Towards Forward Propagation of Reynolds Stress Model Uncertainty

Todd A. Oliver
Vikram Garg and Robert Moser

Center for Predictive Engineering and Computational Sciences
Institute for Computational Engineering and Sciences
The University of Texas at Austin

July 29, 2015

Outline

Representing Model Inadequacy

Motivation

- Many engineering models known to be wrong, but used anyway
- RANS with eddy-viscosity-based closure is perfect example
- Impractical to always correct models prior to making predictions

Goal

- Represent effects of inadequacy via uncertainty in predictions

Source of Model Inadequacy in RANS

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

Cannot recover exact $\overline{u_i' u_j'}$ by changing typical model parameters

Overview of Bayesian UQ Approach

Three Steps

- Model:

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

  where ζ_{ij} is random tensor field
- Calibrate using DNS and/or experimental data
- Predict non-deterministic mean flow (forward propagation)

Hurdles to a practical, Bayesain model UQ capability for RANS:

1. Developing a plausible stochastic model of the Reynolds stress
2. Computational cost of traditional UQ algorithms

Example Reynolds Stress Error Model

Motivation/Inspiration

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

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

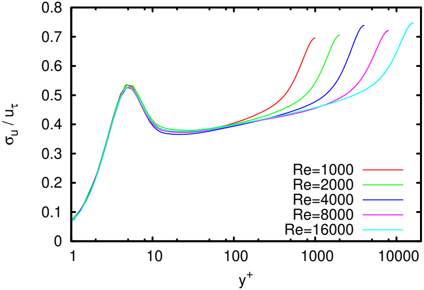
The model (for channel flow case)

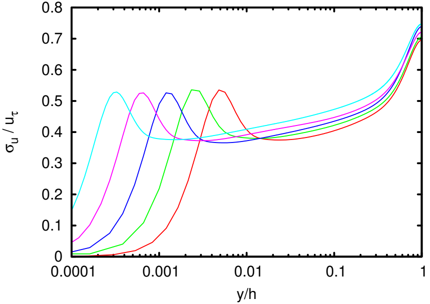
$$\underbrace{-C_p \frac{d\bar{u}}{dy}\zeta}_{\text{“Production”}} \underbrace{+C_p \frac{3}{2}\frac{\sqrt{\tau^m}}{y}\zeta}_{\text{“Dissipation”}} \underbrace{-\frac{d}{dy}\left((\nu + C_\nu \nu_t(\bar{u})) \frac{d\zeta}{dy} \right)}_{\text{“Diffusion”}} = C_\sigma \underbrace{\sqrt{\frac{s^2}{\ell}}\frac{dW}{dy}}_{\text{“Residual”}}$$

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

Example Reynolds Stress Error Model





- 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

Derivative Enhanced UQ Techniques

Forward UQ

- Sensitivity Derivative Enhanced Monte Carlo (SDEMC) [Cao et al., 2006]
  - Linear surrogate using derivative at mean
- Local SDEMC (LSDEMC and LSHEMC) [Garg et al., 2013]
  - Piecewise linear surrogate at multiple samples
  - Can use derivative alone or derivative and hessian

Inverse Problems

- Stochastic Newton Method [Martin et al., 2012]
- Metropolis Adjusted Langevin algorithm [Roberts and Tweedie, 1996]
- Bayesian Optimal Maps [El Moselhy and Marzouk, 2012]

LSDEMC Surrogate Construction

- Random parameters: $\boldsymbol{\xi}$
- QoI: $Q(\boldsymbol{\xi})$
- Associate each sample $\{\boldsymbol{\xi}_i\}_{i=1}^{N_s}$ with a Voronoi cell $\{R_i\}_{i=1}^{N_s}$
- Draw another set of samples $\{\boldsymbol{\xi}_j\}_{j=1}^{N_{ss}}$ where $N_{ss} >> N_s$
- Discontinuous piecewise linear surrogate for $\boldsymbol{\xi}_j \in R_i$:

$$Q_1(\boldsymbol{\xi}_j) = Q(\boldsymbol{\xi}_i) + Q^{'}(\boldsymbol{\xi}_i)(\boldsymbol{\xi}_j - \boldsymbol{\xi}_i)$$

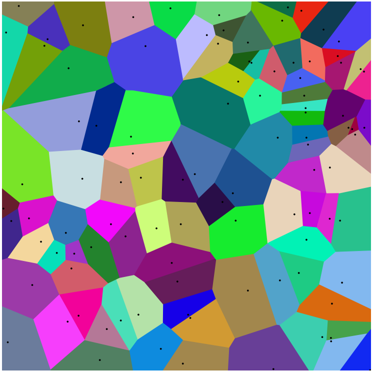
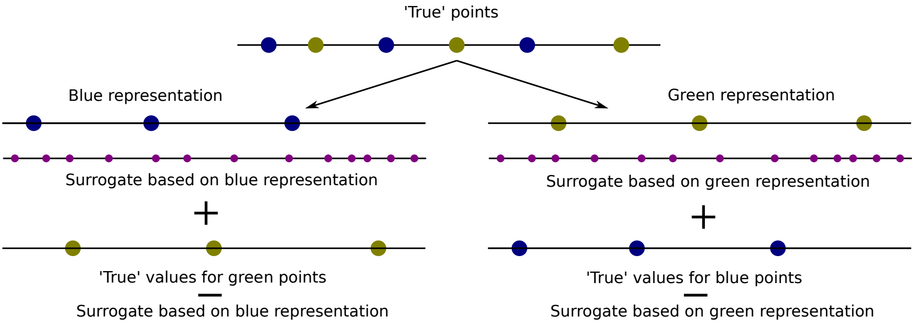


Figure: 2-d Voronoi diagram

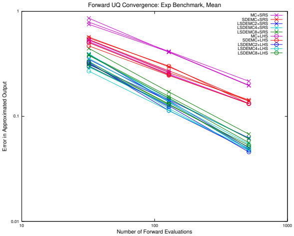
Bias Correction



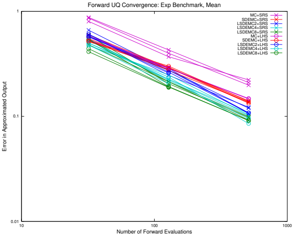
Unbiased estimator for the mean

$$\frac{1}{N_R}\sum_{r=1}^{N_R}\left(\frac{1}{N_{ss}}\sum_{l=1}^{N_{ss}} Q_{r,1}(\boldsymbol{\xi}_l) + \frac{1}{N_s - \frac{N_s}{N_R}}\sum_{c=1}^{N_s-\frac{N_s}{N_R}} \left(Q(\boldsymbol{\xi}_c) - Q_{r,1}(\boldsymbol{\xi}_c)\right)\right)$$

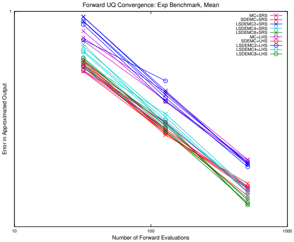
Results for Toy Problem



4 Parameters



16 Parameters



64 Parameters

- Can prove LSDEMC converges asymptotically faster than MC
- Benefit decays as dimensionality grows
- Potential to overcome this decay by incorporating Hessian information (Vikram, is this a reasonable statement? Could I strengthen it?)

Adjoint-Based Sensitivities

- High dimensional inputs $\Rightarrow$ use adjoints to evaluate sensitivities
- Discrete Case
  - Forward model: $R(U;\zeta) = 0$ where R is governing eqns, U is solution vector, and ζ is parameter vector
  - Quantity of interest: $q = Q(\zeta) = J(U(\zeta);\zeta)$
  - Quantity of intersest sensitivity:

$$\frac{dQ}{d\zeta} = \frac{\partial \mathcal{J}}{\partial \zeta} - Z^T \frac{\partial R}{\partial \zeta}$$

where φ is the adjoint vector, defined by

$$\frac{\partial R}{\partial U}^T Z = \frac{\partial J}{\partial U}$$

- Can extend results to the continuous setting

Adjoint-Based Sensitivities for RANS

General Case

For a Reynolds stress perturbation field ζ_{ji}:

$$\Delta Q = \underbrace{\int_\Omega \frac{\partial \varphi_{u_i}}{\partial x_j}\zeta_{ji}}_{\text{From momentum eqns}} + \underbrace{\int_\Omega \varphi^T_{turb} r'_{turb}[\zeta]}_{\text{From turbulence model eqns}}$$

- In following, we use Spalart-Allmaras (SA) turbulence model
- SA model equation has no direct dependence on Reynolds stress:

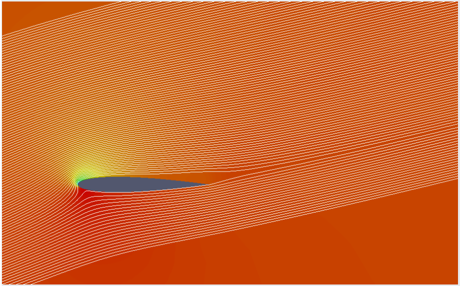
$$\Delta Q = \int_\Omega \frac{\partial \varphi_{u_i}}{\partial x_j}\zeta_{ji}$$

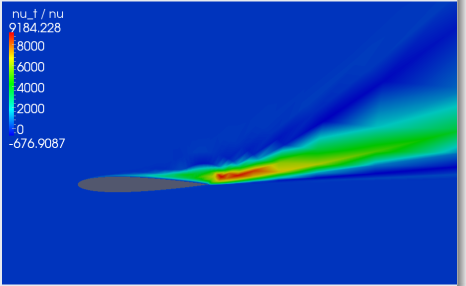
- Momentum adjoint gradient encodes everything about QoI sensitivity!
- Gives insight into what's important about model to the QoI

Results: Case Overview

- Incompressible RANS w/ SA turbulence model
- $Re = 6 \times 10^6$, $\alpha = 0, 16°$
- GRINS Code (https://github.com/GRINSfem/GRINS)

$\alpha = 16°$

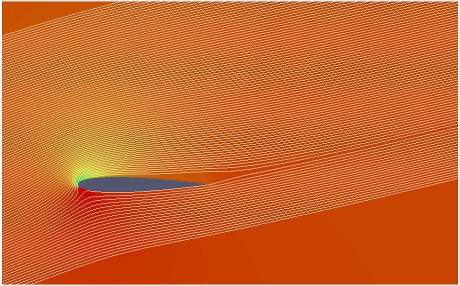


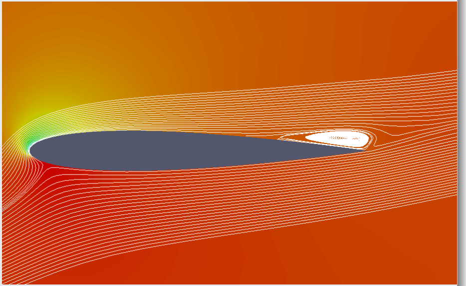


Results: Case Overview

- Incompressible RANS w/ SA turbulence model
- $Re = 6 \times 10^6$, $\alpha = 0, 16^\circ$
- GRINS Code (https://github.com/GRINSfem/GRINS)

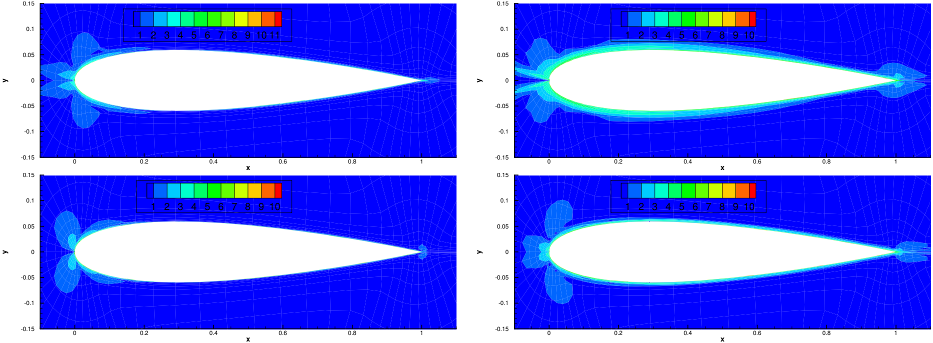
$\alpha = 16^\circ$





Results: Adjoint Gradient

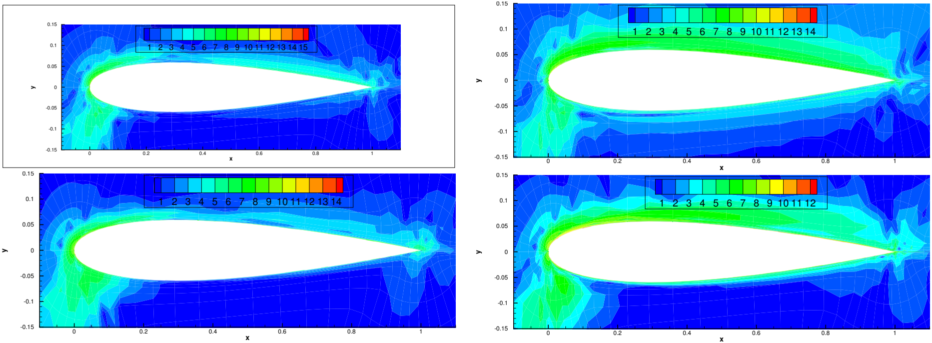
$\alpha = 0$, QoI = Drag



- All plots show $\log\left(\left|\frac{\partial \varphi_{u_i}}{\partial x_j}\right| + 1\right)$

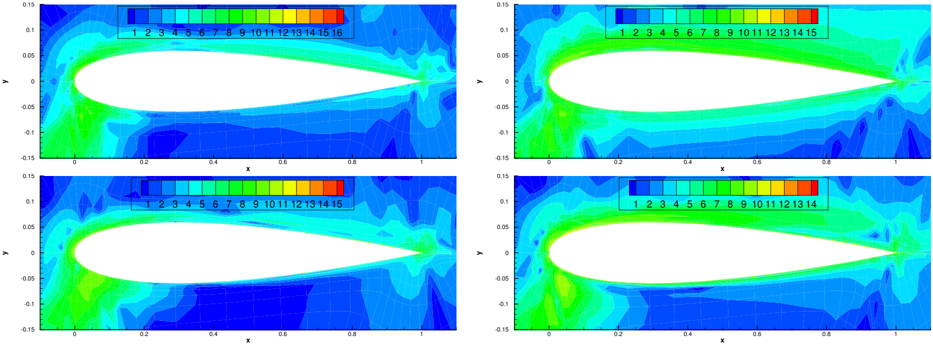
Results: Adjoint Gradient

$\alpha = 16$, QoI = Drag



Results: Adjoint Gradient

$\alpha = 16^\circ$, QoI = Lift



Summary

By computing QoI sensitivity w.r.t. Reynolds stress, we hope to

- Improve forward propagation efficiency for random Reynolds stress
- Gain insight regarding modeled features most important to QoI

Future Work

- Further develop stochastic Reynolds stress inadequacy models
- Use LSDEMC to propagate Reynolds stress uncertainty
- Incorporate Hessian information (LSHEMC)
- Mine Reynolds stress sensitivities to understand critical features

Bibliography I

Cao, Y., Hussaini, M., Zang, T., and Zatezalo, A. (2006).
A variance reduction method based on sensitivity derivatives.
Applied numerical mathematics, 56(6):800–813.

El Moselhy, T. A. and Marzouk, Y. M. (2012).
Bayesian inference with optimal maps.
Journal of Computational Physics, 231(23):7815–7850.

Garg, V., R.H., S., and Willcox, K. (2013).
Local sensitivity derivative enhanced monte carlo.
SIAM CSE, Boston.

Martin, J., Wilcox, L. C., Burstedde, C., and Ghattas, O. (2012).
A stochastic newton mcmc method for large-scale statistical inverse problems with application to seismic inversion.
SIAM Journal on Scientific Computing, 34(3):A1460–A1487.

Bibliography II

Roberts, G. O. and Tweedie, R. L. (1996).
Exponential convergence of langevin distributions and their discrete approximations.
Bernoulli, pages 341–363.