Uncertainty Quantification in the Prediction of Turbulent Flows

Gianluca Iaccarino
Saman Ghili, Michael Emory, Aashwin Mishra

Uncertainty Quantification Lab
Institute for Computational Mathematical Engineering
Department of Mechanical Engineering
Stanford University

Funding from: Darpa, DoE/NNSA
UQ applications in fluid mechanics

Research focused on numerical algorithms and physical models!
Uncertainty Quantification - UQLab

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Projects I am NOT going to discuss today...

- Particle-Laden Turbulent Flow Subject to Radiation
  - Particle Solar Receivers
  - Multiphase Flow
  - Exascale computing

- Complex Fluids in Complex Geometries
  - Immersed Boundary Method
  - Non-Newtonian Fluids
  - Fluid-Structure Interactions
A Simple Fluid Dynamics Design Problem

Objective

"Turn" the flow 180°
while minimizing the
pressure losses

Design variables

The shape of the curved
section...

Examples of Geometrical Modifications

Up to 15% difference in pressure loss
A Simple Fluid Dynamics Design Problem

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Complexities

- The inflow velocity profile might be distorted
Objective

"Turn" the flow 180deg while minimizing the pressure losses

Design variables

The shape of the curved section...

Examples of Inflow Distortion in Baseline Geometry

Up to 8% difference in pressure loss
A Simple Fluid Dynamics Design Problem

Objective
"Turn" the flow 180deg while minimizing the pressure losses

Design variables
The shape of the curved section...

Complexities
1. The inflow velocity profile might be distorted
2. Turbulent separated flows are *difficult* to simulate accurately
A Simple Fluid Dynamics Design Problem

Objective
"Turn" the flow 180deg while minimizing the pressure losses

Design variables
The shape of the curved section...

Velocity Magnitude

Difference Turbulence Models in Baseline Geometry
Up to 6% difference in pressure loss
A Simple Fluid Dynamics Design Problem

Objective

"Turn" the flow 180deg while minimizing the pressure losses

Design variables

The shape of the curved section...

Complexities

1. The inflow velocity profile might be distorted
2. Turbulent separated flows are difficult to simulate accurately

This Talk

Introduce a framework to characterize variability related to operating conditions and potential bias introduced by modeling assumptions
Uncertainty Quantification - UQLab

Variability

Operating Conditions

Manufacturing Process

Inputs

Virtual Model

Outputs

?
Uncertainty Quantification - UQLab

Inputs → Virtual Model → Outputs

- Bias
- Combustion Kinetics Assumptions
- Turbulence Modeling
  - $k-\varepsilon$

Virtual Model
Uncertainty Quantification - UQLab

Virtual Model

Variability
Operational Conditions
- Manufacturing Process

Bias
- Combustion Kinetics Assumptions
- Turbulence Modeling
  - k-ε

Inputs

Outputs
Outline

1. Capturing Variability
   - Non-intrusive Polynomial Chaos
   - Weighted Least Squares Quadrature
   - Work by Saman Ghili

2. Representing Bias
   - Turbulence Modeling Assumptions
   - Enveloping Models
   - Work by Michael Emory & Aashwin Mishra

3. Design Under Uncertainty
   - U-duct design

4. Conclusion & Discussion
1 – Capturing Variability

Variability

Operating Conditions

Manufacturing Process

Inputs

Virtual Model

Outputs

?
1 – Capturing Variability

Variability → Operating Conditions → Manufacturing Process → Inputs → Ensemble of Computations → Outputs
Problem Setup

Define $f(\xi)$ as the a quantify of interest – the output of a CFD simulation

Let $\xi = (\xi_1, \cdots, \xi_d)$:

- Parametric representation of the uncertain inputs – boundary conditions, operating scenario, etc.
- Each component $\xi_k$ is a random variable with PDF $\rho_k(\xi_k)$.
- The random variables are bounded and defined in an interval $D_k$.
- They are also independent: $\xi$ will have joint PDF $\rho(\xi) = \rho_1(\xi_1) \times \cdots \rho_d(\xi_d)$, and take values in $D = D_1 \times \cdots D_d$.

Goal

Construct an approximate functional relationship between $\xi$ and the output of interest $f(\xi)$ to construct an optimal ensemble
Polynomial Chaos expansions

- $f(\xi)$ admits a polynomial chaos expansion:

$$f(\xi) = \sum_{\mathbf{j} \in \mathbb{N}_0^d} \hat{f}_\mathbf{j} \psi_\mathbf{j}(\xi) = \sum_{j_1=0}^{\infty} \cdots \sum_{j_d=0}^{\infty} \hat{f}_{j_1,\ldots,j_d} \psi_{j_1;1}(\xi_1) \cdots \psi_{j_d;d}(\xi_d).$$

where $\mathbf{j} = (j_1, \ldots, j_d) \in \mathbb{N}_0^d$ is a multi-index set, and $\{\psi_{j_k;k}(\xi_k)\}_{j_k=0}^{\infty}$ are orthonormal polynomials with respect to $\rho_k(\xi_k)$. 

In practical terms we need to use a truncated expansion, i.e. a finite subset $\Lambda \subset \mathbb{N}_0^d$ and therefore

$$f(\xi) \approx P_\Lambda f(\xi) = \sum_{\mathbf{j} \in \Lambda} \hat{f}_\mathbf{j} \psi_\mathbf{j}(\xi).$$

Need to define $\Lambda$ and compute the coefficients $\hat{f}_\mathbf{j}$. 

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- In practical terms we need to use a truncated expansion, i.e. a finite subset $\Lambda \subset \mathbb{N}_0^d$ and therefore

$$f(\xi) \approx \mathcal{P}_\Lambda f(\xi) = \sum_{j \in \Lambda} \hat{f}_j \psi_j(\xi).$$
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- In practical terms we need to use a truncated expansion, i.e. a finite subset $\Lambda \subset \mathbb{N}_0^d$ and therefore

$$f(\xi) \approx \mathcal{P}_\Lambda f(\xi) = \sum_{j \in \Lambda} \hat{f}_j \psi_j(\xi).$$

- Need to define $\Lambda$ and compute the coefficients $\hat{f}_j$
The coefficients (for \( j \in \Lambda \)) are defined as

\[
\hat{f}_j = \int_D f(\xi) \psi_j \rho(\xi) d\xi.
\]

resulting in a truncation error:

\[
\| f - P_\Lambda f \|_{L^2(D, \rho)}^2 = \sum_{j \in \mathbb{N}_0^d \backslash \Lambda} \hat{f}_j^2.
\]
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\[
\| f - \mathcal{P}_\Lambda f \|_{L^2(D, \rho)}^2 = \sum_{j \in \mathbb{N}_0^g \setminus \Lambda} \hat{f}_j^2.
\]
We also need to approximate the integrals numerically. This introduces an additional aliasing error:
\[
\| f - \tilde{\mathcal{P}}_\Lambda f \|_{L^2(D, \rho)}^2 = \| \tilde{f}_\Lambda - \hat{f}_\Lambda \|_2^2 + \sum_{j \in \mathbb{N}_0^g \setminus \Lambda} \hat{f}_j^2.
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Polynomial Chaos expansions

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\]

**Goal**

Construct an *approximate* functional relationship \( \mathcal{P}_\Lambda f(\xi) \) based on a PC Expansion *balancing* both errors
How to pick the index set: $\Lambda \subset \mathbb{N}_0^d$?
Polynomial Chaos expansions
Choosing index-sets

How to pick the index set: $\Lambda \subset \mathbb{N}_0^d$?

- **Commonly used:**
  - **Tensor product:**
    $\Lambda_{\text{TP}}^n = \{ \mathbf{j} \in \mathbb{N}_0^d | j_k \leq n, \forall 1 \leq k \leq d \}$, with size
    $N = (n + 1)^d$
    
    $\Lambda_{\text{TP}}^n$ is impractical in almost all cases ($N$ grows too quickly)
  - **Total order:**
    $\Lambda_{\text{TO}}^n = \{ \mathbf{j} \in \mathbb{N}_0^d | \sum_{k=1}^d j_k \leq n \}$, with size
    $N = \binom{n+d}{d} = O\left(\frac{n^d}{d!}\right)$
    
    in some problems (elliptic sPDEs), $\Lambda_{\text{TO}}^n$ is the optimal choice.

- **General anisotropic basis:**
  $\Lambda_{\text{AB}}^n = \{ \mathbf{j} \in \mathbb{N}_0^d | g(j_k) \leq g_n \}$
Polynomial Chaos expansions
Computing expansion coefficients

How to compute the coefficients $\hat{f}_j$?

In general:

$$\hat{f}_j = \int_D f(\xi) \psi_j(\xi) \rho(\xi) \, d\xi \approx \tilde{f}_j = M \sum_{i=0}^{\infty} \alpha_i f(\xi_i) \psi_j(\xi_i)$$

A number of strategies have been proposed in the literature.

d = 2 point sets:

- $\xi_i = (\xi_{i,1}, \xi_{i,2})$

- Monte Carlo Integration
- Gaussian Quadrature
- Sparse Grid Quadrature
Polynomial Chaos expansions
Computing expansion coefficients

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In general:

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- A number of strategies have been proposed in the literature.

$d = 2$ point sets: $\xi^{(i)} = (\xi_1^{(i)}, \xi_2^{(i)})$

Monte Carlo Integration
Gaussian Quadrature
Sparse Grid Quadrature
A Balanced PCE approximation is obtained by

1. selecting $\Lambda(\rightarrow N)$ depending on the required accuracy of the approximation (low truncation error)
2. building a quadrature $Q$ optimized w.r.t. to the basis in $\Lambda$
3. finding the smallest $M$ that gives low aliasing error
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The ratio $r = \frac{M}{N}$ is the over-sampling factor
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The ratio $r = \frac{M}{N}$ is the over-sampling factor

- Gaussian quadrature has low aliasing error but $M$ grows too quickly, i.e. If $\Lambda = \Lambda^{TO}$ then $r = \mathcal{O}(d!)$
The Challenge

Can we achieve the accuracy of Gaussian quadratures with $M$ very close to $N$ for any $\Lambda$ index-set?
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Can we achieve the accuracy of Gaussian quadratures with $M$ very close to $N$ for any $\Lambda$ index-set?

The Key observation
Gaussian quadratures are weighted least squares!

$$\tilde{f}_\Lambda = \arg\min_{a \in \mathbb{R}^N} \sum_{m=1}^{M} w^{(m)} \left( f(\xi^{(m)}) - \sum_{i=1}^{N} a_i \psi_{ji}(\xi^{(m)}) \right)^2$$
Weighted Least Squares (WLS)

The WLS-PCE least square problem:

$$\tilde{f}_{\Lambda} = \arg\min_{a \in \mathbb{R}^N} \sum_{m=1}^{M} w^{(m)} \left( f(\xi^{(m)}) - \sum_{i=1}^{N} a_i \psi_j(\xi^{(m)}) \right)^2$$

can be rewritten as

$$\Psi^T W \Psi \tilde{f}_{\Lambda} = \Psi^T W b.$$

where

- $N$ is the number of basis corresponding to the PCE index-set $\Lambda$
- $M$ is the number of function evaluations $f(\xi^{(i)})$
- $\Psi$ is an $M \times N$ matrix with elements: $\Psi_{m,i} = \psi_j(\xi^{(m)})$
- $W$ is an $M \times M$ diagonal matrix with $W_{i,i} = w^{(i)}$
- $b$ is an $M \times 1$ vector with elements $b = [f(\xi^{(1)}), \cdots, f(\xi^{(M)})]^T$
The WLS-PCE problem is \( \psi^T W \psi \tilde{f}_\Lambda = \psi^T W b \)

We define \( K = \| (W^{\frac{1}{2}} \psi)^\dagger \|_2 \) as the condition number of the WLS.

**Observation**

For Gaussian quadrature over \( \Lambda = \Lambda^{TP} \) we have

\[ \psi^T W \psi = I \]

and therefore \( K = 1 \) independently of \( d' \).

Gaussian quadrature over tensor-product index-sets (\( \Lambda^{TP} \)) leads an *optimally conditioned* WLS with \( M = N \) (\( r = 1 \)).
Optimization problem

Minimizing the aliasing error for a given truncation error

Starting Point

\[
\begin{align*}
\text{Aliasing:} & \quad \| \hat{f}_\Lambda - \tilde{f}_\Lambda \|_2 \\[10pt]
\text{Truncation:} & \quad K \| f - \mathcal{P}(f) \|_{L_2(Q_Y,W)}.
\end{align*}
\]

Strategy

Given \( \Lambda (\rightarrow N) \) and \( M \) (close to \( N \)), find \( M \) points and weights that make the upper bound on the aliasing error as small as possible.
Optimization problem
Minimizing the aliasing error for a given truncation error

Starting Point

\[
\begin{align*}
\text{Aliasing} & \quad \| \hat{f}_\Lambda - \tilde{f}_\Lambda \|_2 \leq K \| f - \mathcal{P}(f) \|_{L^2(Q_{y,W})}. \\
\text{Truncation} & \quad \| f - P(f) \|_{L^2(Q_{y,W})}.
\end{align*}
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Strategy

Given \( \Lambda (\rightarrow N) \) and \( M \) (close to \( N \)), find \( M \) points and weights that make the upper bound on the aliasing error as small as possible.

Optimization

Given

\[ \Psi^T W \Psi \tilde{f}_\Lambda = \Psi^T W b. \]

minimize \( K \); i.e. find the \( M \) weights \( \{ w^{(1)}, \ldots, w^{(M)} \} \) and points \( \{ \xi^{(1)}, \ldots, \xi^{(M)} \} \) such that the condition number of \( \Psi^T W \Psi \) is minimal.
The general WLS-PCE problem is $\Psi^T W \Psi \tilde{f}_\Lambda = \Psi^T W b$

In the special case of Gaussian quadrature over $\Lambda = \Lambda^{TP}$ we have

$$\Psi^T W \Psi = I \quad \rightarrow \quad \tilde{f}_{\Lambda^{TP}} = \Psi^T W b$$

Remark: The solution of the optimization problem $(W, \{\xi(1), \cdots, \xi(M)\})$ does NOT depend on the function $f$ (i.e. the vector $b$). Can be precomputed.
The general WLS-PCE problem is \( \Psi^T W \Psi \tilde{f}_\Lambda = \Psi^T W b \)

In the special case of Gaussian quadrature over \( \Lambda = \Lambda^{TP} \) we have

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\Psi^T W \Psi = I \quad \rightarrow \quad \tilde{f}_{\Lambda^{TP}} = \Psi^T W b
\]

In the general case the coefficients \( \tilde{f}_\Lambda \) are coupled:

\[
\tilde{f}_\Lambda = \left( \Psi^T W \Psi \right)^{-1} \Psi^T W b
\]
Optimization problem

Remarks

- The general WLS-PCE problem is $\Psi^T W \Psi \tilde{f}_\Lambda = \Psi^T W b$
- In the special case of Gaussian quadrature over $\Lambda = \Lambda^{TP}$ we have
  $$\Psi^T W \Psi = I \quad \rightarrow \quad \tilde{f}_{\Lambda^{TP}} = \Psi^T W b$$

- In the general case the coefficients $\tilde{f}_\Lambda$ are coupled:
  $$\tilde{f}_\Lambda = \left( \Psi^T W \Psi \right)^{-1} \Psi^T W b$$

- Remark: The solution of the optimization problem ($W$, $\{\xi^{(1)}, \ldots, \xi^{(M)}\}$) does NOT depend on the function $f$ (i.e. the vector $b$). Can be precomputed.
Point Sets - $d=2$ - Close-form Solution

- Gauss Quadrature
- Gauss-Lobatto
- Present Optimization

Gauss Points - $\Lambda^{TP}$ (N=8)

Padua Points $\Lambda^{T0}$ (N=10)
Numerical experiments, #1

\[ d = 2, \ \Lambda^{TO} \]

\[ f(\xi_1, \xi_2) = \frac{1}{1 + 9\xi_1^2} \times \frac{1}{1 + 9\xi_2^2} \]
Numerical experiments, #2

- $d = 3$, $\Lambda^{AB} = \mathbf{j} \in \mathbb{N}_0^3 | j_1 + 2j_2 + 4j_3 < n$

$$f(\xi_1, \cdots \xi_3) = \frac{0.5}{1 + (4.9668\xi_1)^2} \times \frac{0.5}{1 + (2.4346\xi_2)^2} \times \frac{0.5}{1 + (1.1260\xi_3)^2}$$

![Graphs showing error and condition number](image)

**Total Error**

**Condition number**
Numerical experiments, #3

- \( d = 3, \; \Lambda^{TP}; \; \Lambda^{TO}; \; \Lambda^{AB} = \xi_1^\alpha (1 + \xi_3^\beta) \)

\[
f(\xi_1, \cdots \xi_3) = 7 \sin(\pi \xi_1) + \sin(\pi \xi_2) \sin(\pi \xi_3) + \xi_3^4 \sin(\pi \xi_1)
\]

<table>
<thead>
<tr>
<th>Basis</th>
<th>Quadrature</th>
<th>N</th>
<th>M</th>
<th>r</th>
<th>( \epsilon_{\text{mean}} )</th>
<th>( \epsilon_{\text{var}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Lambda^{TP} )</td>
<td>Gauss</td>
<td>125</td>
<td>729</td>
<td>5.9</td>
<td>(&lt; 0.01% )</td>
<td>(&lt; 0.01% )</td>
</tr>
<tr>
<td>( \Lambda^{TO} )</td>
<td>Sparse Grid</td>
<td>35</td>
<td>495</td>
<td>14.1</td>
<td>(&lt; 0.01% )</td>
<td>(&lt; 0.01% )</td>
</tr>
<tr>
<td>( \Lambda^{AB} )</td>
<td>Sparse Grid</td>
<td>25</td>
<td>64</td>
<td>2.6</td>
<td>14.3%</td>
<td>11.8%</td>
</tr>
<tr>
<td>( \Lambda^{AB} )</td>
<td>Optimized</td>
<td>25</td>
<td>30</td>
<td>1.2</td>
<td>0.3%</td>
<td>0.7%</td>
</tr>
<tr>
<td>( \Lambda^{AB} )</td>
<td>Monte Carlo</td>
<td>25</td>
<td>729</td>
<td>30</td>
<td>4.5%</td>
<td>8.6%</td>
</tr>
</tbody>
</table>

\[ n = 4; \; N^{TP} = (n + 1)^3 = 125; \; N^{TO} = \binom{n+3}{3} = 35 \]
Goal

Construct an *approximate* functional relationship between $\xi$ and the output of interest $f(\xi)$ to construct an optimal ensemble

- A novel formulation of the *pseudo-spectral* polynomial chaos approach is described (Balanced PCE)
- It is non-intrusive and adapted to the index-set, i.e. the selected polynomial basis
- It uses an optimization procedure to balance aliasing and truncation error
- The accuracy is better than randomly generated points (for a given number of function evaluations) by at least one order of magnitude
2 – Representing Bias

Combustion Kinetics Assumptions
Turbulence Modeling

Inputs

Virtual Model

Outputs

Bias

k-ε
2 – Representing Bias

Inputs → Enveloping Models → Outputs

Combustion Kinetics Assumptions
Turbulence Modeling

Bias

k-ε
Simulation of Turbulent Flows

- Direct simulations of turbulent flows require resolution of both temporal and spatial scales and lead to largely unfeasible computations.

- In engineering application typically only mean quantities are of interest (Reynolds Averaged Navier-Stokes equations):

\[
\frac{\partial (U_i)}{\partial t} + \frac{\partial U_i (U_j)}{\partial x_j} = \frac{1}{\rho} \frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial u'_i u'_j}{\partial x_j}; \quad \frac{\partial U_i}{\partial x_i} = 0
\]
Direct simulations of turbulent flows require resolution of both temporal and spatial scales and lead to largely unfeasible computations. In engineering application typically only mean quantities are of interest (Reynolds Averaged Navier-Stokes equations):

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\]

The solution requires an estimate of the Reynolds stresses: \( u'_i u'_j \)
Simulation of Turbulent Flows

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\]

- The solution requires an *estimate* of the Reynolds stresses: \( \overline{u_i' u_j'} \)

**Goal**

Derive *bounds* for the Reynolds stresses describing the potential bias induced by turbulence models.
Example: $k-\epsilon$ Turbulence Model

- Multiple **assumption** and **coefficients** are introduced...

\[ a_{ij} = \frac{u_i'u_j'}{k} - \frac{2}{3} \delta_{ij} \approx -C_{\mu} \frac{k}{\epsilon} S_{ij} \quad k = \frac{1}{2} u'_i u'_i \]

where

\[ \frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \epsilon + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] \]

\[ \frac{\partial \epsilon}{\partial t} + U_j \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon 1} P_k - C_{\epsilon 2} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] \]

- **Closure constants** ($C_{\mu}$, $\sigma_k$, $\sigma_\epsilon$, $C_{\epsilon 1}$, $C_{\epsilon 2}$) are often **calibrated**
Example: $k-\epsilon$ Turbulence Model

Multiple **assumption** and **coefficients** are introduced...

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a_{ij} = \frac{u_i'u_j'}{k} - \frac{2}{3} \delta_{ij} \approx -C_\mu \frac{k}{\epsilon} S_{ij} \quad k = \frac{1}{2} u_i'u_i'
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\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \epsilon + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right]
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**Closure constants** ( $C_\mu$, $\sigma_k$, $\sigma_\epsilon$, $C_{\epsilon 1}$, $C_{\epsilon 2}$ ) are often **calibrated**

**Goal**

Derive **bounds** for the Reynolds stresses describing the potential bias induced by **assumptions** used in turbulence models
Virtually ALL models used are **local**, i.e. define closure based on resolved local quantities.

The Reynolds stress tensor is a **symmetric and semi-positive definite** $3 \times 3$ matrix

$$-u'_i u'_i = 2k \left( \frac{\delta_{ij}}{3} + a_{ij} \right)$$

The equation for $k$ can be derived **directly** from the Navier-Stokes equations:

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = -u'_i u'_j \frac{\partial U_j}{\partial x_i} - 2\nu \bar{s}'_{ij} \bar{s}'_{ij} - \frac{\partial}{\partial x_i} \left( \bar{u}'_i u'_j u'_j + \bar{u}'_i p' / \rho - 2\nu \bar{u}'_i s'_{ij} \right)_{P_k}$$
Uncertainty in Turbulence Models

Objective

- Replace assumptions and functional relationships used in the turbulence models with *extreme-possible-values* based on theory
- Construct an ensemble of enveloping models

Strategy

- Define the amplitude \(k\), the shape \(\Lambda_{ij}\) and the orientation \(v_{ij}\) of the Reynolds stress tensor
- Describe ALL the possible stress states of turbulence
- Bound the energy transfer between mean flow and turbulent motion
The eigenvalues of $a_{ij}$ are constrained by realizability conditions:

\[
1/3 \leq a_{\alpha\alpha} \leq 2/3; \quad -1/2 \leq a_{\alpha\beta} \leq 1/2
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Expanding in terms of basis tensors:
\[
a_{ij} = C_1 c \hat{a}^{1c}_{ij} + C_2 c \hat{a}^{2c}_{ij} + C_3 c \hat{a}^{3c}_{ij}
\]

The coefficients determine how close the stresses are to the asymptotic states.
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The coefficients determine how close the stresses are to the asymptotic states.

There is a one-to-one relationship between the eigenvalues of $a_{ij}$ ($\Lambda_{ij}$) and the coefficients $C_{1c}$, $C_{2c}$ and $C_{3c}$.

$C_{1c} = \lambda_1 - \lambda_2$; $C_{2c} = 2(\lambda_2 - \lambda_3)$; $C_{3c} = 3\lambda_3 + 1$
The eigenvalues of $a_{ij}$ are constrained by realizability conditions:
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Expanding in terms of basis tensors:

$$a_{ij} = C_1 c \hat{a}_{ij}^1 + C_2 c \hat{a}_{ij}^2 + C_3 c \hat{a}_{ij}^3$$

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$$C_1 c = \lambda_1 - \lambda_2; \quad C_2 c = 2(\lambda_2 - \lambda_3); \quad C_3 c = 3\lambda_3 + 1$$

**Enveloping behavior** can be observed by forcing the $\overline{u_i u_j}$ eigenvalues to represent 1C, 2C, 3C states!
Once the eigenvalues are defined, we can obtain the eigenvectors by computing bounds on the energy transfer between mean flow and turbulent motion.

Kinetic energy production $P_k = -u'_i u'_j \frac{\partial U_j}{\partial x_i}$

$\frac{\partial U_j}{\partial x_i}$ is the known mean velocity gradient tensor.

$u'_i u'_j$ is a symmetric matrix with known eigenvalues.

Which $u'_i u'_j$ set of eigenvectors leads to $\text{Max}(P_k)$ and $\text{Min}(P_k)$?
Enveloping Models

Anysotropy eigenvectors - $\nu_{ij}$ and $k$

- $P_k = -u'_i u'_j \frac{\partial U_j}{\partial x_i}$ is the d-dot product of $3 \times 3$ symmetric matrices
- $\frac{\partial U_j}{\partial x_i}$ has known eigenvectors $w_{ij}^U$ and known eigenvalues
- $u'_i u'_j$ has known eigenvalues but unknown eigenvectors $\nu_{ij}$

Max ($P_k$) $\rightarrow \nu_{ij} = w_{ij}^U$

Min ($P_k$) $\rightarrow \nu_{ij} = w_{ij}^U$

$P_k$ (with $P_k = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$)
Enveloping Models
Anysotropy eigenvectors - $v_{ij}$ and $k$

- $P_k = -u'_i u'_j \frac{\partial U_j}{\partial x_i}$ is the d-dot product of $3 \times 3$ symmetric matrices
- $\frac{\partial U_j}{\partial x_i}$ has known eigenvectors $w_{ij}^U$ and known eigenvalues
- $u'_i u'_j$ has known eigenvalues but unknown eigenvectors $v_{ij}$
- It can be proven that
  \[
  \text{Max}(P_k) \rightarrow v_{ij} = w_{ij}^U \\
  \text{Min}(P_k) \rightarrow v_{ij} = w_{ij}^U \mathcal{P} \quad (\text{with } \mathcal{P} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix})
  \]
We construct a family of models that represents possible Reynolds stresses states without introducing assumptions.
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- Chosen eigenvalues (1C, 2C and 3C) lead to asymptotic behavior (shape) of the stresses.
- Chosen eigenvectors ($w_{ij}^U$ and $Pw_{ij}^U$) lead to formal bounds for the kinetic energy production mechanism.
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Considering 6 computations \{1C, 2C, 3C | $w_{ij}^U$ \} and \{1C, 2C, 3C | $w_{ij}^U P$ \} we recover ALL possible RANS model predictions!
Turbulent flow over a backward facing step – $Re_h = 5100$
Numerical experiments, #2

Turbulent flow over an asymmetric diffuser – $Re_h = 2000$
## Numerical experiments, #3

<table>
<thead>
<tr>
<th>Case</th>
<th>Notes</th>
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<tbody>
<tr>
<td>1</td>
<td>Backward-facing step</td>
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<tr>
<td>2</td>
<td>Asymmetric diffuser</td>
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<td>3</td>
<td>Jet efflux of the NASA ARNozzle</td>
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<td>Heated jet efflux in Seiner nozzle</td>
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<td>ONERA Wing</td>
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<td>6</td>
<td>NACA 0012 airfoil at different angles of attack</td>
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<td>7</td>
<td>30P30N, Multi-element Airfoil</td>
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<td>8</td>
<td>JAXA wing body aircraft model</td>
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</tbody>
</table>
Summary – Part 2

Goal

Derive bounds for the Reynolds stresses describing the potential bias induced by assumptions used in turbulence models.

- Asymptotic states of the turbulence componentality determine the eigenvalues of the Reynolds stress.
- Max/Min of the energy transfer from mean flow to turbulent motion determine the eigenvectors of the Reynolds stresses.
- 6 solutions are required to construct envelopes to the actual model behavior. In practice, only 2 computations (1C and 3CP) appear to be sufficient.
- Approach is intrusive!
3 – Combining Uncertainty Estimates

Variability

Operating Conditions

Manufacturing Process

Bias

Combustion Kinetics Assumptions

Turbulence Modeling

$k$-$\varepsilon$

Inputs

Outputs

Ensemble of Enveloping Models
Design Under Uncertainty

**Design Goal:**
Minimize pressure loss in U-turn under uncertain inflow distortion

- Inflow described by 4 parameters; uncertainty quantified using PCE with $\Lambda^{TO}$, $n = 3$ and $r = 1.1$
- Shape defined by 8 FFD control points
- Turbulence model uncertainty described by e-space perturbations
- Simplex optimizer with single objective
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Effect of the inflow uncertainty:
- More distortion
- Less distortion
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- 1C Baseline 3CP
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**Effect of the inflow uncertainty:**
- More distortion
- Less distortion

**Effect of the turbulence model:**
- 1C Baseline 3CP

**Effect of design changes:**
Design Under Uncertainty

Design Goal:
Minimize pressure loss in U-turn under uncertain inflow distortion

<table>
<thead>
<tr>
<th></th>
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<tr>
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<td>191.1</td>
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Best Design

Worst Design
Design Under Uncertainty

Design Goal:
Minimize pressure loss in U-turn under uncertain inflow distortion

Best Design

Worst Design

Pressure Loss (Pa)

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Design Conclusion
Accounts for variance induced by inflow distortion and bias induced by modeling assumptions
Other Applications

PSAAP Program
Particle-laden Turbulence in a Radiation Environment

Experiments

Multifidelity UQ Analysis
Other Applications

CFM56 High Power Conditions

From deterministic to stochastic simulations, to tackle the effect of air temperature and fuel flow rate uncertainty.

Temperature duration ~20 ms

Intermittent, hot “bursts” on liner caused by unsteady JICF wakes

Temperature excursion on the combustor liners

Higher T in near field does not always mean higher T at exit

Temperature (normalized)

One standard deviation above and below the mean Temperature

Top liner

Bottom liner
Other Applications

- Multifidelity/Multidisciplinary Analysis
- Includes Turbulence Model uncertainty (Data-free and Data-driven UQ)
- Constrain Optimization Strategies
- Develop a comprehensive open-source framework for UQ+Design
Conclusions

This talk

Introduce a framework to characterize *variability* related to operating conditions and potential *bias* introduced by modeling assumptions.
Conclusions

This talk

Introduce a framework to characterize *variability* related to operating conditions and potential *bias* introduced by modeling assumptions

- Capture *Variability*: Balanced non-Intrusive Polynomial Chaos Approach
- Represent *Bias*: Enveloping (Intrusive) Turbulence Models
- Combined Approach to Perform *Design Under Uncertainty*


Thank you

Questions?
Discussion – Open Questions

Part 1
- How to handle cases with large number of uncertainties ($d > 10$)?
- The uncertainties are assumed to be bounded and independent. Can this be generalized?

Part 2
- Reynolds stress e-space definition is only based on local quantities. Can this represent spatially varying bias?
- The equation for the kinetic energy $k$ still includes unclosed terms...

Part 3
- What is the correct way of combining bias and variability measures? i.e. combined uncertainties?
- How do you formulate more comprehensive optimization objectives?