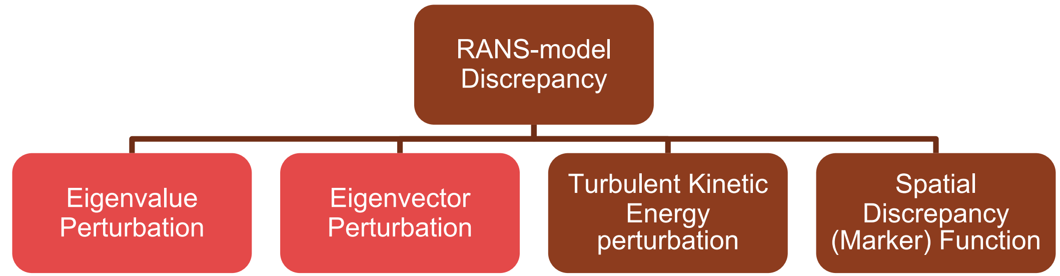
Intended Features

- *Versatility*: cater to the needs and abilities of beginners and experts.
- *Rigorous theoretical foundations.*
- *Reliability*: Tested and validated across flows of disparate types.
- *Computationally inexpensive:* only 5 additional RANS solutions.
- *Computationally flexibility*: Parallelized or sequential execution.
- *Ancillary*: open source; part of a widely used suite.

Eigenspace Perturbation Framework

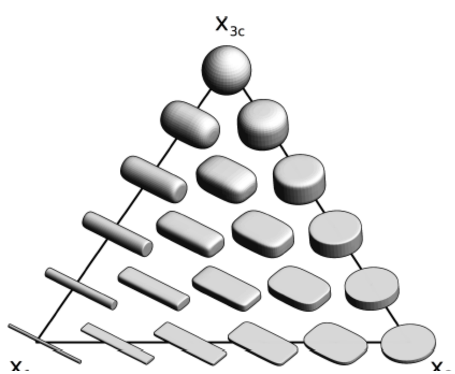
- Introducing perturbations directly into the modeled Reynolds stress:

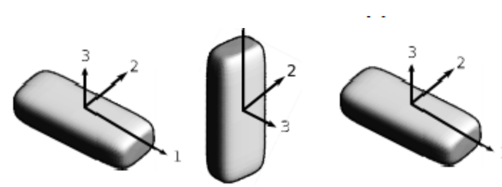
$$R^*_{ij} = 2k^*(\frac{\delta_{ij}}{3} + v^*_{in}\Lambda^*_{nl}v^*_{lj})$$



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

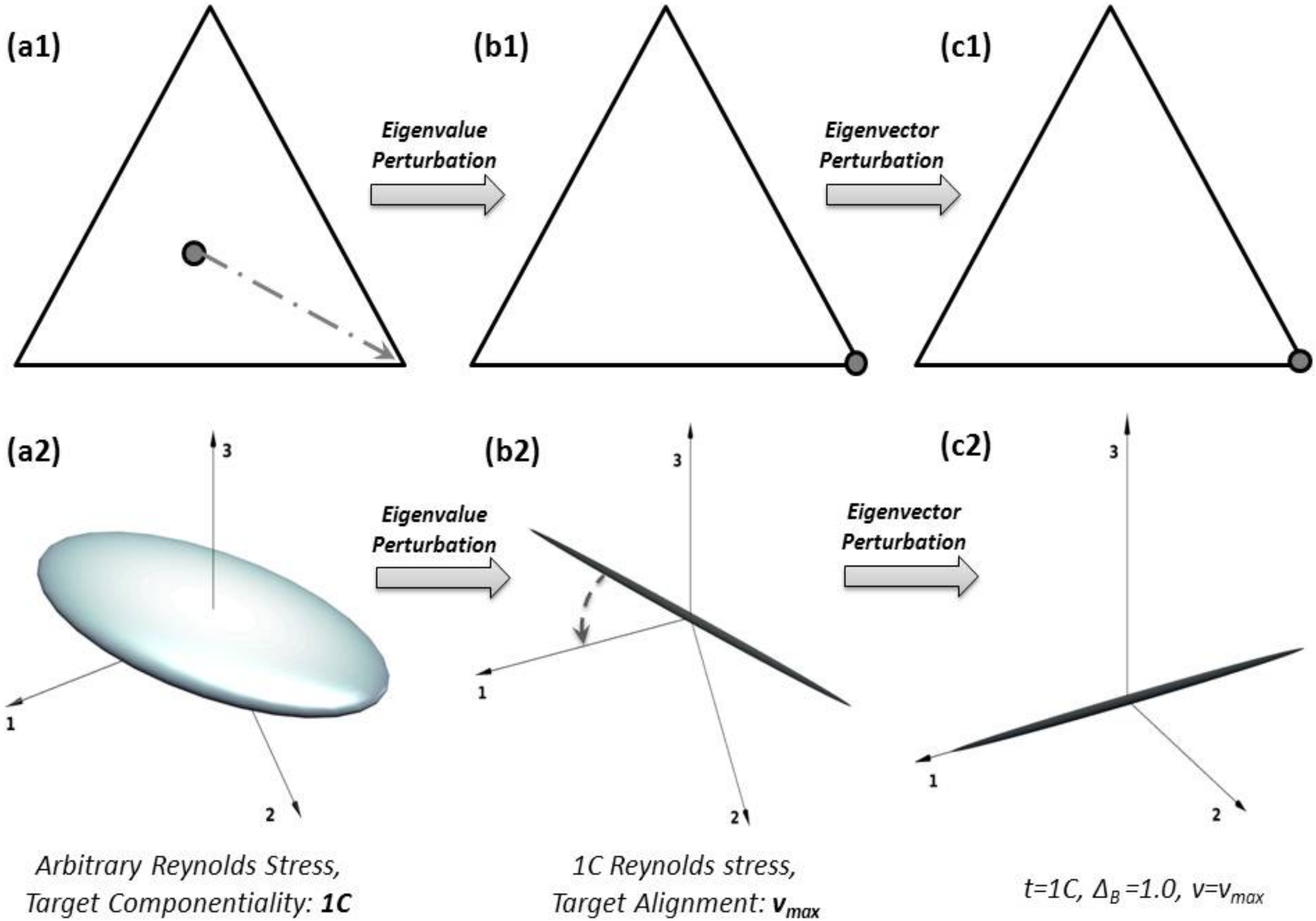
- *Functional utility:*
  Eigenvalue perturbations → Shape of Reynolds stress ellipsoid,
  Eigenvector perturbations→ Alignment of Reynolds stress ellipsoid





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

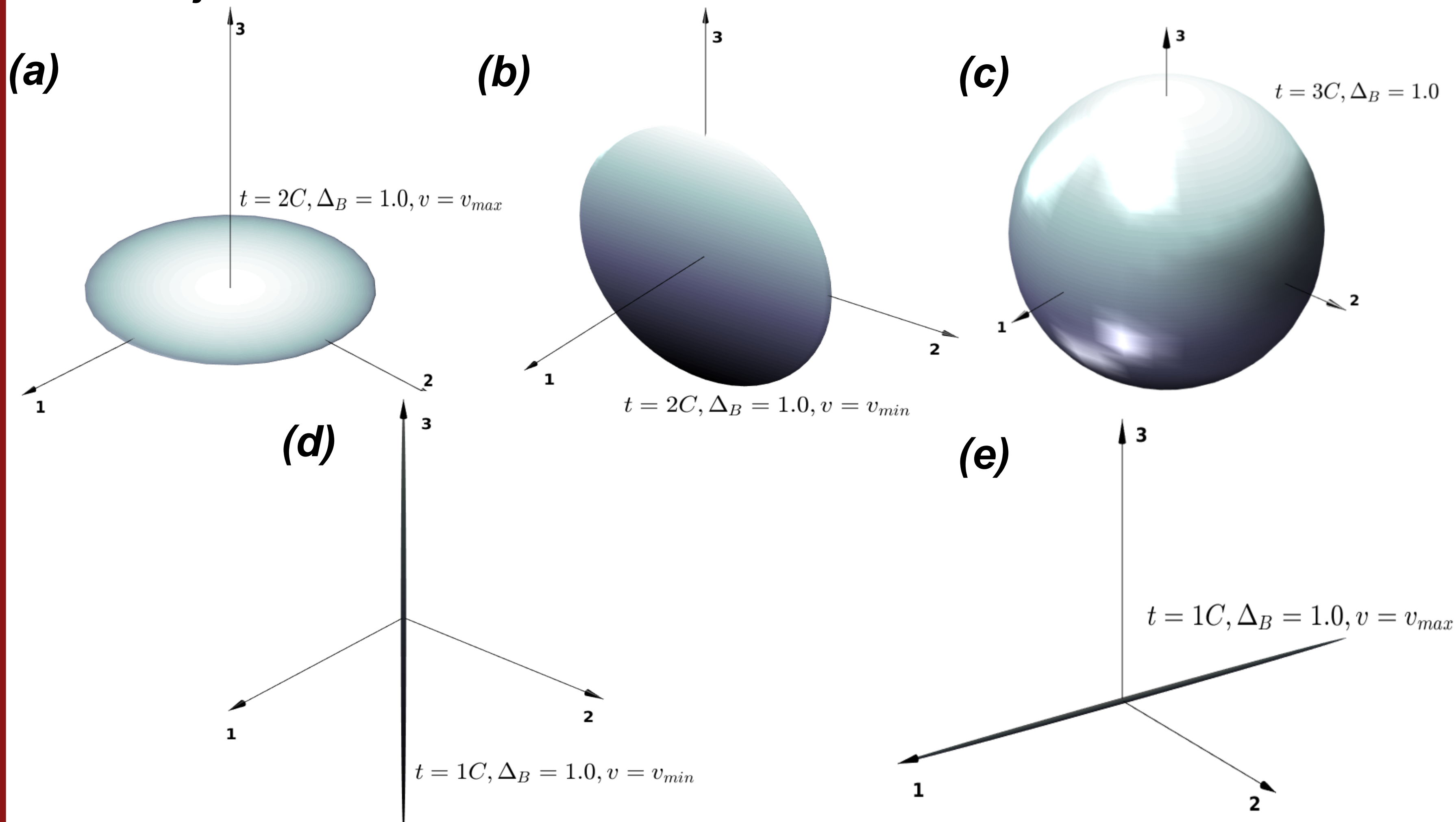
Eigenspace Perturbation Framework: Visualization



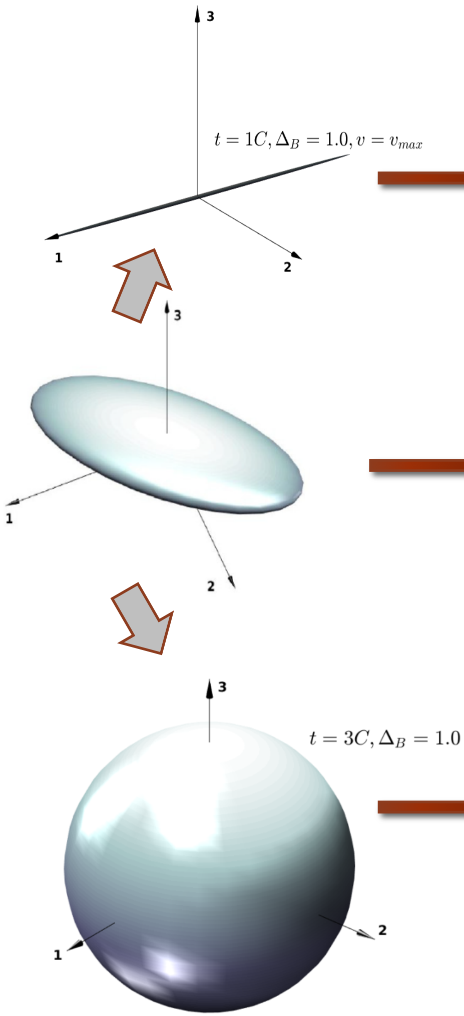
Mishra & Iaccarino,"Uncertainty Estimation for Reynolds-Averaged Navier–Stokes Predictions of High-Speed Aircraft Nozzle Jets." *AIAA Journal* (2017)
Iaccarino, Mishra & Ghili, “Eigenspace perturbations for uncertainty estimation of single-point turbulence closures”, *Physical Review Fluids* (2017)

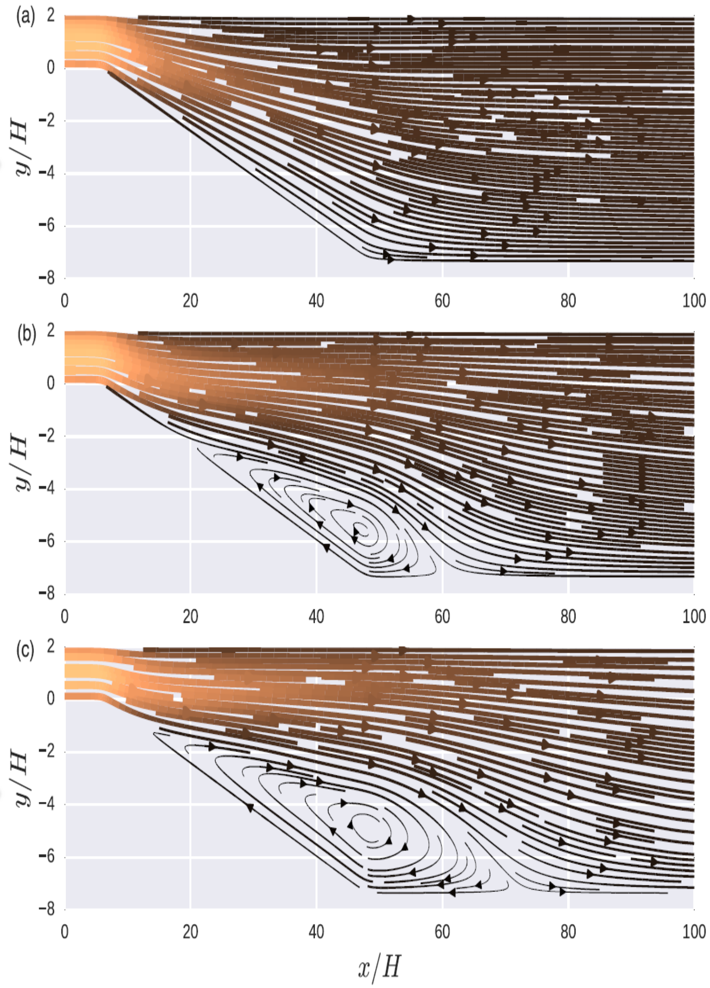
Eigenspace Perturbation Framework: Extremal States

- **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*



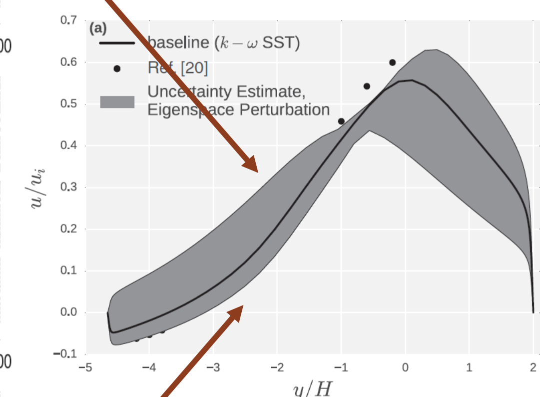
Overview of the Methodology





Perturbations correlate to physics

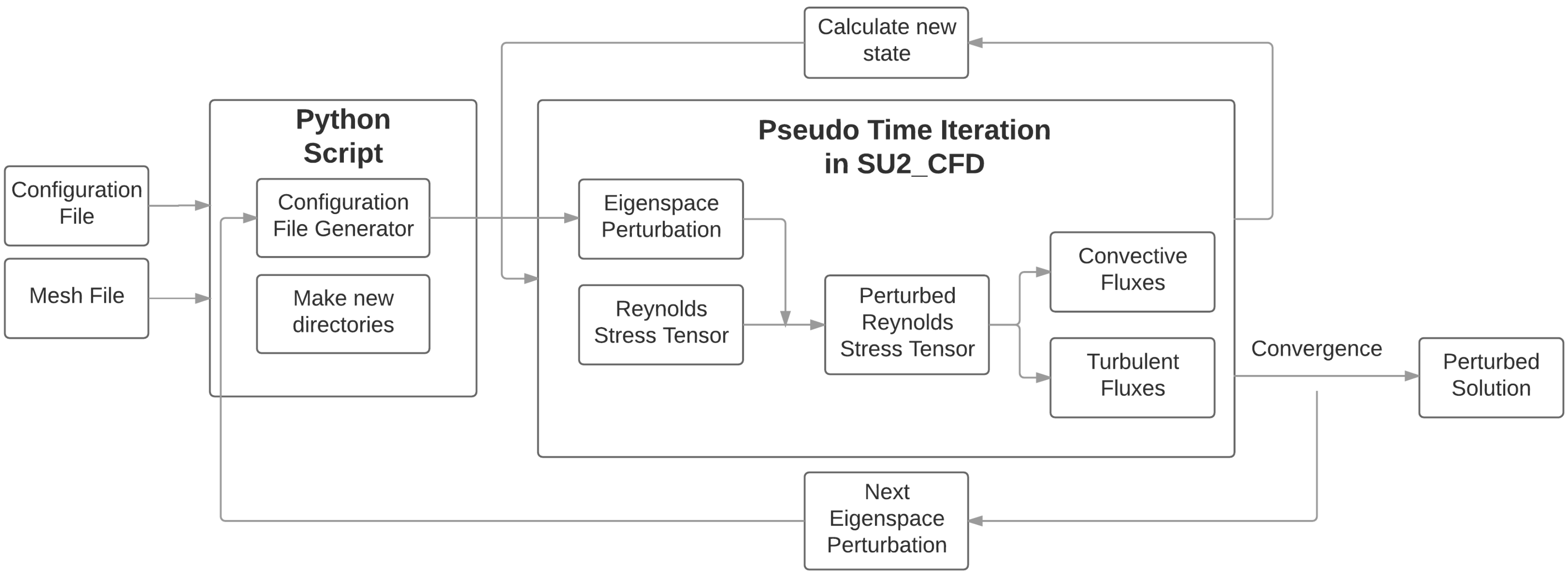
Maximize turbulence production:
Suppress flow separation



Minimize turbulence production:
Increase flow separation

Bounds represent the "envelope" of 5+1 RANS simulations

SU2 Implementation

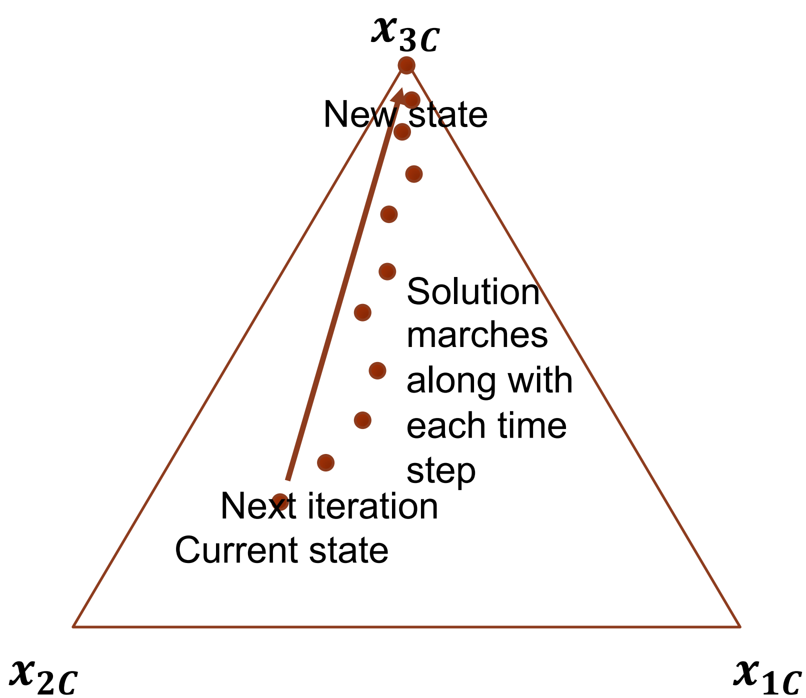


- The methodology works on the exact same mesh and input files as a baseline RANS simulation.
- UQ module built with ***versatility*** in mind. Non-experts can use it as a black-box tool without changing any settings, while expert users can customize the module to their specific needs.

Eigenspace Perturbation Procedure

For each cell in the mesh:

1. Use mean velocity gradients to calculate the Reynolds Stress
2. Find location of stress state on barycentric map using eigenvalues
3. Perturb eigenvectors and eigenvalues
4. Create new Reynolds Stress state using perturbed eigenvectors and eigenvalues
5. Use new state in flux calculations for next time step
6. Repeat for each iteration until convergence



Test & Validation Cases

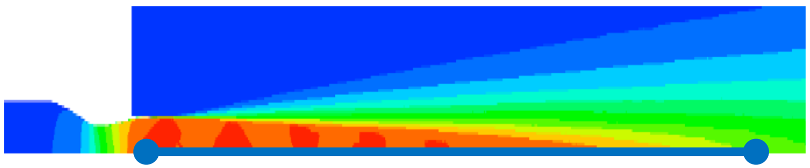
	Case	Rationale	Notes
I.	Flow over a Backward-Facing Step	Benchmark flow	2D Steady Simulation
II.	Flow through an asymmetric diffuser	Benchmark flow	2D Steady Simulation
III.	Jet efflux of the NASA Acoustic Response Nozzle	Engineering case	3D subsonic flow
IV.	NACA 4412 airfoil at different angles of attack	Engineering case	Range of 2D simulations with separation & stall.
V.	**NACA 0012 airfoil at different angles of attack**	**Engineering case**	**Mesh Refinement Study, 2D Subsonic**
VI.	**Heated jet efflux via a Seiner nozzle**	**Engineering case**	**3D supersonic flow**
VII.	**30P30N, Multi-element Airfoil**	**Engineering case**	**3D, subsonic, compressible simulation.**
VIII.	**ONERAM6 Transonic Wing**	**Engineering case**	**3D, transonic, compressible simulation.**

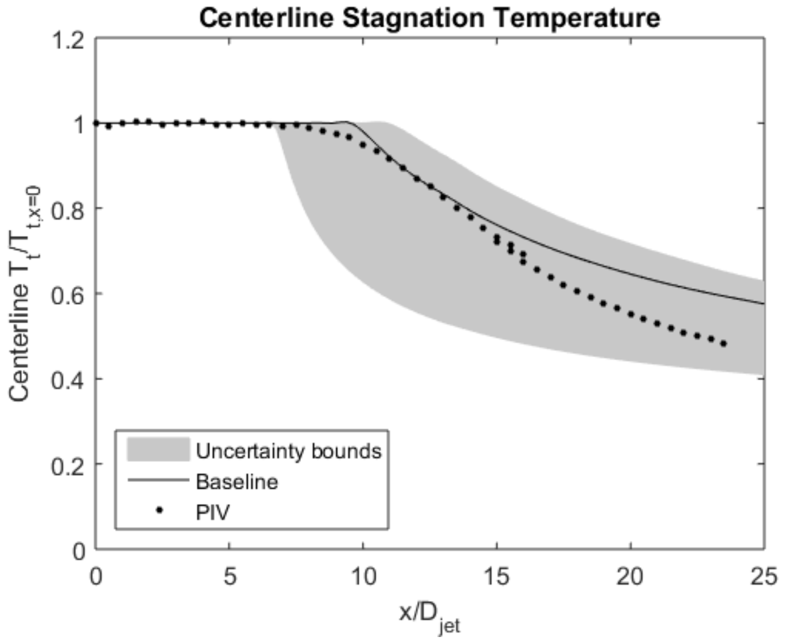
Jet Efflux of the Seiner Supersonic Nozzle

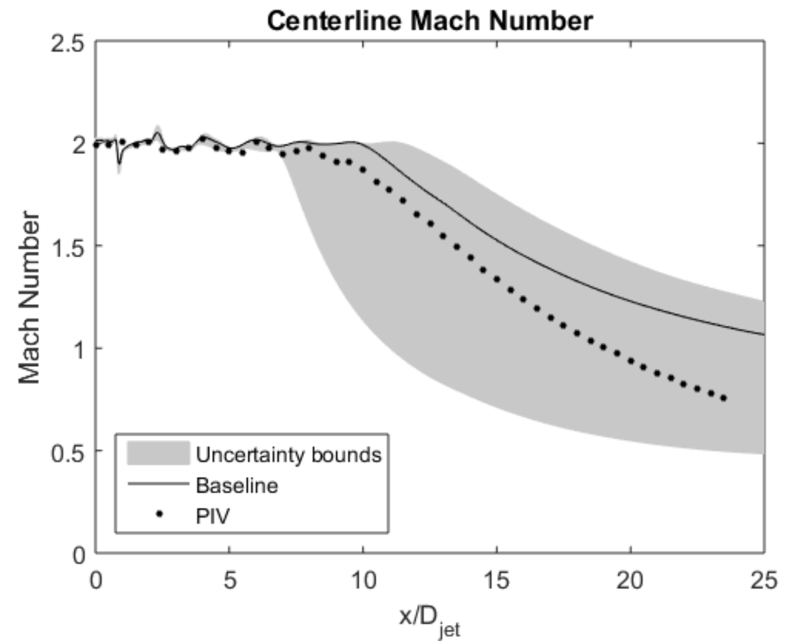
- Nozzle Mach Number= 2.0
- Temperature Ratio= 4.017
- Pressure Ratio= 7.824

Note the discrepancy in baseline turbulence prediction, and experimental data

UQ bounds encapsulate experimental data very well



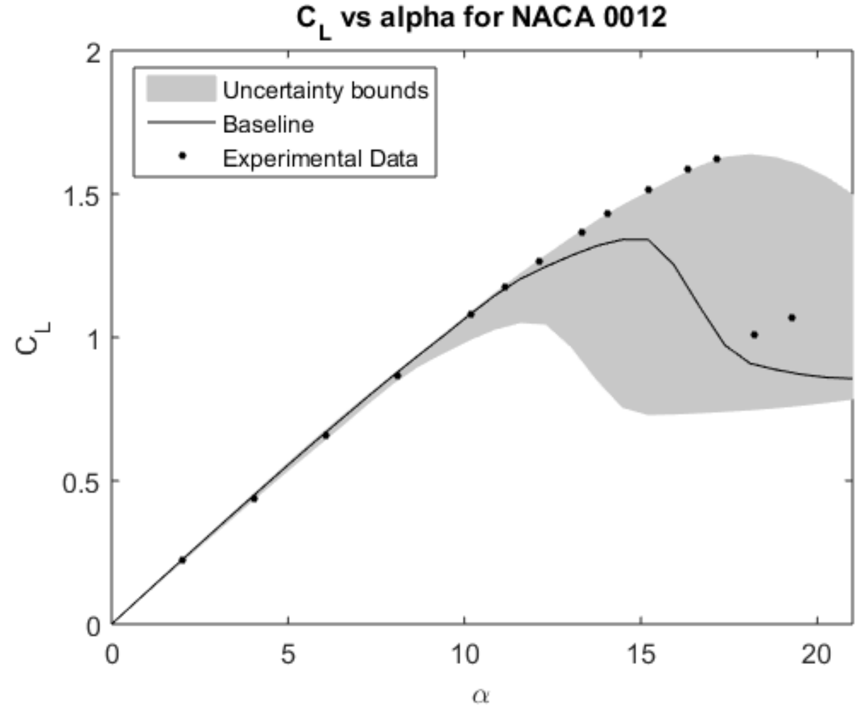


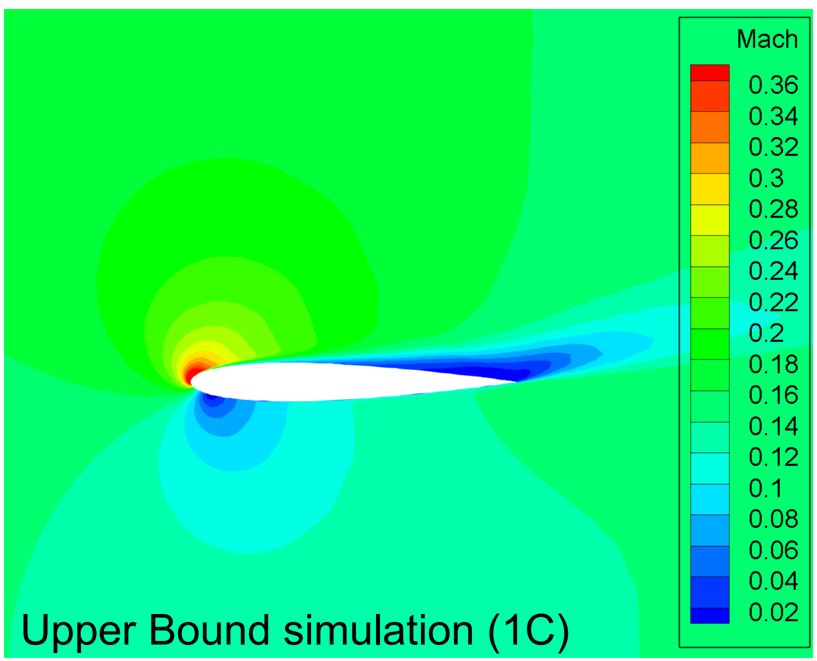


NASA TMR case: https://turbmodels.larc.nasa.gov/jetsupersonichot_val.html

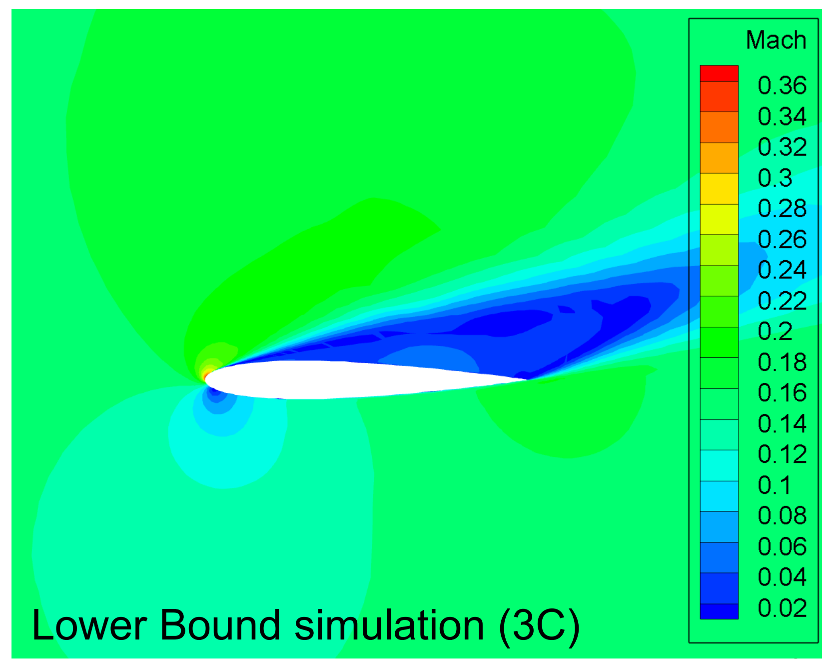
NACA 0012

- Mach= 0.15
- Re = 6×10^6
- AOA $\alpha \in \{0, 3, 6, 9, 12, 15, 18\}$
- Notice how the error bars get larger the closer we get to stall
- Plots below show the Mach contours for $\alpha = 18°$



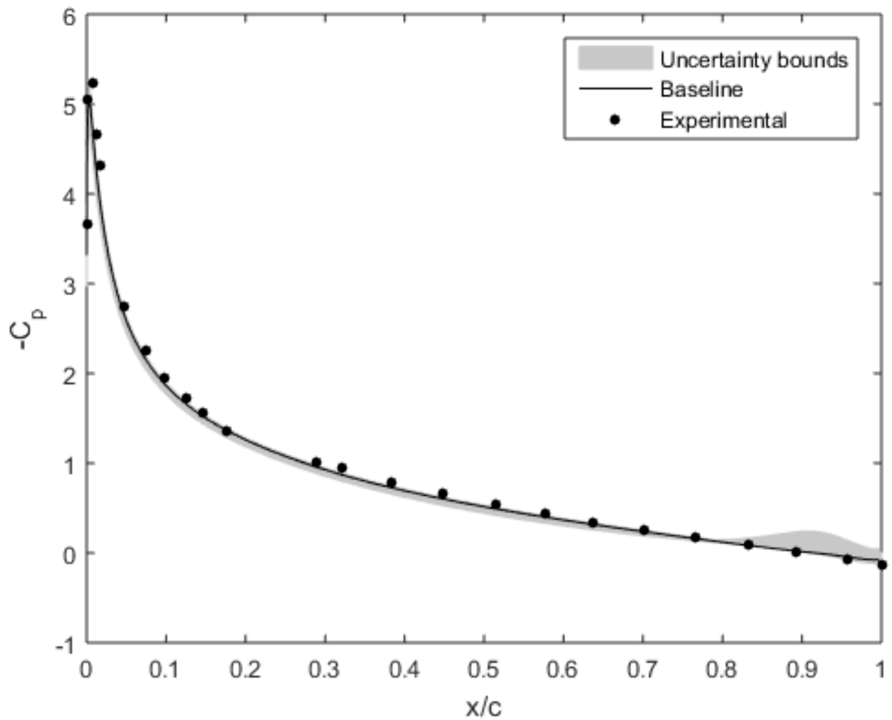


Upper Bound simulation (1C)

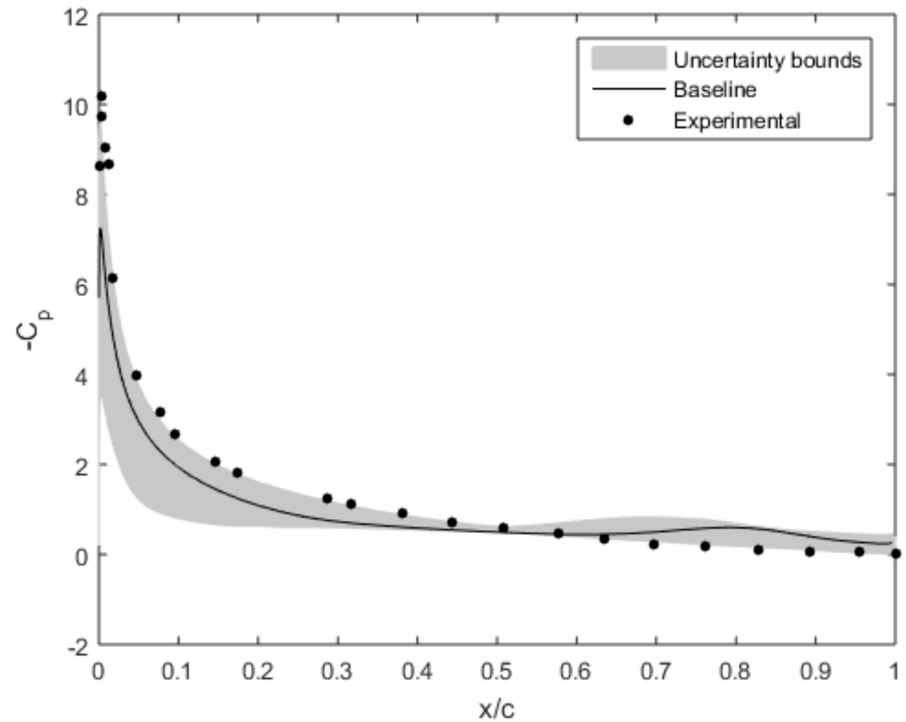


Lower Bound simulation (3C)

Flow over a NACA 0012 Airfoil



Angle of Attack: 10
Low discrepancy
Negligible uncertainty bounds

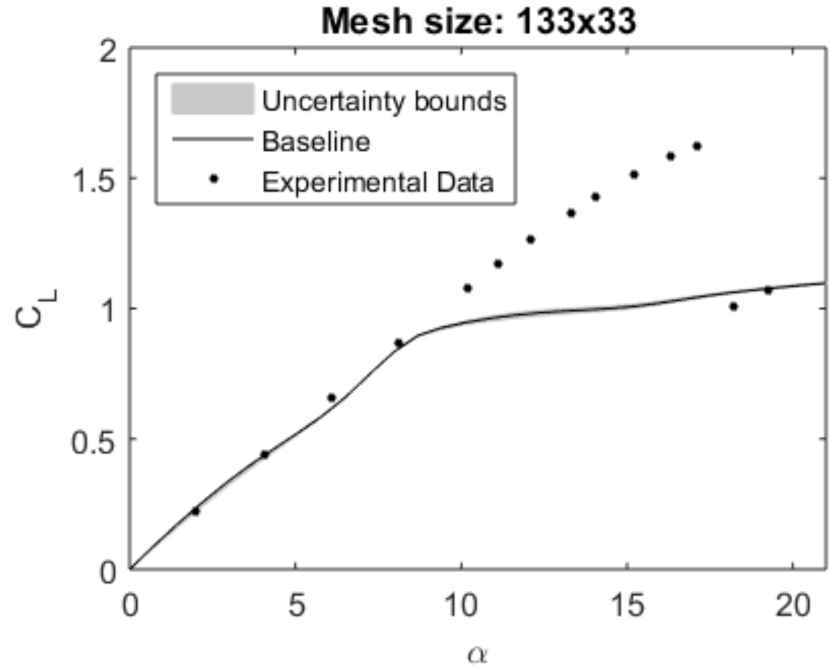


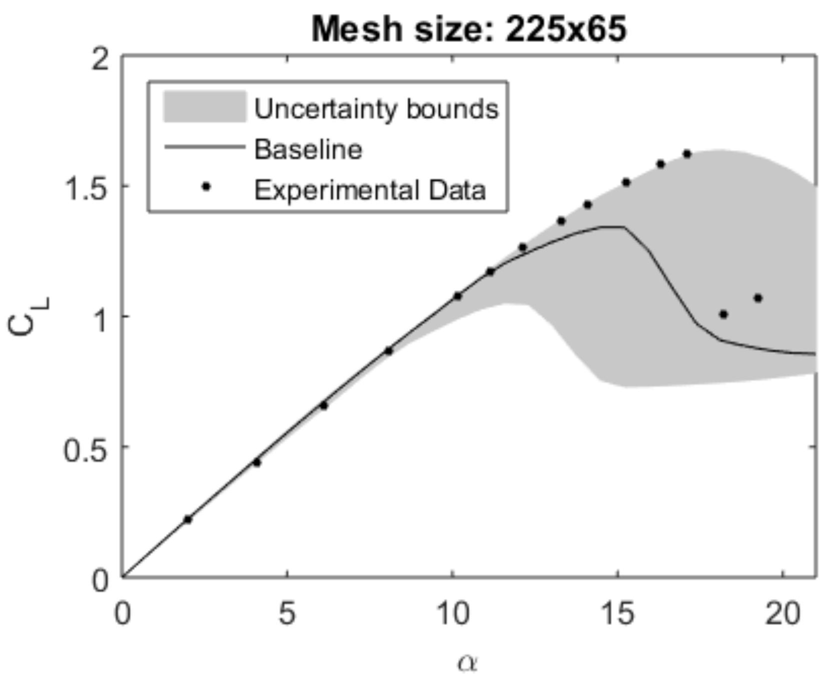
Angle of Attack: 15
Significant discrepancy
Substantial uncertainty bounds

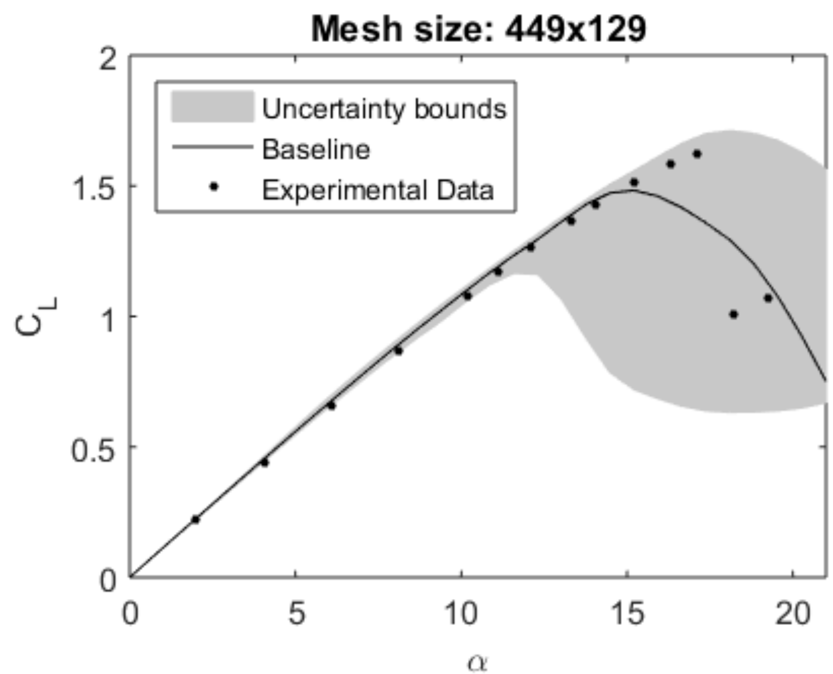
Stanford University

Mesh Refinement Study

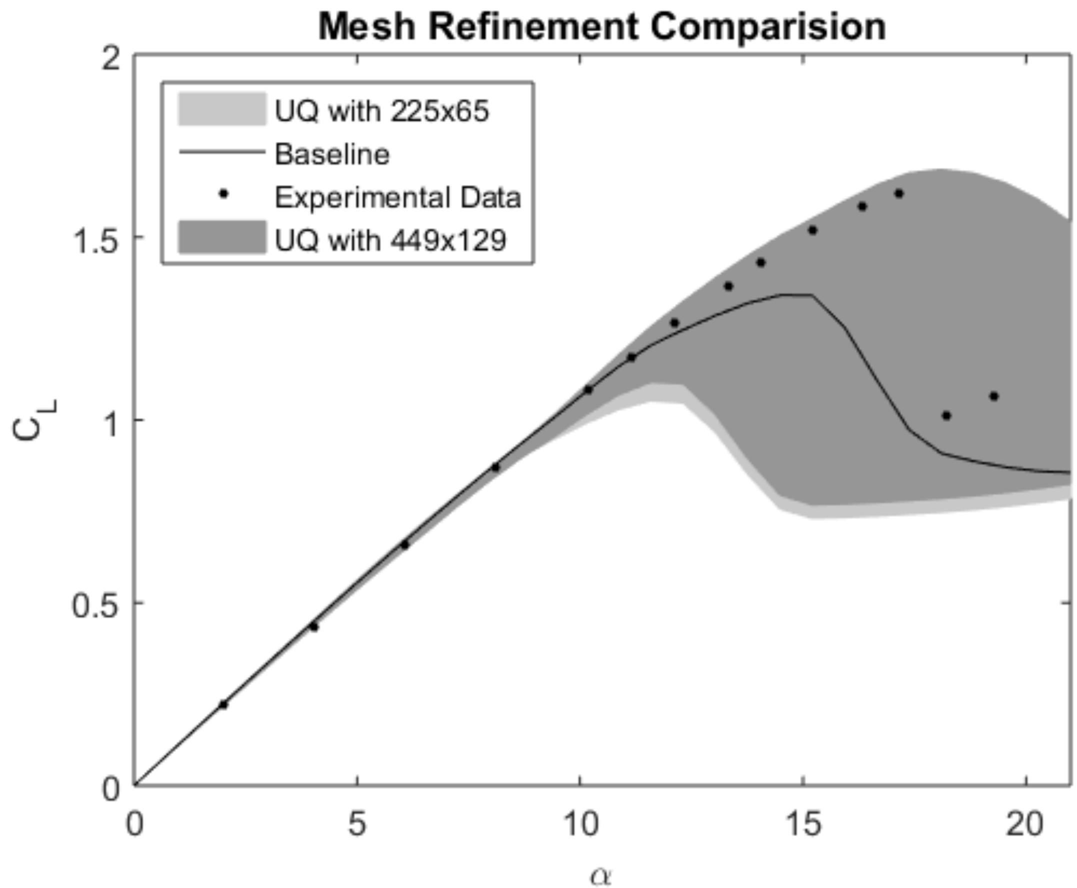
- First mesh is too coarse to capture any flow features
- Medium and fine mesh give similar results
- Gives confidence that numerical and model-form errors are “mesh independent” for reasonable resolutions







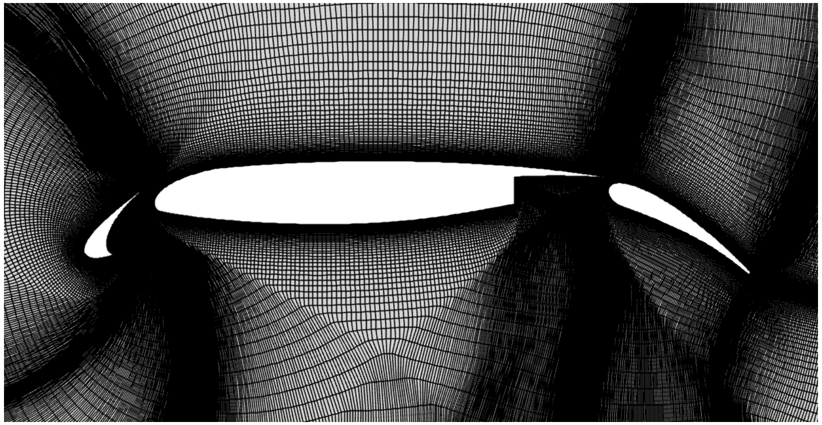
Mesh Refinement Study

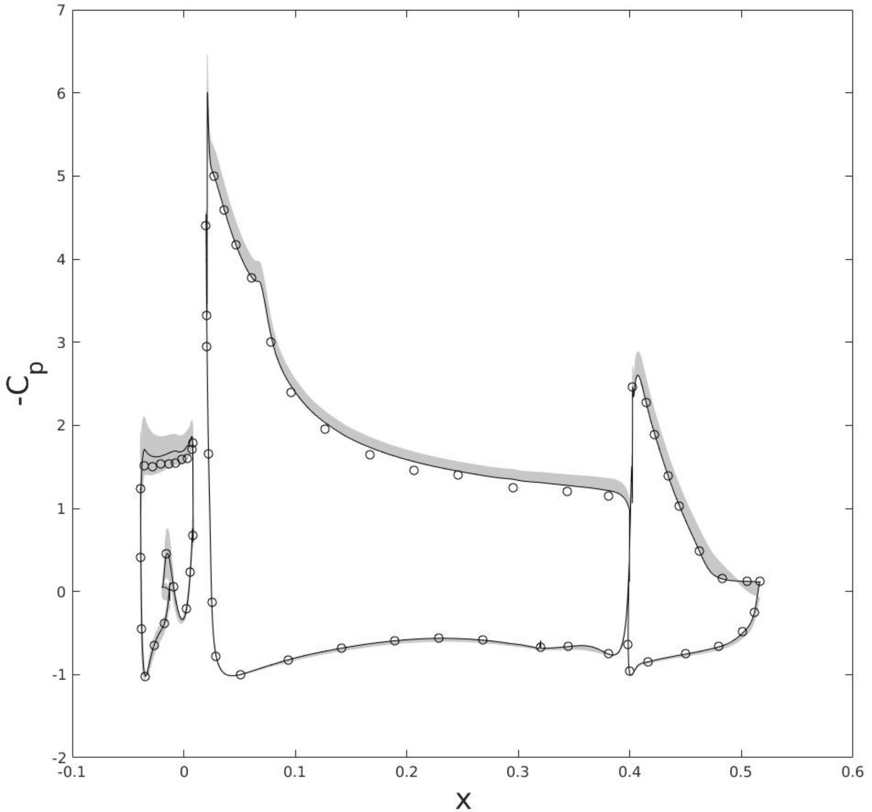


- The numerical discretization error is reduced by using a finer mesh
- The model-form error is mostly unchanged, with just a shift of the uncertainty bounds upwards

30P30N Airfoil

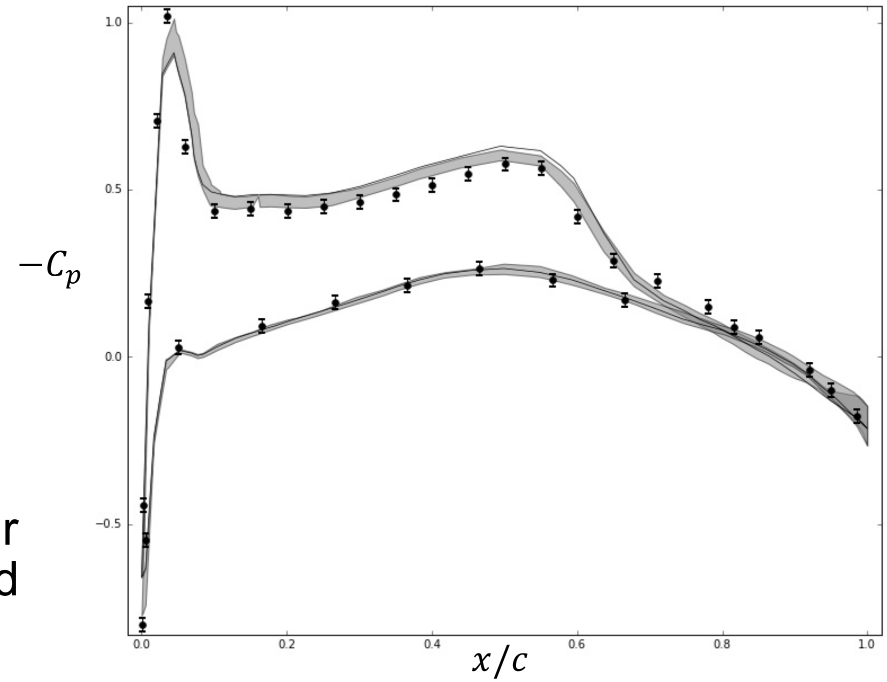
- Mach= 0.2
- Re = 9×10^6
- $\alpha = 8°$
- Uncertainty bounds are negligible for most of the airfoil except
    - Slat upper surface: some separation exists
    - Flap trailing edge: separation also present
    - Main element upper surface
- Some issues with convergence of eigenvector perturbations which might be enhanced at higher angles of attack
- Need to do an angle of attack sweep similar to what was done with the NACA 0012 airfoil

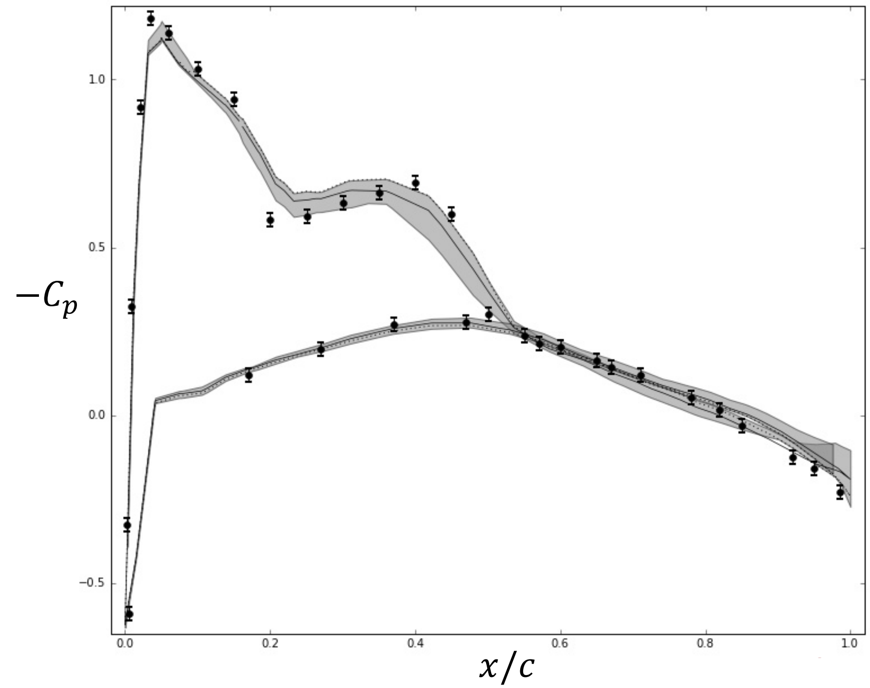


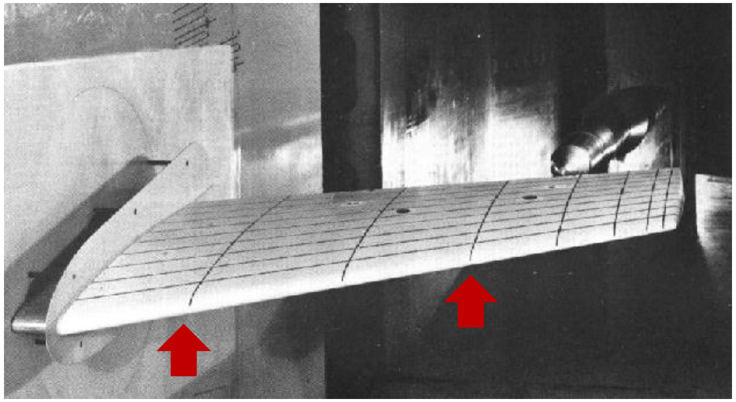


ONERA M6 Wing

- Mach= 0.8395
- Re = 11.72×10^6
- $\alpha = 3.06$
- Coefficient of pressure plots at locations indicated below
- Most experimental data points or their error bars are encapsulated within the error bars



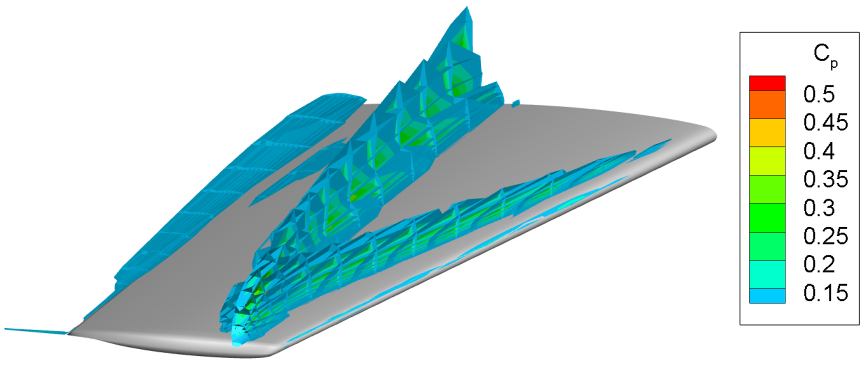




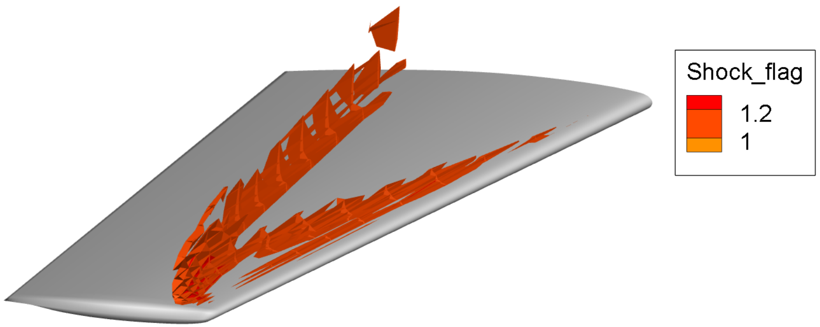
ONERA M6 Wing

- Uncertainty in C_P is maximum in 2 main areas:
  - Near the shock
  - Just behind trailing edge and wing tip
- Visualizing areas of maximum uncertainty can inform higher-fidelity evaluations
- Wind-tunnel tests can explore operating space based on uncertainty bounds of lower fidelities
- Can inform sensor placement

Areas where $C_P$variability > 0.1

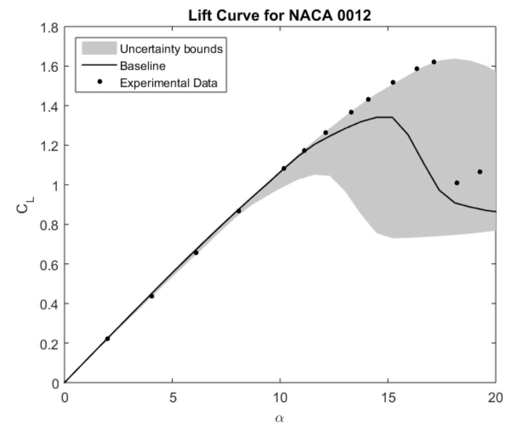


Shock Visualization over the wing



Summary

- Added **UQ module** to SU2 focusing on **uncertainties from turbulence models**
- Usable by experts and non-experts alike
- Ready for release (pull request is in)
- Tutorial is ready to be uploaded onto the website
- AIAA paper is currently under review



Goals

This tutorial covers the EQUiPS (Enabling Quantification of Uncertainty in Physics-based Simulations) module implemented in SU2 that allows for the estimation of epistemic uncertainties arising from structural assumptions in RANS turbulence closures. The test case chosen for this is the NACA0012 airfoil where we will estimate the uncertainty in surface C_p predictions at two different angles of attack. Instructions for running an angle of attack sweep to estimate the uncertainty in C_L predictions are also provided. The following capabilities of SU2 will be showcased in this tutorial:

- Uncertainty Quantification (UQ) of the SST Turbulence Model
- compute_uncertainty.py: automates the UQ module
- Manual configuration options to perform UQ analysis

Resources

The resources for this tutorial can be found in the UQ_NACA0012 directory in the project website repository. You will need the configuration file (turb_NACA0012_uq.cfg) and the mesh file (mesh_n0012_225-65.su2).

Details about the methodology and implementation in SU2 is available as a pre-print

Tutorial

The following tutorial will walk you through the steps required when using the EQUiPS module for estimating uncertainties in CFD predictions arising due to assumptions made in turbulence models. The tutorial will also address procedures for both serial and parallel computations. To this end, it is assumed you have already obtained and compiled SU2_CFD. If you have yet to complete these requirements, please see the Download and Installation pages.

Questions

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- Mishra & Iaccarino,"Uncertainty Estimation for Reynolds-Averaged Navier–Stokes Predictions of High-Speed Aircraft Nozzle Jets." *AIAA Journal* (2017)
- Iaccarino, Mishra & Ghili, “Eigenspace perturbations for uncertainty estimation of single-point turbulence closures”, *Physical Review Fluids* (2017)
- Mishra & Iaccarino,"RANS predictions for high-speed flows using enveloping models”, *CTR Annual Research Briefs* (2016)

NACA 4412

- Mach= 0.15
- Re = 6×10^6
- AOA $\alpha \in \{0, 3, 6, 9, 12, 15, 18\}$
- Similar trends to NACA 0012 case are observed
- Baseline overpredicts the C_L in this case
- Contour below showcases baseline prediction for

$$\alpha = 13.87°$$