Robust Bayesian calibration of a RANS model for jet-in-crossflow simulations

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Introduction

- **Aim:** Enable predictive RANS simulations of compressible jet-in-crossflow configurations (JIC)

- **Problem:** JIC simulations not very predictive; suffer from:
  - Model-form errors i.e., missing physics
  - Use of constants derived from incompressible canonical flows

- **Hypothesis:** Prediction errors are caused mostly by wrong constants
  - Calibration solves this problem (quantify estimation uncertainty!)
  - Fixing model-form error has a smaller effect
  - Approximate the new constant using an analytical model
    - i.e., show that the calibrated constants are physical, not just a “curve-fit”
  - Explore if there exists a calibration that works across a set of JIC configurations
The equations

- **The model**
  - Devising a method to calibrate 3 k-ε parameters $\mathbf{C} = \{C_\mu, C_1, C_2\}$ from expt. data
    
    \[
    \frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_i} \left[ \rho u_i k - \left( \mu + \frac{\mu T}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] = P_k - \rho \varepsilon + S_k
    \]
    
    \[
    \frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_i} \left[ \rho u_i \varepsilon - \left( \mu + \frac{\mu T}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] = \frac{\varepsilon}{k} \left( C_1 f_1 P_k - C_2 f_2 \rho \varepsilon \right) + S_\varepsilon
    \]
    
    \[
    \mu_T = C_\mu f_\mu \rho \frac{k^2}{\varepsilon}
    \]

- **Calibration parameters**
  - $\mathbf{C} = \{C_\mu, C_1, C_2\}$; $C_\mu$: affects turbulent viscosity; $C_1$ & $C_2$: affects dissipation of TKE

- **Model-form error**
  - \(- \tau_{ij} = -u_i' u_j' = \frac{2}{3} k \delta_{ij} - \nu_T S_{ij} + \nu_T \frac{k}{\varepsilon} \sum_{l=1}^{3} c_l f_l(S, \omega) + \nu_T \left( \frac{k}{\varepsilon} \right)^2 \sum_{l=4}^{7} c_l f_l(S, \omega)\)

- Currently only linear terms are used (linear eddy viscosity model, LEVM); does adding more terms help in increasing prediction accuracy?
Target problem - jet-in-crossflow

- A canonical problem for spin-rocket maneuvering, fuel-air mixing etc.
- We have experimental data (PIV measurements) on the cross- and mid-plane
- Will calibrate to vorticity on the crossplane and test against mid-plane
RANS (k-$\omega$) simulations - crossplane results

- Crossplane results for stream
- Computational results (SST) are too round; Kw98 doesn’t have the mushroom shape; non-symmetric!
- Less intense regions; boundary layer too weak
Calibration

- **Bayesian calibration** – Develop a PDF for \((C\mu, C_2, C_1)\)
  - Captures the uncertainty in the estimation
  - Will be performed for 4 (Mach, J) combinations, to see how generalizable the calibration is

- **We pose the calibration as a statistical/Bayesian inverse problem**
  - Solve it using Markov chain Monte Carlo (MCMC)
  - Requires \(O(10^4)\) samples/generations to give converged PDFs
    - Implies \(O(10^4)\) invocations of the forward problem
  - Samples taken sequentially, not concurrently, so takes a long time

- **Observational data for calibration:** velocity measurements (PIV) on the midplane
  - 5 streamwise locations with 63 measurement points per location ~ 315 “probes”

- **Observational data for testing:** vorticity measurements on the crossplane
The Bayesian calibration problem

- Model experimental values at probe $j$ as $v^{(j)}_{ex} = v^{(j)}(C) + \varepsilon^{(j)}$, $\varepsilon^{(j)} \sim \text{N}(0, \sigma^2)$

$$
\Lambda(v_{ex}|C) \propto \prod_{j \in P} \exp \left( -\frac{\left( v^{(j)}_{ex} - v^{(j)}(C) \right)^2}{2\sigma^2} \right)
$$

- Given prior beliefs $\pi$ on $C$, the posterior density (‘the PDF’) is

$$
P(C, \sigma | v_{ex}) \propto \Lambda(v_{ex}|C) \pi(C, \sigma)
$$

- $P(C|v_{ex})$ is a complicated distribution that has to be visualized by drawing samples from it

- This is done by MCMC
  - MCMC describes a random walk in the parameter space
  - Each step of the walk requires a model run to check out the new parameter combination
Forward model and surrogates

- 3D, finite volume, unsteady Roe solver
  - $10^7$ mesh, $10^4$ CPU hours to steady state. Can’t be used in MCMC

- Surrogate models: A “curve-fit” replacement for aero solver
  - $v^{(j)} = a^{(j)0} + a^{(j)1}C_\mu + a^{(j)2}C_2 + a^{(j)3}C_1 + a^{(j)4}C_\mu C_2 + a^{(j)5}C_\mu C_1 + ...$

- Making surrogates
  - Generate $\sim 5000$ ($C_\mu$, $C_2$, $C_1$) samples (bounds are known); run RANS
  - For the rest, OLS fitting for $a^{(j)1}$
    - Simplify using AIC
  - If within 10% of RANS, accept surrogate as being “accurate enough”

- Usually left with $\sim 50 / 315$ probes where we can make sufficiently good surrogates
Solution of the inverse problem

- We estimated $\mathbf{C} = (C_\mu, C_2, C_1)$ for 4 $(M, J)$ cases
  - $M = [0.6, 0.7], J = 10.2$
  - $M = 0.8, J = [10.2, 16.7]$

- A few commonalities
  - $C_2$ is higher than nominal
  - $C_1$ (nominal) is probably OK
  - $C_\mu$ – probably does not affect mean flow much and is not constrained by it

- $\sigma$ show that
  - $M = 0.7$ case probably best fit
  - $M = 0.6$ case worst fit

Vertical green lines:
- Dashed: nominal value
- Solid: Analytical model’s estimate
Check # 1 – point vortex summary

- Same 100 C from the PDF, run them forward
- Use the crossplane vorticity fields from the ensemble to compute
  - Total circulation, centroid of vorticity field, radius of gyration of vorticity field
  - Normalize each by their experimental counterpart
- We expect to get an ensemble of values for each metric around 1
  - We also find a $C_{opt} = \{0.1025, 2.09, 1.42\}$ that provides the best predictions

Jet–in–crossflow predictions for $M = 0.8$ and $J = 10.2$

The spread of point vortex summaries are tightly distributed around 1. The red circles are the predictions from the nominal values of $C$. 

Normalized predictions (numerical / experimental)
Check # 2 – the vorticity field

- Contours are plotted using the experimental measurements
- The improvement is significant

RANS predictions with $C_{\text{nom}}$

RANS predictions with $C_{\text{opt}}$
Check # 3 – mid-plane comparisons

- $M = 0.8$, $J = 10.2$, case
Check # 4 – $M = 0.7$ case

- $M = 0.7$, $J = 10.2$
Combining PDFs

- The 4 PDFs have overlaps
  - Could \( (C_\mu, C_2, C_1) \) samples from the overlap region be predictive for all 4 cases?

- Take 100 samples each from the 4 PDFS; simulate all 4 cases with them
  - Call each RANS run, seeded with a \( (C_\mu, C_2, C_1) \) sample, a separate “model”
    - We have an ensemble of 400 models

- Could a weighted average of 400 models reproduce experimental velocities for all 4 cases? BMA!
  - If yes, then the weights of each model i.e., \( (C_\mu, C_2, C_1) \) combination, could be used to make a PDF over them
  - That becomes a PDF that’s useable for all 4 cases
  - But only if they cluster in a region, to make a unimodal PDF
Combining PDFs - results

- 22/400 account for 99.9% of the probability mass
- They don’t cluster. Failed!
Model-form error

- **Hypothesis:** The simple form of the EVM is responsible for lack of predictive skill
  - Can enriching it fix the problem?
  - \(- \tau_{ij} = -\overline{u_i' u_j'} = \frac{2}{3} k \delta_{ij} - \nu_T S_{ij} + \nu_T \frac{k}{\epsilon} \sum_{i=1}^{3} c_i f_i(S, \omega) + \nu_T \left( \frac{k}{\epsilon} \right)^2 \sum_{i=4}^{7} c_i f_i(S, \omega)\)
  - We do have estimates of \(c_i\) from incompressible canonical flow
  - Which terms do we include? We don’t have enough expt data to estimate all 7 terms

- **Pose a shrinkage problem**
  - We have measurements of \(k, S, \omega\) and \(\tau_{ij}\) on the midplane; no \(\epsilon\)
  - Approximate \(\epsilon\) as Production = destruction
  - \(\min_{\mathbf{c}} \| \tau_{ij} - A(k, \epsilon, S, \omega) \mathbf{c} \|_2^2 + \lambda \| \mathbf{c} \|_1\)
  - This will retain only those \(c_i\) that are supported by observations

- Note that the values of \(c_i\) so obtained are not trustworthy
Model-form error results

- Good value of $\lambda$ obtained via 7-fold cross-validation
- Final chosen value of $\lambda$ retains one extra quadratic term ($\omega^2$) in the EVM
Calibrating QEVM

- While we have an enriched EVM, we still have a problem values of constants
- Calibration shows (again) that appropriate values of $C_2$ are different from nominal
  - And $C_1$ is close to OK
- We’ll check the calibration via a ”pushed-forward posterior”
Vorticity, crossplane

- Experiments: Contours
- Significant improvement
Velocities, midplane

- Velocities on the mid plane match experiments, after calibration
- Neither QEVM and LEVM, before calibration, are predictive
Discussion

- We have shown how Bayesian calibration improves predictive skill
  - New \((C_\mu, C_2, C_1)\) could be a mere artefact to fitting to data; may have no physical significance
  - But analytical model predictions very close to predictions with \(C_{\text{opt}}\)
    - Next talk: \(C_{\text{opt}} \sim C_{\text{analytical}}\)
  - Our calibration does yield physically realistic constants
- We’ve also explored enriching the LEVM, but no great improvements
  - For this particular configuration, it does not seem to be about model-form errors, but inappropriate constants
  - Dechant (next talk) will show how and why the calibrated constants are the good ones
Conclusions

- We have explored the causes behind non-predictive JIC RANS computations
  - We think we should be using very different constants
  - We inferred the “good” values of the constants via Bayesian calibration
  - Calibrated PDFs more accurate than the nominal values
  - Also, calibration supported via analytical verification

- We addressed model-form error too
  - In this case, the inappropriate constants overwhelmed model-form error
  - Regardless, the model-form error exists, and manifests itself in the turbulent stresses
  - They don’t match measurements
BACKGROUND
RANS \((k-\omega)\) simulations – midplane results

- Experimental results in black
- All models are pretty inaccurate (blue and red lines are the non-symmetric results)