Uncertainty Quantification in Turbulence Modeling

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July 12, 2017

Outline

The Turbulence Prediction Problem

Turbulence ubiquitous feature of high Re fluid flows

- Has an $O(1)$ affect on the flows in which it occurs
  - Transport of momentum, heat, species $\Rightarrow$ drag and separation resistance, surface heating/cooling, surface reactions
  - Mixing of heat, species... $\Rightarrow$ quenching, enhanced combustion
- Need to predict effects on turbulence for design & operations
  - Solve the Navier-Stokes equations for turbulence (DNS)
  - Model the effects of turbulence: RANS or LES

- We understand the microphysics (i.e. the N-S equations), but struggle to predict the macroscopic behavior (a common situation)
- Critical to know what we are trying to predict (the QoI)

The Pedigree of a RANS Model

Predict Some Average Properties of Turbulent Flow

- Turbulence is chaotic, but averages appear stable (predictable)
- Averages (e.g. heat flux, heat release) of primary interest
- Sufficient to solve for just the average flow

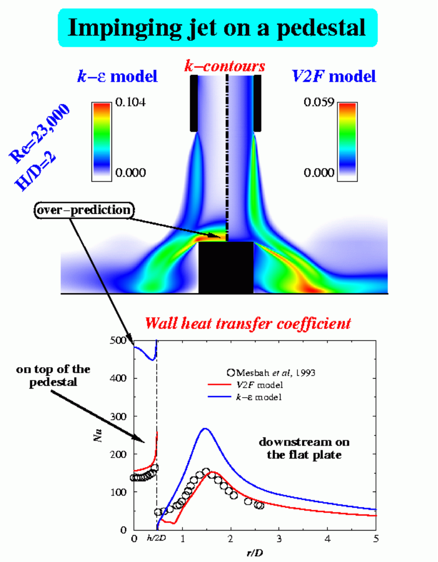
- Conservation of mean momentum (e.g. incompressible):

$$\partial_t U_i + \partial_j U_i U_j = -\partial_i P + \partial_j (\nu \partial_j U_i - \overline{u'_i u'_j})$$

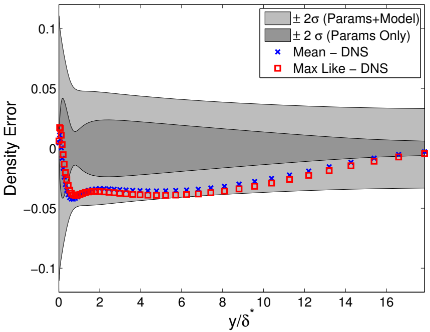
  - Where applicable, validity of RANS equations is NOT in doubt
  - But, $\overline{u'_i u'_j}$ is not known in terms of U_i (closure problem)
- Closed models for $\overline{u'_i u'_j}$ are generally "derived" based on usually well articulated but questionable modeling assumptions
  - These models are known to be unreliable
  - These models are widely used in engineering

A RANS Prediction Failure

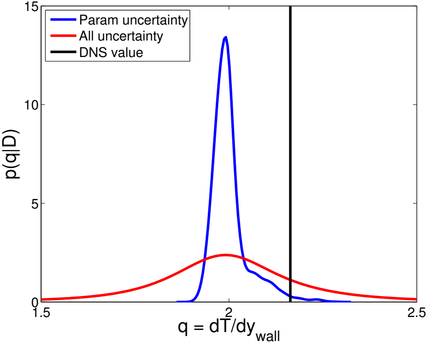
- k–ϵ model used to predict heat transfer from a computer chip with an impinging air flow
  - Heat transfer over-predicted
  - Cooling fans under-sized
  - Computers overheated
- Now understood as the “stagnation point anomaly” (Durbin)
  - Durbin developed $v^2 f$ model to correct
  - Better to detect effect of k–ϵ inadequacy



Parameter Uncertainty Not Enough: Compressible TBL



Predicting the Data



Predicting a QoI ($\partial T/\partial y\big|_{wall}$)

- Errors (compared to DNS) are too large to be explained by uncertainty in the model parameters
- Representation of model inadequacy is consistent with the errors
- Ignoring inadequacy yields invalid predictions

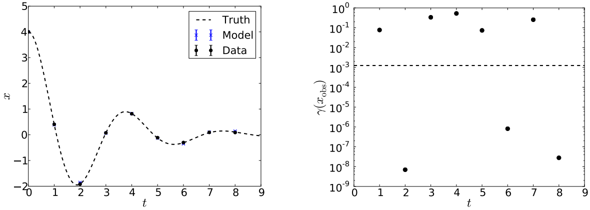
Why Model & Simulate Turbulent Flows?

- We want to make predictions about the flow
  - Support design & decision making
- Predictions are calculations of specific quantities (quantities of interest, QoIs) for which no corroborating data are available.
  - Fundamentally an extrapolation from available information
  - e.g. predict performance before a device is built, or response to a new condition
- But, our (turbulence) models are not reliable.
  - They do not rise to the status of reliable scientific theory
  - They are known to be inconsistent with observations

What gives us the right to make such predictions?

Validation for Predictions

- In comparing models to experiments there are always discrepancies, what do they mean?
  - Discrepancies within the uncertainties of the experiments and models are expected–UQ is necessary for meaningful validation
  - What about larger discrepancies?



  - The calibrated model and the observations in excellent agreement
  - It is highly improbable that data and model are consistent
  - I want to use this model! It is "inadequate," does it matter?

Interpreting Validation Results

A Validation Paradox

- Consistency with observations $\not\Rightarrow$ valid predictions
  - Observation may be insensitive to errors that the QoI is sensitive to
- Inconsistency with observations $\not\Rightarrow$ invalid predictions
  - Observation may be sensitive to errors that the QoI is insensitive to

- If the validation data is not consistent with the model, we have no "right" to make a prediction.
  - The model errors responsible for the observed discrepancies could also produce significant errors in the QoI.
  - But then again, they might not
  - To know which, need to represent the uncertainty due to the model error
- Enrich the erroneous model with a probabilistic representation of the model error

RANS as a "Composite Model"

A composite model is the combination of a reliable but unclosed theory, with a generally less reliable *embedded model* for closure

- Reliable theory: Conservation of mean mass, momentum & energy, e.g.:

$$\partial_t U_i + \partial_j U_i U_j = -\partial_i P + \partial_j(\nu \partial_j U_i - \overline{u_i' u_j'})$$

  - Validity not in question in scenarios of interest
- Embedded model: Reynolds stress closure $\overline{u_i' u_j'} \approx \overline{u_i' u_j'}^m$
  - This is the source of modeling errors
  - Assuming reliable auxiliary data (e.g. BCs) and reliable measurements, this is the cause of discrepancies with observations
- Representation of error determined from observations as

$$\overline{u_i' u_j'} \approx \overline{u_i' u_j'}^m + \epsilon_m$$

- Composite structure allows error to propagate through reliable theory to unobserved QoI

Reliable Predictions with RANS? Really?

- Yes if:
  - Model formulated within a reliable theory (e.g. conservation laws)
  - Unreliable components (embedded models such as Reynolds stress closure) enriched with a probabilistic representation of uncertainty due to any model error
  - Probabilistic model error representations account for all discrepancies between model and observations
  - In the prediction, enriched embedded models are used in conditions for which they have been well calibrated and validated
- In this case, we extrapolate with the reliable theory, but not the unreliable embedded model.

Two common challenges

- Obtaining sufficient data that is informative for parameters/model inadequacy and relevant to prediction
- Representing the uncertainty introduced by model error

Outline

Challenges with data

- Data is required to
  - Inform model parameters and inadequacy representation
  - Assess performance of calibrated model away from calibration scenario
- Data used must be informative to the model in the context of the prediction scenario
- Can be a problem for turbulent flow: Despite plethora of turbulence data sets from both experiment and DNS, data required for a particular application may be sparse

Example: High-speed, reacting, turbulent boundary layers

- Existing high-quality experimental data sets not sufficiently informative
- Existing DNS data sets not sufficiently rich (e.g., not much with reactions and pressure gradients)
- Solution: Formulate new DNS model problem to supply directly relevant data

Experimental Data Literature Search

Data Selection Criteria (Settles and Dodson [1993])

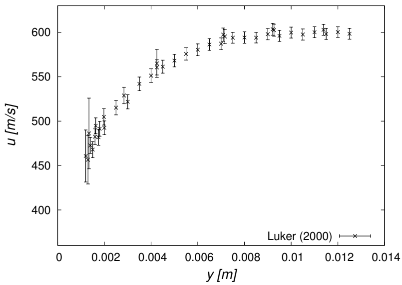
- **Applicability:** Experimental scenario and observables must be relevant to turbulence model predictions for supersonic BL
- **Simplicity:** Experiment must be simple enough to simulate relatively easily and cheaply
- **Characterized BCs:** Data set should supply BC information
- **Uncertainty Analysis:** Data set must provide measurements *and* quantitative, systematic uncertainty estimates

Results

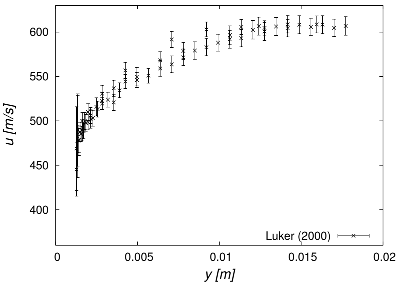
- BC and uncertainty requirements difficult to satisfy
- Identified work of Bowersox and co-authors as a good source of data from compressible, non-reacting, boundary layer flow

Sample Bowersox Supersonic BL Data

ZPG Velocity



FPG Velocity



- **Applicability:** ZPG and FPG, mean and turbulence measurements
- **Simplicity:** Experimental geometry and scenarios well-defined
- **Characterized BCs:** Mean velocity profile measured upstream
- **Uncertainty Analysis:** "Textbook" assessment (linearized propagation, independent effects) provides confidence intervals

Calibration via Baysian Inference

$$p(\theta|D) \propto p(D|\theta)p(\theta)$$

Bayes' theorem yields parameter uncertainties given data uncertainties

Problem Statement

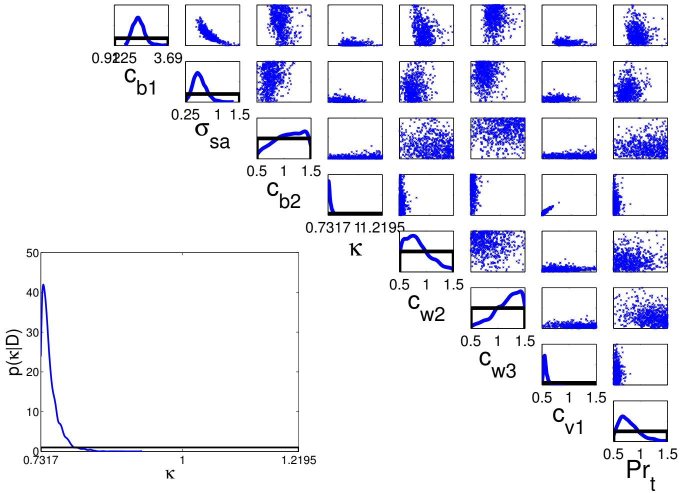
- Physical model: RANS+Spalart-Allmaras
- Prior: Uniform
- Likelihood: Gaussian

$$p(D|\theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi(\sigma_{exp}^2 + \sigma_{cal}^2)}} \exp\left[-\frac{1}{2}\frac{(D_i - f_i(\theta))^2}{\sigma_{exp}^2 + \sigma_{cal}^2}\right]$$

Comments

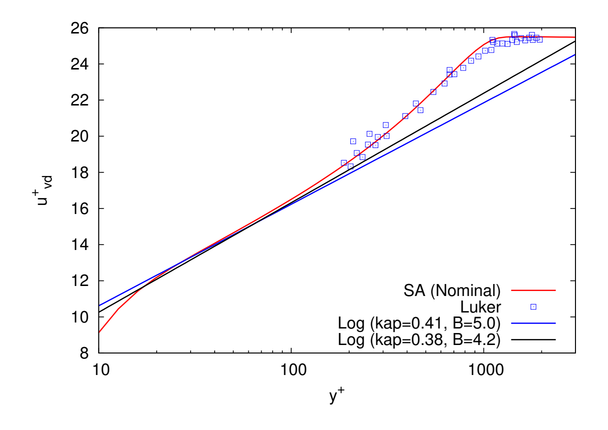
- These choices are overly simplistic
- Seek to understand the effect of the data

Posterior PDF



$\kappa/\kappa_0 \leq 0.75$ strongly conflicts with prior knowledge

What is going on? Lack of Near Wall Data



- Closest measurement point is at $y^+ \approx 180$
- Very few (zero?) points in log-layer
- κ not constrained as it should be $\Rightarrow$ abused to fit outer layer

Observations

From this compressible calibration effort

- Lack of near-wall data means some parameters not appropriately informed
- Model inadequacy results in those parameters being abused to correct errors *when allowed by the prior*
- Can overcome this behavior using a stronger prior, but near-wall data is necessary to appropriately inform model parameters

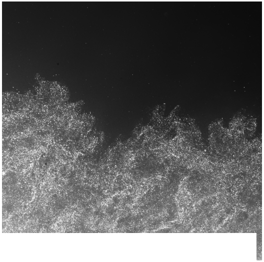
More generally

- Data sparsity *worsens* as problem becomes more complex. E.g. Reentry vehicle heat shield BL
  - Cold, ablating wall
  - Chemically reacting flow
- To capture these phenomena and get near-wall data, need to look beyond legacy data for calibration purposes

Options for Generating Calibration Data

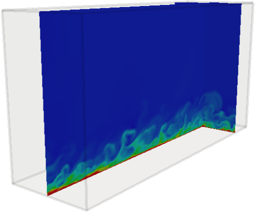
TBL Experiments

Advantages	*Disadvantages*
• Physical reality	• Difficult to obtain near-wall data
• Higher Re	• Uncertainty characterization



Direct Numerical Simulation

Advantages	*Disadvantages*
• Measure any statistic	• A model
• Better control	• Low Re



Conclusion

Use DNS primarily for calibration; reserve experiments for validation

Slow Growth Formulation Background

Difficulty with spatially developing BL DNS

- Complicated by streamwise inhomogeneity
  - Must generate inflow data
  - Long streamwise domain required to “wash out” inflow effect
- Do we need true spatially developing boundary layer data?
  - Probably not: Use multiple scale analysis to model “slow” spatial development
  - Resulting problem is homogeneous in streamwise direction
  - Successful TBL DNS using homogenized equations
    - Spalart (1988): Incompressible TBL
    - Guarini et al. (2000): Compressible TBL

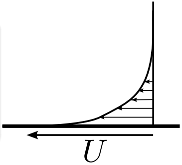
Difficulty with Guarini approach

- Fairly complex modeling required would be difficult to pursue in context of turbulence model equations
- Need the homogenization terms to be closed in RANS

Temporal Slow Growth Formulation

Motivating flow: Rayleigh Problem

- At $t = 0$, impulsively start infinite plate with velocity U
- BL homogeneous in space but *not stationary*



Slow temporal development

- Define two time variables: $t_f = t$, $t_s = \epsilon t$ where $\epsilon \ll 1$
- Assume mean and RMS depend only on slow time variable:

$$U(x, y, z, t) = \overline{U}(y, t_s) + U_{RMS}(y, t_s)U'(x, y, z, t_f)$$

- Navier-Stokes equations become

$$\frac{\partial U}{\partial t_f} + \epsilon \frac{\partial U}{\partial t_s} + N(U) = 0$$

- Idea: Simulate at single point in slow time by *modeling* slow evolution

Slow Growth Source Terms

- Model slow time evolution:

$$S(U) \approx -\epsilon \frac{\partial U}{\partial t_s} \Rightarrow \frac{\partial U}{\partial t_f} + N(U) = S(U)$$

- Assuming similarity in mean and RMS quantities, i.e.,

$$\bar{U}(y, t_s) = U_\infty(t_s) F(\eta), \quad U_{RMS}(y, t_s) = U_{RMS,A}(t_s) G(\eta)$$

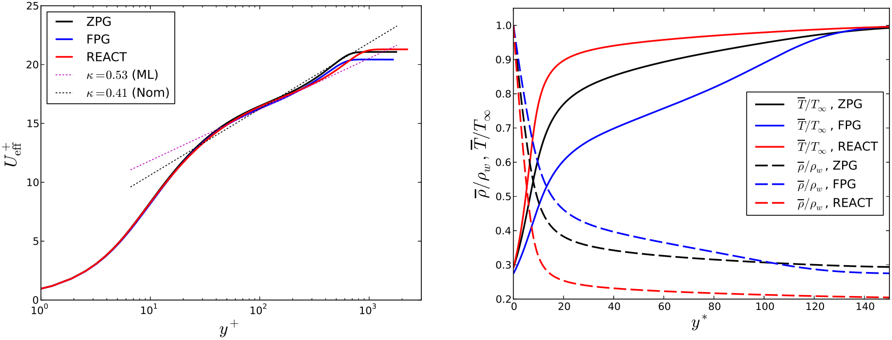
where $\eta = y/\Delta(t_s)$ and Δ is an appropriate length scale

- The source term can be shown to be

$$S(U) = -\frac{U}{U_\infty} \frac{\partial U_\infty}{\partial t_s} + \frac{\partial \Delta}{\partial t_s} \frac{y}{\Delta} \left(\frac{\partial \overline{U}}{\partial y} + \frac{U'}{U_{RMS}} \frac{\partial U_{RMS}}{\partial y} \right)$$

These models have been developed for compressible reacting flows with pressure gradients, and are easily closed in common RANS formulations

DNS Results



3 Cases Inspired by reentry vehicle heat shields

- ZPG: Zero pressure gradient, Non-reacting, $M_\infty = 1.2$, $Re_\theta = 420$, $T_{wall}/T_\infty = 0.29$, $v^+_{wall} = 0.019$
- FPG: Favorable pressure gradient, Non-reacting, $M_\infty = 0.8$, $Re_\theta = 368$, $T_{wall}/T_\infty = 0.27$, $v^+_{wall} = 0.020$
- REACT: Zero pressure gradient, 5 species air $M_\infty = 1.2$, $Re_\theta = 438$, $T_{wall}/T_\infty = 0.29$, $v^+_{wall} = 0.019$

Calibration Overview

Physical Model and Parameters

- Favre-averaged Navier-Stokes + Spalart-Allmaras turbulence model
- 9 physical model parameters (7 SA model parameters, Pr_t, Le_t)

Data and Data Uncertainty

- Three DNS cases from previous slide
- Data uncertainty from sampling error estimate

Model Uncertainty

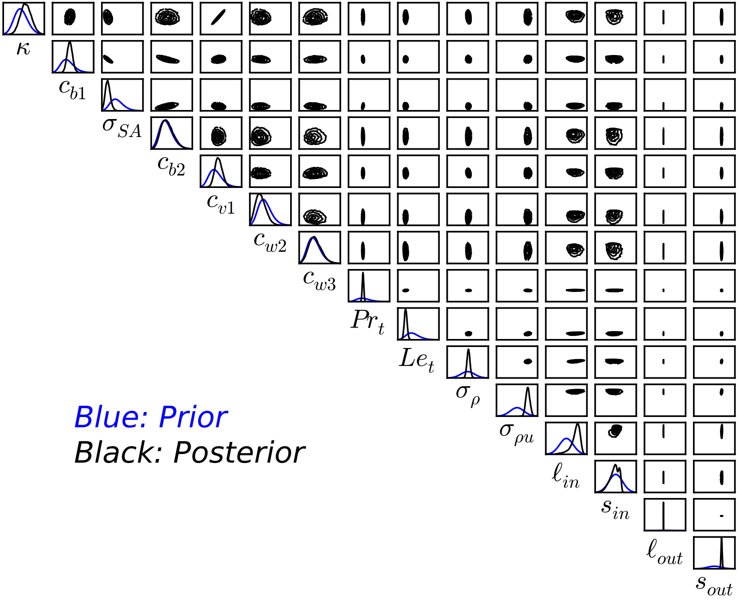
- Variable length scale multiplicative Gaussian process, e.g., for density

$$\rho_{\text{true}} = (1 + \epsilon_\rho)\rho_{\text{rans}}, \quad \epsilon_\rho \sim N(0, k(y, y')),$$

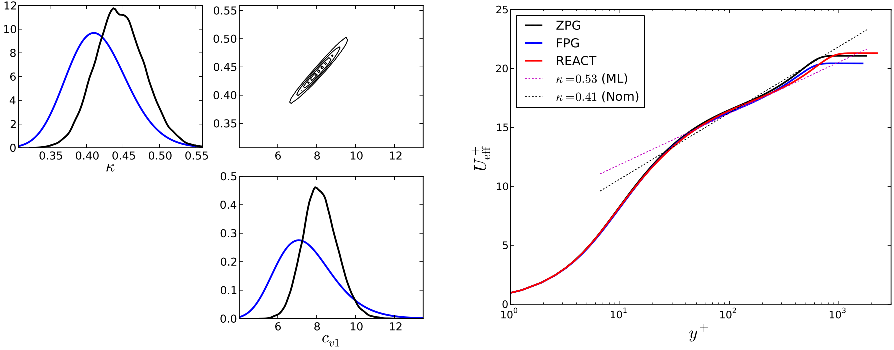
$$k(y, y') = \sigma_\rho^2 \left(\frac{2\ell(y)\ell(y')}{\ell^2(y) + \ell^2(y')} \right)^{1/2} \exp\left[\frac{-(y - y')^2}{\ell^2(y) + \ell^2(y')} \right]$$

- Adds total of 6 parameters to calibration problem

Sample Calibration Results: All Parameters



Sample Calibration Results: κ, c_{v1}



Observations

- Posterior for Karman constant κ shifted to the right relative to prior
- Posterior for c_{v1} also shifts to right b/c of correlation
- Large values for κ are consistent with low Re effects

Outline

Model Inadequacy in RANS

Mean conservation of momentum

$$\partial_t U_i + \partial_j U_i U_j = -\partial_i P + \partial_j(\nu \partial_j U_i - \overline{u_i' u_j'})$$

- Where applicable, validity of RANS equations is NOT in doubt
- But, $\overline{u_i' u_j'}$ is not known in terms of U_i (closure problem)

Standard eddy-viscosity-based closure

$$-\overline{u_i' u_j'} = \tau_{ij} = 2\nu_t S_{ij} - \frac{2}{3} k \delta_{ij}$$

where S_{ij} is mean strain rate tensor

Model inadequacy idea

$$-\overline{u_i' u_j'} = \tau_{ij} = 2\nu_t S_{ij} - \frac{2}{3} k \delta_{ij} + \zeta_{ij}$$

where ζ_{ij} is *random tensor field*

Channel Flow Example

Incompressible, fully-developed channel flow

- Simplest possible wall-bounded flow
- Calibrate and assess stochastic model using DNS
  - $Re_\tau = 944,\ 2003$ [del Alamo et al., 2004; Hoyas et al., 2006]
  - $Re_\tau \approx 5200$ [Lee et al., 2013]

Mean Momentum

$$-\frac{d}{d\eta}\left(\frac{1}{Re_\tau}\frac{d\langle u\rangle^+}{d\eta} + \tau^+\right) = 1$$

Errors

- Mean velocity: $e^+ = \langle u\rangle^+ - \bar{u}^+$
- Reynolds shear (a priori): $\zeta = \tau^+ - \nu_t(\langle u\rangle^+)\, d\langle u\rangle^+/dy$

Channel Flow Uncertainty Propagation

Following the a priori approach:

$$-\frac{d}{d\eta}\left[\left(\frac{1}{Re_\tau}+\nu_t(\bar{u}^+)\right)\frac{de^+}{d\eta}+\Delta\nu_t\left(\frac{d\bar{u}^+}{d\eta}+\frac{de^+}{d\eta}\right)\right]=\frac{d\zeta}{d\eta}$$

where

$$\Delta\nu_t=\nu_t(\bar{u}^+ + e^+)-\nu_t(\bar{u}^+)$$

- Clearly do not know ζ exactly $\Rightarrow$ Need a model
- Use probability to represent uncertainty $\Rightarrow$ Random field models
- Would like ζ to be consistent with knowledge of physics

A Model For Reynolds Stress Error

Motivation/Inspiration

- True Reynolds stress satisfies Reynolds stress transport equation
- Modeled Reynolds stress does not, but residual is not computable

$$\mathcal{R}(\tau) = \mathcal{R}(\tau^m + \zeta) = 0 \quad \Rightarrow \quad \mathcal{R}'[\tau^m](\zeta) \approx -\mathcal{R}(\tau^m)$$

The model (for channel flow case)

$$\underbrace{-C_p \frac{d\bar{u}}{dy}\zeta}_{\text{“Production”}} \underbrace{+C_p \frac{3}{2}\frac{\sqrt{\tau^m}}{y}\zeta}_{\text{“Dissipation”}} \underbrace{-\frac{d}{dy}\left((\nu + C_\nu \nu_t(\bar{u}))\frac{d\zeta}{dy}\right)}_{\text{“Diffusion”}} = C_\sigma \underbrace{\sqrt{\frac{s^2}{\ell}}\frac{dW}{dy}}_{\text{“Residual”}}$$

where $s = u_\tau^3$, $\ell = u_\tau/(\partial u/\partial y)$

- LHS: Simplistic modeling and dimensional analysis
- RHS: Don’t know correct residual, so choose white noise
- Set parameters C_p, C_ν, and C_σ via Bayesian calibration

Bayesian Calibration Problem

- Most obvious approach uses only DNS mean velocity:

$$p(C_p, C_\nu, C_\sigma | \langle u \rangle^+) \propto p(\langle u \rangle^+ | C_p, C_\nu, C_\sigma)\, p(C_p, C_\nu, C_\sigma)$$

- Challenging because $p(\langle u \rangle^+ | C_p, C_\nu, C_\sigma)$ is difficult to evaluate
  - Requires forward propagation of high-dimensional uncertainty
- Alternatively, using DNS mean velocity and Reynolds stress, can treat the true error ζ_{true} as the observable:

$$p(C_p, C_\nu, C_\sigma | \zeta_{true}) \propto p(\zeta_{true} | C_p, C_\nu, C_\sigma)\, p(C_p, C_\nu, C_\sigma)$$

- Evaluating $p(\zeta_{true} | C_p, C_\nu, C_\sigma)$ is easy (it's Gaussian!)

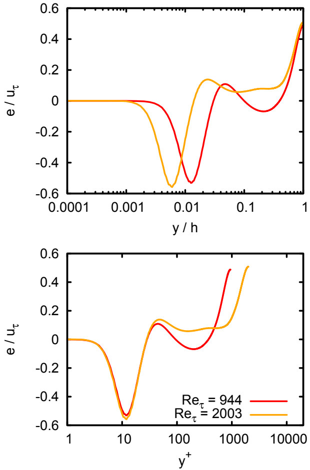
The likelihood becomes

$$p(\zeta_{true} | C_p, C_\nu, C_\sigma) = \frac{\exp\left(-\frac{1}{2} \zeta_{true}^T (L^{-1} M L^{-T})^{-1} \zeta_{true}\right)}{\sqrt{(2\pi)^N \det(L^{-1} M L^T)}}$$

where L and M are discrete operators that depend on C_p, C_ν, C_σ

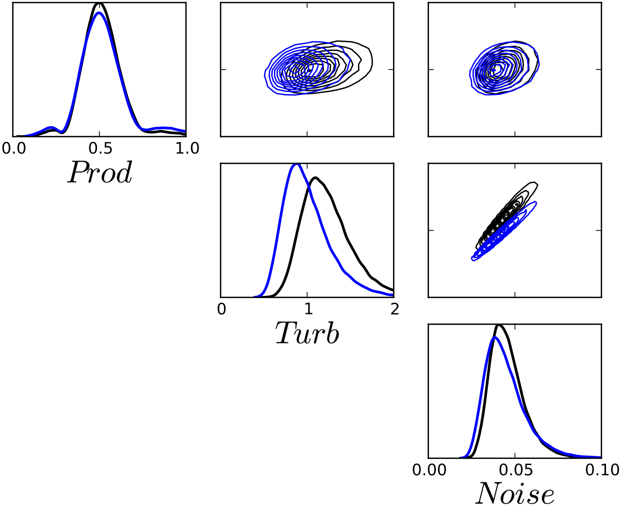
Channel Flow Results Overview

- Fully-developed, incompressible channel flow
- Turbulence model: Spalart–Allmaras
  - Similar results with other models
- Available DNS data
  - $Re_\tau = 944, 2003$ [del Alamo et al., 2004; Hoyas et al., 2006]
  - $Re_\tau \approx 5200$ [Lee et al., 2013]
- Calibrate with $Re_\tau = 944, 2003$ DNS
- Test against $Re_\tau \approx 5200$ DNS



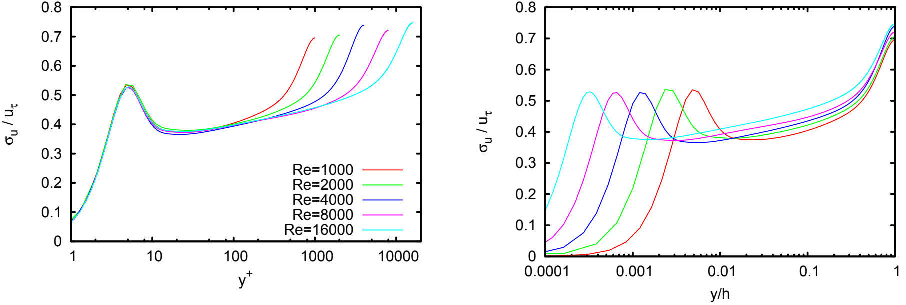
Look for expected collapse in inner and outer layers as well as any Re dependence in inverse or forward results

Calibration Results



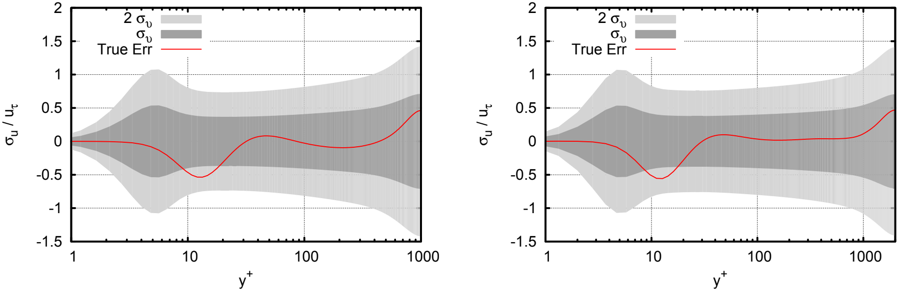
Black: $Re_\tau = 1000$, Blue: $Re_\tau = 2000$

Forward Propagation: Scaling with Re



- Forward propagate ζ uncertainty to $\langle u \rangle$ using posterior mean for C_p, C_ν, C_σ obtained at $Re_\tau = 1000$
- Resulting standard deviation of u shows good collapse with usual non-dimensionalizations
- Inner peak qualitatively similar to true error

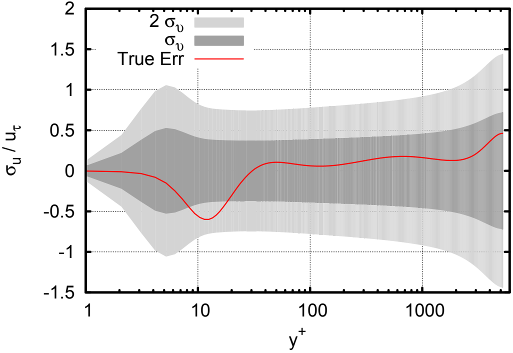
Forward Prop: Comparison Against Calibration Data



$Re_\tau = 1000$ $Re_\tau = 2000$

- $\pm 2\sigma$ covers true velocity error in both cases
- Shape of σ is qualitatively similar to true error
- But, inner peak is in the wrong location ($y^+ \approx 6$ instead of 12)
- Some potential to improve by relaxing relation between production and dissipation terms in model (adds another calibration parameter)

Forward Propagation: Comparison Against $Re_\tau = 5200$



- Qualitatively the same as lower Re results
- Gives confidence that model can successfully extrapolate in Re

RANS/Flamelet Modeling for Turbulent Reacting Flow

- Model equations for $\tilde{u}$, $\tilde{v}$, $\bar{p}$, k, ϵ, $\tilde{z}$, $\widetilde{z''^2}$
  - Typical RANS modeling: eddy viscosity, gradient diffusion, etc.
- Resulting PDEs depend on mean temperature, which depends on chemistry
  - Chemistry uncertain due to Arrhenius rate parameter uncertainty and/or mechanism inadequacy
- Closure for mean temperature based on "flamelet library":

$$\tilde{T} = \int_0^\infty \int_0^1 \underbrace{T(z, \chi_{st})}_{\text{Laminar diffusion flame}} \underbrace{\tilde{p}(z) p(\chi_{st})}_{\text{Assumed PDFs}} \, dz \, d\chi_{st}$$

  - Basic enabling assumption: Chemical length & time scales small relative to turbulence ⇒ May represent turbulent flame via ensemble of laminar flames
  - $T(z, \chi_{st})$ is random field because of uncertain chemistry
  - Many other potential inadequacy sources (e.g., assumed PDF forms)

Inadequacy of flamelet model

- Even when basic enabling assumption is reasonable, the flamelet model of average thermodynamic and chemical state suffers from many modeling errors, e.g.
  - Errors in the model equations for $\tilde{z}$ and $\widetilde{z''^2}$
  - Errors in the reconstruction of $\tilde{\chi}$ and $\widetilde{\chi''^2}$
  - Errors due to choice of dependencies for thermo-chemical state
  - Errors in the assumed PDF for z and χ_{st}
- All these errors manifest as uncertainties in the reconstructed average thermo-chemical state

Stochastic Assumed PDF Model: Main Ideas

1. Represent inadequacies as uncertainties in the PDF for z and χ_{st}
2. Generate PDF perturbations by maximizing the KL divergence relative to original PDF for a given moment perturbation
3. Enrich deterministic model with stochastic PDEs to generate uncertain moment perturbations

Example Uncertain PDF Model (1)

- Standard assumed PDF $q(z)$ is β-distribution with parameters determined by $\tilde{z}$ and $\widetilde{z''^2}$
- Main idea: Given perturbation of implied third moment δ, determine new PDF $p(z)$ that maximizes $D_{KL}(p||q)$ while matching $\tilde{z}$, $\widetilde{z''^2}$ and perturbed third moment
- Solution of this problem given by

$$p(z) = \exp\left[\sum_{n=0}^{3} \lambda_n z^n - 1\right] q(z).$$

  where λ_n are Lagrange multipliers
- In discretized combustion model, requires nonlinear system for λ_n at each quadrature point
- Simplify by linearizing about q

Example Uncertain PDF Model (2)

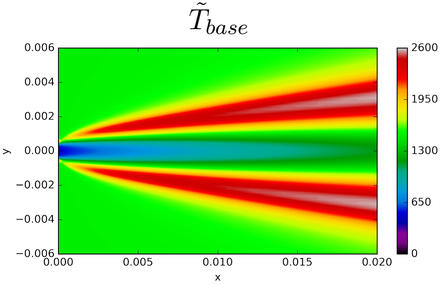
- To complete model, provide a perturbation of the third moment
- Based on exact transport equation for $\widetilde{z''^3}$, a plausible stochastic model for $\widetilde{z''^3}$ is

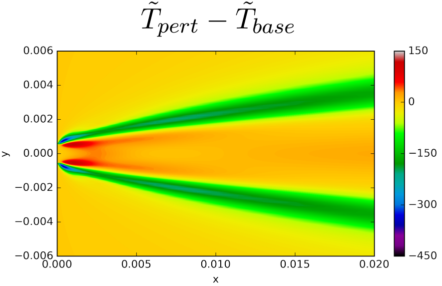
$$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{z''^3}\right) + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\widetilde{z''^3}\right) = \frac{\partial}{\partial x_i}\left(\bar{\rho}(\bar{\mathcal{D}} + \mathcal{D}_t)\frac{\partial\widetilde{z''^3}}{\partial x_i}\right) + 3\frac{\mu_t}{Sc_t}\frac{\partial\tilde{z}}{\partial x_i}\frac{\partial\widetilde{z''^2}}{\partial x_i} - 6C_3\,\frac{\bar{\rho}\widetilde{z''^3}}{\tau} + R$$

where R is a random forcing term constructed to be non-zero only in the flame zone

Sample Turbulent Jet Flame Results

Infinitely Fast, Irreversible Chemistry

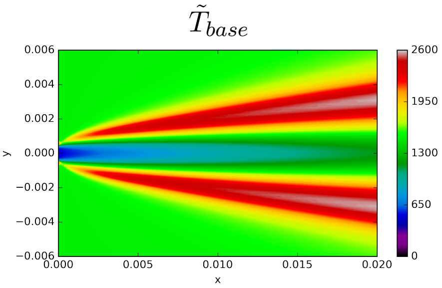


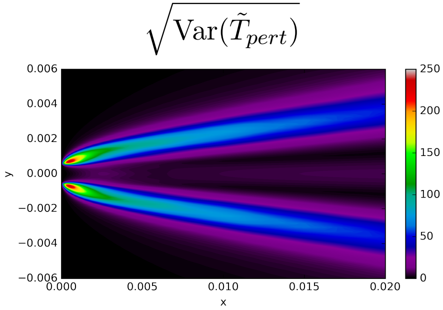


- Left figure: Baseline model predicted mean temperature
- Right figure: Difference between baseline and perturbed model with deterministic $\widetilde{z''^3}$ equation
- Perturbing the assumed PDF can have a substantial impact on $\tilde{T}$

Sample Turbulent Jet Flame Results

Infinitely Fast, Irreversible Chemistry





- Left figure: Baseline model predicted mean temperature
- Right figure: Standard deviation of mean temperature induced by stochastic $\widetilde{z''^3}$ model

Summary

"Predictive validation" provides a coherent, defensible framework for approaching validation of predictions of unobserved quantities based on mixed fidelity models like those commonly used in turbulent flow predictions

Data sufficiency and model inadequacy are common challenges

- Many turbulence problems admit development of computationally tractable DNS model problems for generation of calibration and validation data
- Model inadequacy representations must target the source of modeling errors (turbulence closures)
- SPDEs offer a promising modeling framework for using physical knowledge and intuition while randomly perturbing ad hoc or suspect modeling assumptions that lead to inadequacy