Treating Uncertainty due to Model Error with Applications to RANS Turbulence Models and Chemical Kinetics

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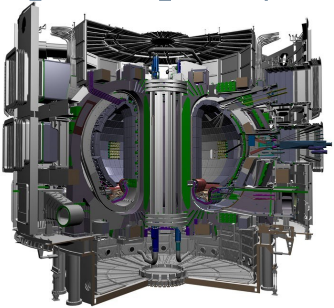
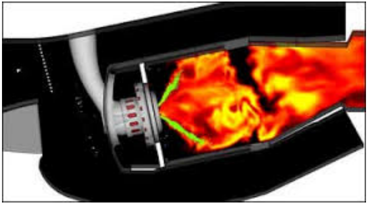
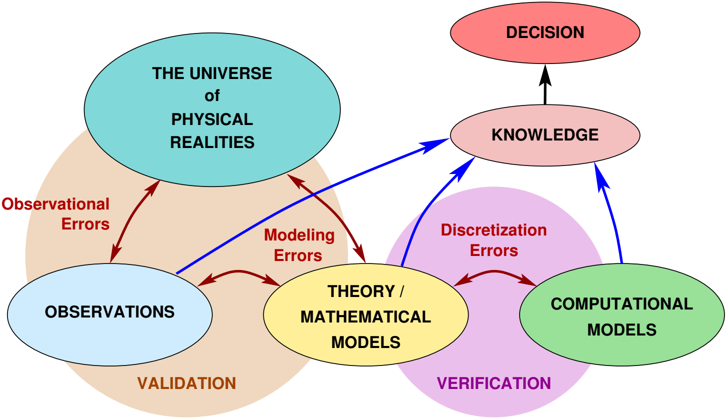
Engineering Complex Systems





Models of such complex system are generally imperfect

Imperfect Paths to Knowledge and Predictive Simulation



Prediction is difficult, especially if it is about the future — N. Bohr

Simulations have a Purpose

To inform some decision (e.g. for design, operations or control)

- Quantities are predicted to inform the decision
- These are the *Quantities of Interest* (QoIs)
- Must predict QoIs for which confirming observational data is not available
  - Otherwise, predictions would not be needed
  - Many reasons why there is no data (e.g. system is not built yet)

Computational models are not scientific theories

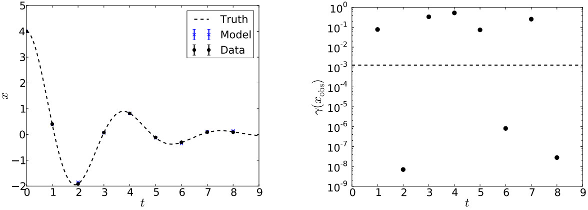
Their validity depends on their purpose:

- The QoIs to be predicted
- The required accuracy

Fundamental question: What entitles us to make predictions?

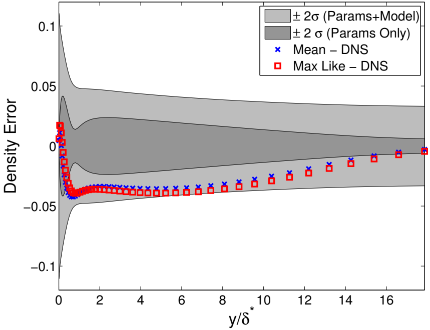
Validation for Predictions

- 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?

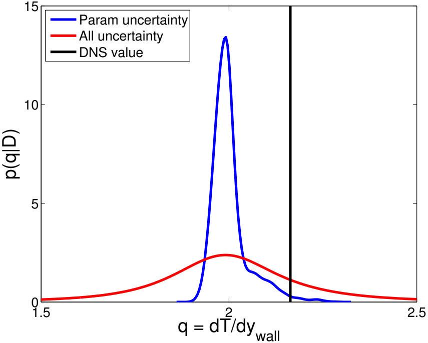


  - The calibrated model and the observations in excellent agreement
  - It is highly improbable that data and model are consistent
  - I want to use this model! It is “inadequate,” does it matter?
- Need to include uncertainty due to model inadequacy!

Realistic Example—A Turbulence Model Prediction



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

Interpreting Validation Results

A Validation Paradox

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

Composite Model Structure

Physics-based composite model:

$$\mathcal{R}(u, \tau; r) = 0 \quad \text{(Highly reliable)}$$

$$\tau = m(u; \theta, s) \quad \text{(Embedded model)}$$

Or

$$\tau = m(u; \theta, s) + \boldsymbol{\epsilon}_{mod}(u; \alpha, s)$$

Measurement model:

$$\mathbf{d} = \mathbf{d}(u, \tau; r) + \boldsymbol{\epsilon}_{exp}$$

Quantity of Interest model:

$$\mathbf{q} = \mathbf{q}(u, \tau; r)$$

- τ: unclosed quantity in $\mathcal{R}$
- θ, α: uncertain model parameters
- r, s: scenario parameters

Model structure allows uncertainty due to model error to be informed by observations and propagated to QoIs

An Example: Spring-Mass-Damper System

Prediction Scenario and QoI

Want to predict the *maximum velocity* of a given mass ($m = 5$) for a given initial condition ($x = 4$, $\dot{x} = 0$)

Physical Model

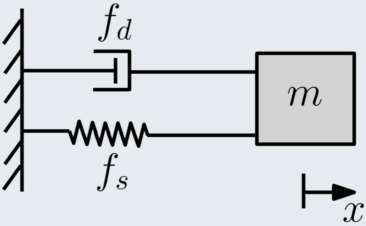
- Reliable model: $F = ma$ implies

$$m\ddot{x} = f_d + f_s$$

- Embedded models:

$$f_s = -kx$$
$$f_d = -c_o\dot{x}$$

with k and c_o constant



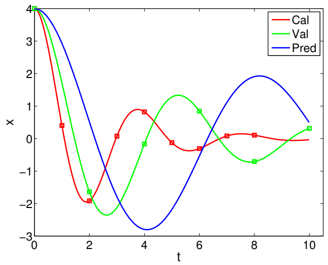
Reality and Data

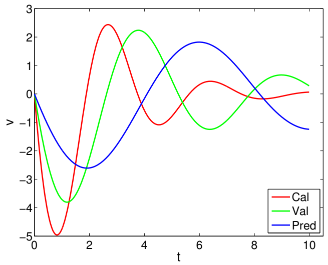
Reality: Damper not constant coefficient

$$f_d = -c(t)\dot{x} \;\Rightarrow\; m\ddot{x} + c(t)\dot{x} + kx = 0$$

where $c(t)$ related to temperature variation in the damping fluid.

Data: “Real” system with correct ICs but smaller masses





- 8 measurements of position vs time for $m = 1$
- 8 measurements of position vs time for $m = 2$

Models of Uncertainty due to Inadequacy

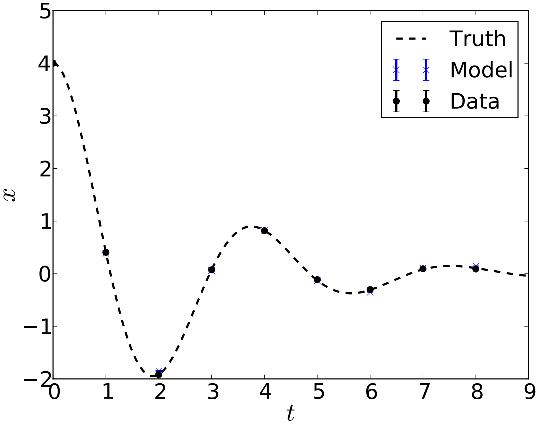
Reflect what we know about the system, so we must be explicit about what we know.

The Denial Model: Parameter Uncertainty Only

- Constant k spring model is presumed a good approximation (no inadequacy)
- Constant c_o damper model is presumed a good approximation (no inadequacy)
- Values of k and c_o not well known

Determine k and c_o via Bayesian inference based on $m = 1$ data

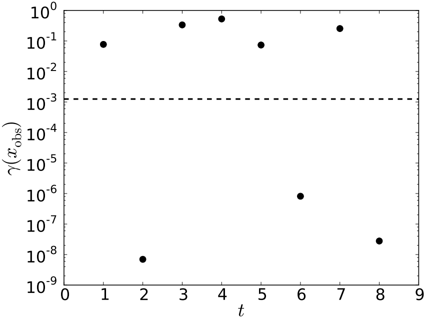
Posterior Predictive Check of Denial Model

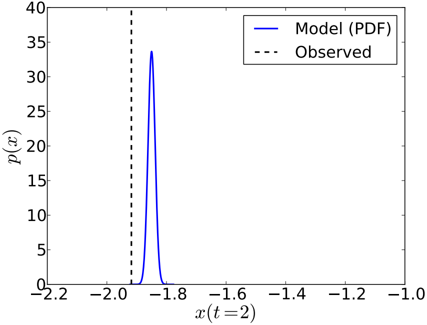


Comments

- Qualitatively, prediction not too bad—trends correct

Posterior Predictive Check of Denial Model





Comments

- Qualitatively, prediction not too bad—trends correct
- But, uncertainties much to small to explain some discrepancies
- γ is HPD metric (highest posterior density)
- Cannot proceed to further validation checks or prediction

The Inadequate Damper Model

Model Uncertainty in Damper Representation

- Constant k spring model is presumed to be a good approximation
- Suspect that a constant c_0 model is inadequate
- Hypothesize that non-constant behavior caused by damper fluid temperature changes
  - e.g. noticed that damper gets warm

- Note: Information about why the model may be inadequate is important
  - Can constrain an inadequacy model
  - Provides a basis for assessing the domain of applicability of models, including inadequacy

The Inadequate Damper Model

Model

- Physics:

$$m\ddot{x} + c\dot{x} + kx = 0$$

- Uncertainty:

$$c \sim \log \mathcal{N}(c_\mu, c_\sigma^2)$$

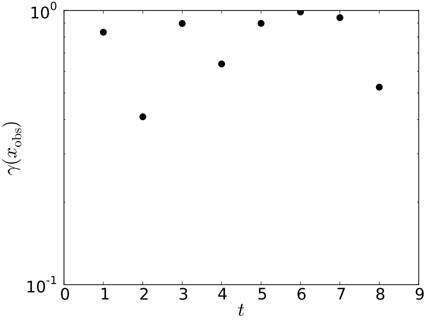
- Joint Bayesian calibration of k, c_μ, and c_σ

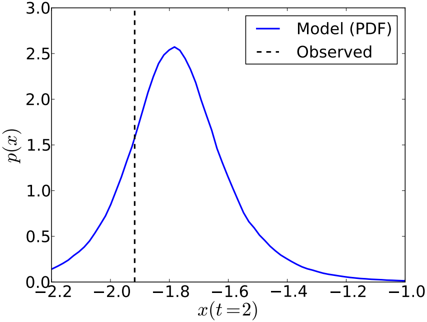
Likelihood

Requires marginalizing c:

$$p(D_i|k, c_\mu, c_\sigma) = \int p(D_i|k, c)p(c|c_\mu, c_\sigma)\, dc$$
$$p(\mathbf{D}|k, c_\mu, c_\sigma) = \Pi_{i=1}^{M} p(D_i|k, c_\mu, c_\sigma)$$

Posterior Predictive Check of Inadequate Damper Model ($m = 1$)

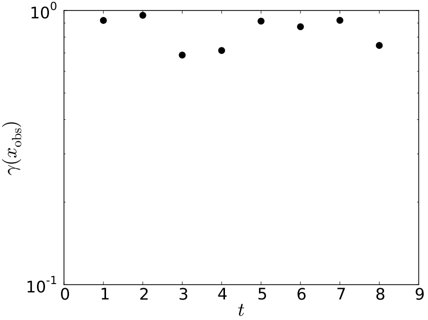


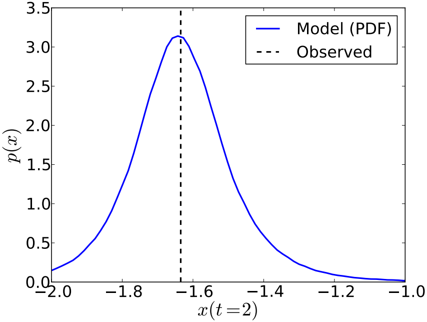


Observations

- All $m = 1$ data within prediction uncertainty
- No small γ values

Posterior Predictive Check of Inadequate Damper Model ($m = 2$)





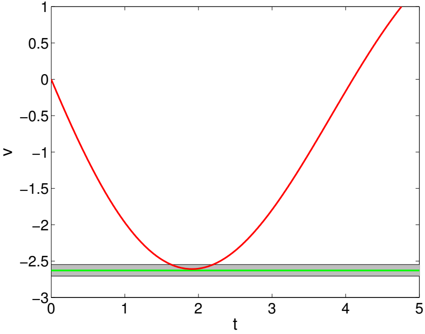
Observations

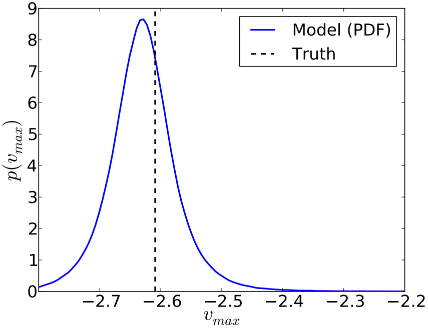
- All $m = 2$ data within prediction uncertainty
- No γ values close to zero

QoI Prediction ($m = 5$) with Inadequate Damper Model

Do Validation Tests give Confidence in the Prediction

- Not in general, need to asses how strong the validation tests are (out of scope for today)
- Conclusion: validation tests are strong enough for this prediction





- As expected, true value of QoI within uncertainty range of prediction

Importance of Inadequacy Representations

- It is common to use embedded models with known flaws; i.e. known to be inconsistent with relevant observations of the phenomena
  - Better models are not tractable
  - Phenomenon is not fully understood, and no better model exists
  - Yet, decision must be made
  - Low fidelity (inexpensive) models are commonly used early in a design process, or for model-based control
- When inadequate (flawed) models are to be used for prediction, inadequacy representations are necessary
- Consider two representative examples
  - Reduced chemical reaction mechanisms
  - RANS turbulence models

Inadequacy of Reduced Chemical Reaction Mechanisms

- Combustion of a fuel can involve 100's or 1000's of reactions and up to 100's of intermediate chemical species.
  - In simulations (e.g. DNS) of turbulent combustion, generally intractable
  - Memory scales with number of species and cost scales with number of reactions
- Instead, use "reduced mechanisms" with many fewer species and reactions
  - Intended to capture specific characteristics of the reaction process
  - Generally need to be calibrated (e.g. against higher fidelity mechanisms or experiments)
  - Introduces modeling errors: need to represent the resulting uncertainties
- Even the most detailed mechanisms are incomplete and are therefore "reduced" relative to reality

Consider the simplest possible example: $\mathrm{H_2/O_2}$ combustion.

Detailed reaction mechanism, where $k = AT^n e^{-E/R^\circ T}$; mol/cm^3, s^{-1}, K, kJ/mol

Reaction	A	n	E
Hydrogen-oxygen chain			
1. $\mathrm{H} + \mathrm{O_2} \longrightarrow \mathrm{OH} + \mathrm{O}$	3.52×10^{16}	-0.7	71.4
2. $\mathrm{H_2} + \mathrm{O} \longrightarrow \mathrm{OH} + \mathrm{H}$	5.06×10^{4}	2.7	26.3
3. $\mathrm{H_2} + \mathrm{OH} \longrightarrow \mathrm{H_2O} + \mathrm{H}$	1.17×10^{9}	1.3	15.2
4. $\mathrm{H_2O} + \mathrm{O} \longrightarrow \mathrm{OH} + \mathrm{OH}$	7.60×10^{0}	3.8	53.4
Direct recombination			
5. $\mathrm{H} + \mathrm{H} + \mathrm{M} \longrightarrow \mathrm{H_2} + \mathrm{M}$	1.30×10^{18}	-1.0	0.0
6. $\mathrm{H} + \mathrm{OH} + \mathrm{M} \longrightarrow \mathrm{H_2O} + \mathrm{M}$	4.00×10^{22}	-2.0	0.0
7. $\mathrm{O} + \mathrm{O} + \mathrm{M} \longrightarrow \mathrm{O_2} + \mathrm{M}$	6.17×10^{15}	-0.5	0.0
8. $\mathrm{H} + \mathrm{O} + \mathrm{M} \longrightarrow \mathrm{OH} + \mathrm{M}$	4.71×10^{18}	-1.0	0.0
9. $\mathrm{O} + \mathrm{OH} + \mathrm{M} \longrightarrow \mathrm{HO_2} + \mathrm{M}$	8.00×10^{15}	0.0	0.0
Hydroperoxyl reactions			
10. $\mathrm{H} + \mathrm{O_2} + \mathrm{M} \longrightarrow \mathrm{HO_2} + \mathrm{M}$	5.75×10^{19}	-1.4	0.0
11. $\mathrm{HO_2} + \mathrm{H} \longrightarrow \mathrm{OH} + \mathrm{OH}$	7.08×10^{13}	0.0	1.2
12. $\mathrm{HO_2} + \mathrm{H} \longrightarrow \mathrm{H_2} + \mathrm{O_2}$	1.66×10^{13}	0.0	3.4
13. $\mathrm{HO_2} + \mathrm{H} \longrightarrow \mathrm{H_2O} + \mathrm{O}$	3.10×10^{13}	0.0	7.2
14. $\mathrm{HO_2} + \mathrm{O} \longrightarrow \mathrm{OH} + \mathrm{O_2}$	2.00×10^{13}	0.0	0.0
15. $\mathrm{HO_2} + \mathrm{OH} \longrightarrow \mathrm{H_2O} + \mathrm{O_2}$	2.89×10^{13}	0.0	-2.1
Hydrogen peroxide reactions			
16. $\mathrm{OH} + \mathrm{OH} + \mathrm{M} \longrightarrow \mathrm{H_2O_2} + \mathrm{M}$	2.30×10^{18}	-0.9	-7.1
17. $\mathrm{HO_2} + \mathrm{HO_2} \longrightarrow \mathrm{H_2O_2} + \mathrm{O_2}$	3.02×10^{12}	0.0	5.8
18. $\mathrm{H_2O_2} + \mathrm{H} \longrightarrow \mathrm{HO_2} + \mathrm{H_2}$	4.79×10^{13}	0.0	33.3
19. $\mathrm{H_2O_2} + \mathrm{H} \longrightarrow \mathrm{H_2O} + \mathrm{OH}$	1.00×10^{13}	0.0	15.0
20. $\mathrm{H_2O_2} + \mathrm{OH} \longrightarrow \mathrm{H_2O} + \mathrm{HO_2}$	7.08×10^{12}	0.0	6.0
21. $\mathrm{H_2O_2} + \mathrm{O} \longrightarrow \mathrm{HO_2} + \mathrm{OH}$	9.63×10^{6}	2.0	2.0

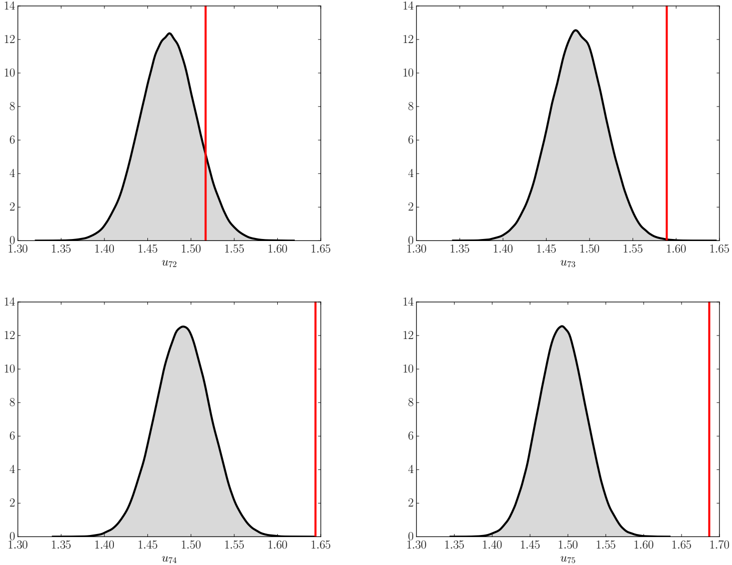
H_2/O_2 reaction[1]

- Detailed reaction model
  - 21 elementary reactions
  - 2 types of atoms (hydrogen and oxygen)
  - 8 species (H_2, O_2, H, O, OH, HO_2, H_2O, H_2O_2), whose concentrations are denoted $\boldsymbol{u} = [u_1, u_2, \ldots, u_8]^T$
  - Yields a set of 8 nonlinear ODEs
- Reduced reaction model
  - Subset of 5 of the previous reactions
  - 7 species are tracked (all but H_2O_2)
  - Set of 7 ODEs, but much simpler than above (fewer reactions)

Bayesian inference to infer reaction parameters from “observations” from detailed mechanism.

[1] F. A. Williams. Detailed and reduced chemistry for hydrogen auto-ignition. *Journal of Loss Prevention in the Process Industries*, 21: 131-135, 2008.

Validation Check of the Reduced Model



Stochastic Operator Inadequacy Model

- Reduced model inconsistent with observations, to be used, we need to represent uncertainty due to model error
- Proposed representation

$$\frac{d\boldsymbol{c}}{dt} = R(\boldsymbol{c}) + \mathcal{A}\boldsymbol{c}$$

  where $\mathcal{A}$ is a stochastic linear operator (matrix).
- But $\mathcal{A}$ must satisfy physical constraints
  - Species concentrations remain non-negative
  - H and O atoms must be conserved
- These constraints imply:
  - Columns of $\mathcal{A}$ sum to 0
  - $\mathcal{A}$ is weakly diagonally dominant
  - $\mathcal{A}$ has non-positive eigenvalues
- But how to construct $\mathcal{A}$ that satisfies the constraints?

Construction of $\mathcal{A}$

It can be shown that the constraints are satisfied if $\mathcal{A} = CQ =$

$$\begin{pmatrix} -1 & 0 & -1/2 & -1/3 & -2/3 & -1/2 \\ 0 & -1 & -1/2 & -2/3 & -1/3 & -1/2 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} q_1 & 0 & -q_2 & 0 & q_3 & q_4 & q_5 & q_6 \\ 0 & q_7 & 0 & -q_8 & q_9 & q_{10} & q_{11} & q_{12} \\ 0 & 0 & 0 & 0 & -q_{13} & q_{14} & q_{15} & q_{16} \\ 0 & 0 & 0 & 0 & q_{17} & -q_{18} & q_{19} & q_{20} \\ 0 & 0 & 0 & 0 & q_{21} & q_{22} & -q_{23} & q_{24} \\ 0 & 0 & 0 & 0 & q_{25} & q_{26} & q_{27} & -\hat{q}_{28} \end{pmatrix}$$

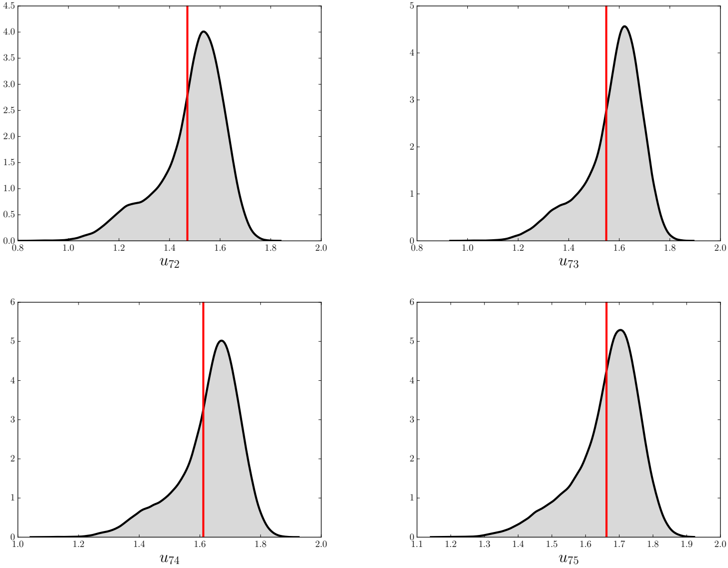
with $\hat{q}_{28} = q_{28} + 2(q_6 + q_{12} + q_{16}/2 + 2q_{20}/3 + 2q_{24}/3)$

- The elements $q_i \geq 0$ and are modeled

$$q_i \sim \log \mathcal{N}(\mu_i, \eta_i)$$

- The (log) mean and variance μ_i and η_i are inferred via (hierarchical) Bayesian inference, along with reaction parameters

Validation Check of Stochastic Inadequacy Model



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

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

Errors

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

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)

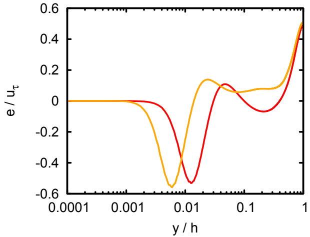
$$\underbrace{-C_p \frac{d\bar{u}}{dy}\zeta}_{\text{“Production”}} \; \underbrace{+C_p \frac{3}{2}\frac{\sqrt{\tau^m}}{y}\zeta}_{\text{“Dissipation”}} \underbrace{-\frac{d}{dy}\left((\nu + C_\nu \nu_t(\bar{u}))\frac{d\zeta}{dy}\right)}_{\text{“Diffusion”}} = C_\sigma \underbrace{\sqrt{\frac{s^2}{\ell}}\frac{dW}{dy}}_{\text{“Residual”}}$$

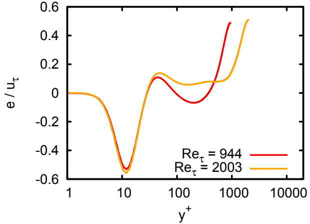
where $s = u_\tau^3$, $\ell = u_\tau/(\partial u/\partial y)$

- 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

Channel Flow Results Overview

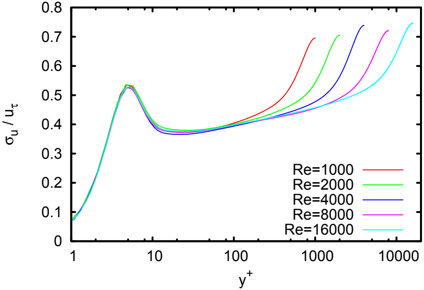
- Fully-developed, incompressible channel flow
- Turbulence model: Spalart–Allmaras
  - Similar results with other models
- Available DNS data
  - $Re_\tau = 944,\ 2003$ [del Alamo et al., 2004; Hoyas et al., 2006]
  - $Re_\tau \approx 5200$ [Lee et al., 2013]
- Calibrate with $Re_\tau = 944,\ 2003$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

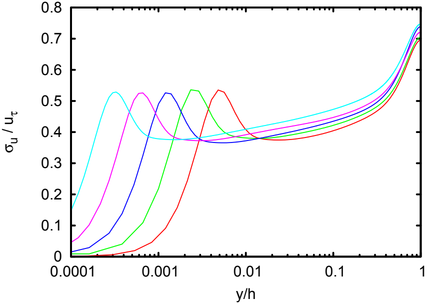




Look for expected collapse in inner and outer layers as well as any Re dependence in inverse or forward results

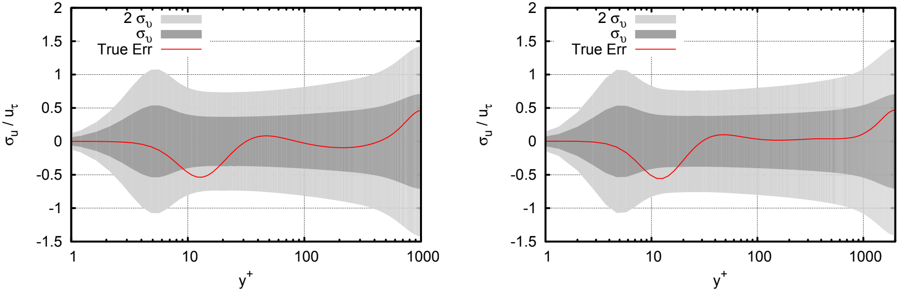
Forward Propagation: Scaling with Re





- 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

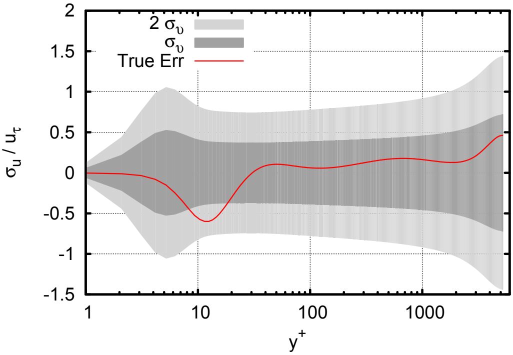
Forward Prop: Comparison Against Calibration Data



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

- $\pm 2\sigma$ 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

Ongoing efforts in model inadequacy

RANS turbulence modeling

- Generalizing SPDEs to govern Reynolds stress uncertainty

Low-fidelity aerodynamic design models

- Potential flow + integral boundary layer model
- Model uncertainty based on indicators of violated modeling assumptions?

Contaminant transport in porous media flow

- Inferring linear operator governing inadequacy of depth-integrated model

Turbulent Combustion

- Inadequacy of reduced kinetics model
- Inadequacy of model for Reynolds averaged reaction rates

Summary

- In Engineering and Science, we commonly use models that are known *a priori* to be inadequate.
- When we do, it is important to consider the uncertainty introduced by model inadequacy
- To represent model inadequacy:
  - Introduce the uncertainty where it occurs in the model: enrich the inadequate imbedded model
  - Make use of all that is known about the phonomenon being modeled and the inadequacy of the embedded model
  - Constrain the inadequacy representation with observations
    - calibration and validation observables need to be sensitive to the inadequacy

Further Reading:
Oliver *et al* 2015 Validating predictions of unobserved quantities, *Comput. Methods Appl. Mech. Engrg.* **283**, 13101335

Moser & Oliver 2015 Validation of physical models in the presence of uncertainty, manuscript for a chapter in *Handbook of Uncertainty Quantification*.

Thank you.

Questions?