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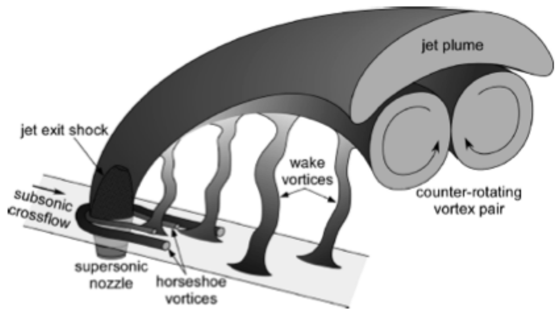

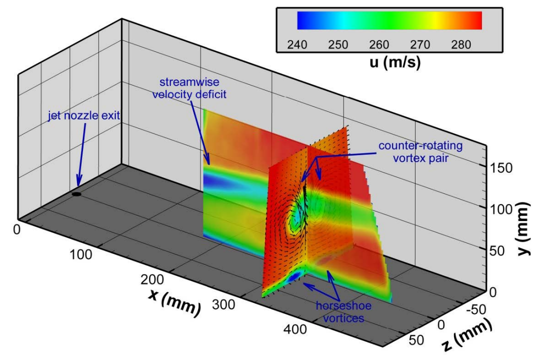

Robust Bayesian calibration of a RANS model for jet-in-crossflow simulations

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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 **C** = {C_μ, C_2, C_1} from expt. data

$$\frac{\partial \rho k}{\partial t}+\frac{\partial}{\partial x_i}\left[\rho u_i k-\left(\mu+\frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right]=P_k-\rho\varepsilon+S_k$$

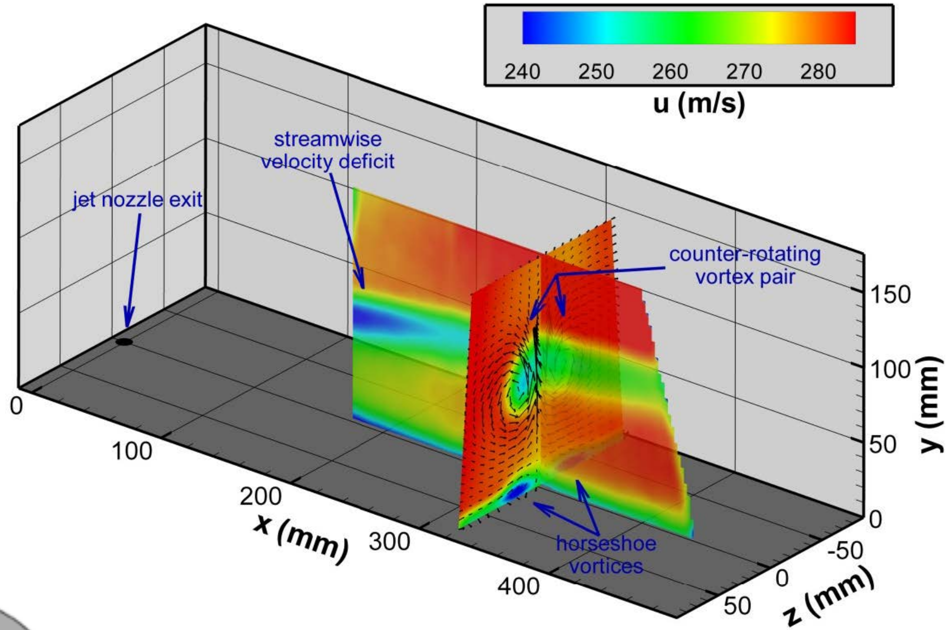
$$\frac{\partial \rho \varepsilon}{\partial t}+\frac{\partial}{\partial x_i}\left[\rho u_i \varepsilon-\left(\mu+\frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right]=\frac{\varepsilon}{k}\left(C_1 f_1 P_k-C_2 f_2\rho\varepsilon\right)+S_\varepsilon$$

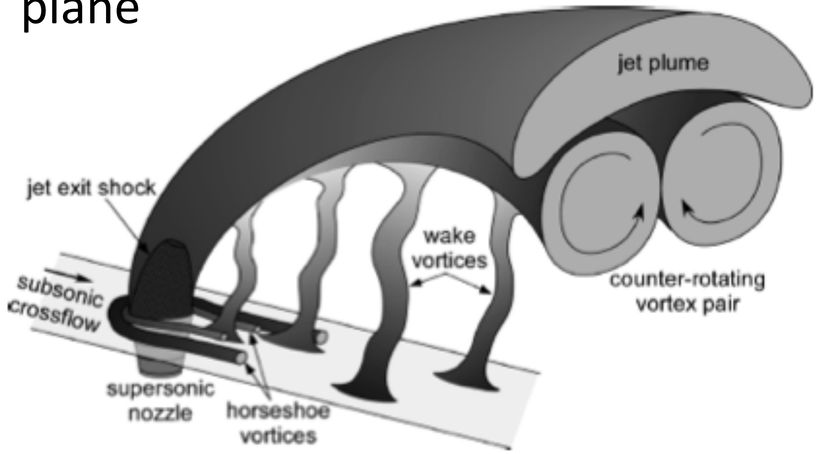
$$\mu_T=C_\mu f_\mu \rho\frac{k^2}{\varepsilon}$$

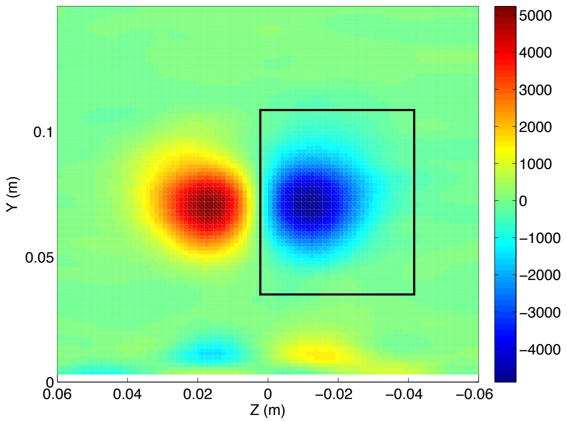
- Calibration parameters
  - **C** = {C_μ, C_1, C_2} ; C_μ: affects turbulent viscosity; C_1 & C_2: affects dissipation of TKE
- Model-form error
- $-\tau_{ij}=-\overline{u_i' u_j'}=\frac{2}{3}\mathrm{k}\delta_{ij}-\nu_T S_{ij}+\nu_T\frac{k}{\epsilon}\sum_{l=1}^{3}c_l f_l(S,\omega)+\nu_T\left(\frac{k}{\epsilon}\right)^2\sum_{l=4}^{7}c_l f_l(S,\omega)$
- 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

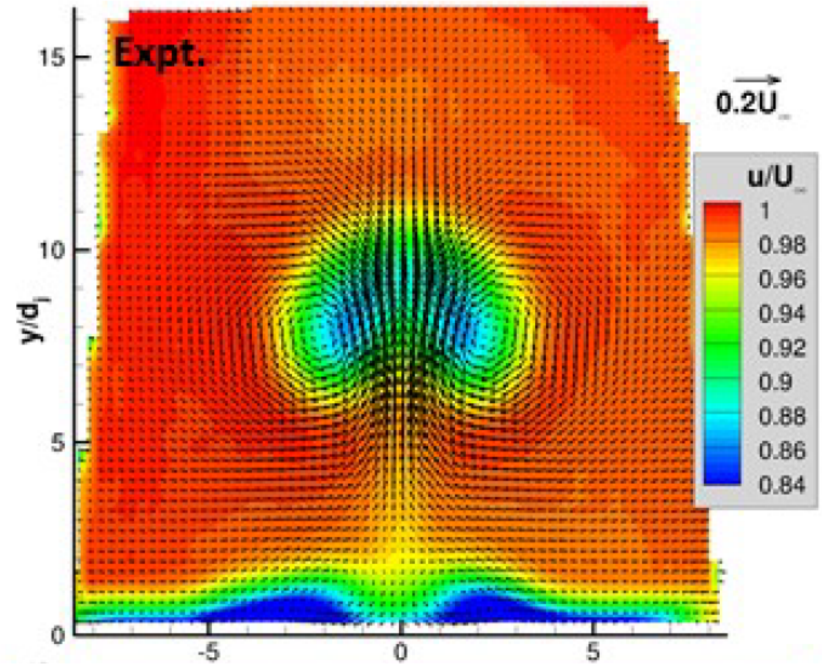
- A canonical problem for spin-rocket maneuvering, fuel-air mixing etc.
- We have experimental data (PIV measurements) on the cross- and mid-plane
- Will calibrate to vorticity on the crossplane and test against mid-plane

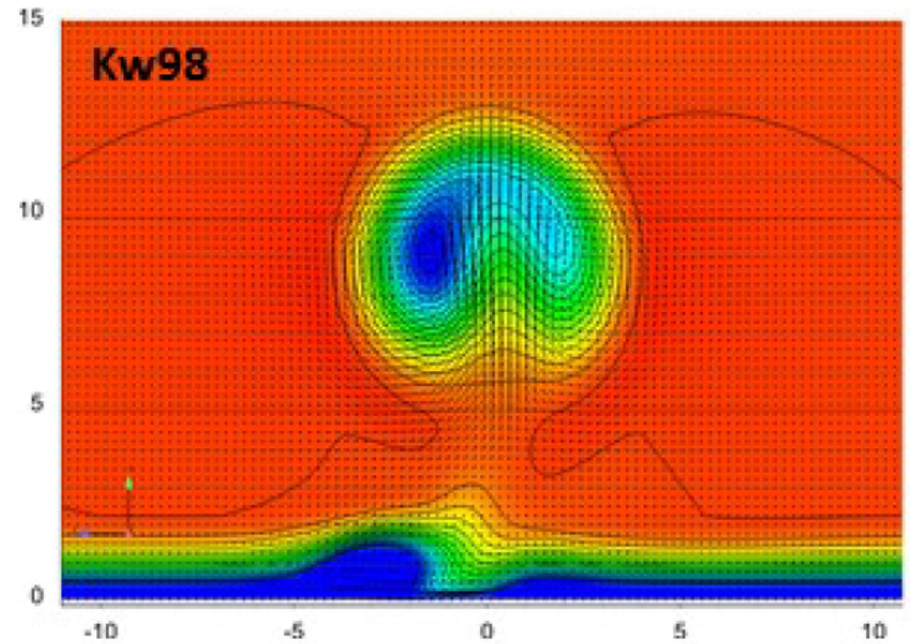






RANS (k-ω) simulations - crossplane results

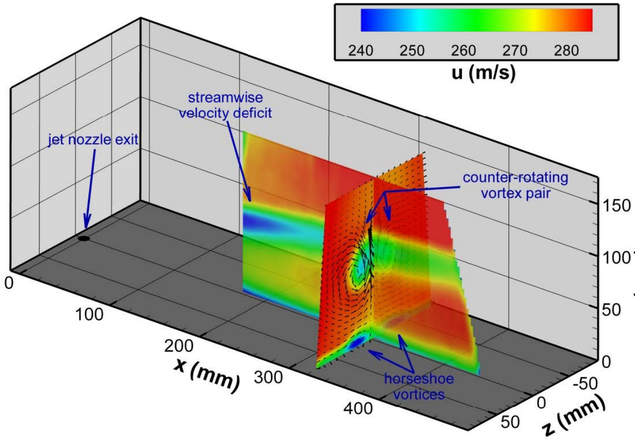




- Crossplane results for stream
- Computational results (SST) are too round; Kw98 doesn't have the mushroom shape; non-symmetric!
- Less intense regions; boundary layer too weak

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 $v^{(j)}_{ex} = v^{(j)}(\mathbf{C}) + \varepsilon^{(j)}$, $\varepsilon^{(j)} \sim N(0, \sigma^2)$

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

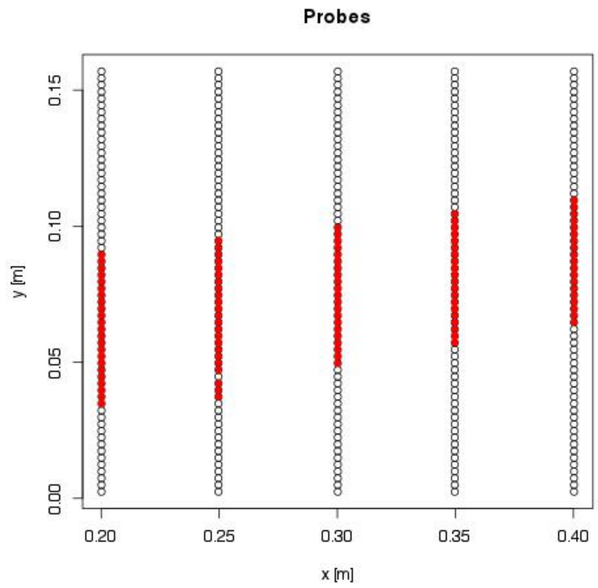
- Given prior beliefs π on **C**, the posterior density (‘the PDF’) is

$$P(C,\sigma\,|\mathbf{v}_{ex}) \propto \Lambda(\mathbf{v}_{ex}|C)\,\pi(C,\sigma)$$

- $P(\mathbf{C}|\mathbf{v}_{ex})$ 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
  - $v^{(j)} = a^{(j)}_0 + a^{(j)}_1 C\mu + a^{(j)}_2 C_2 + a^{(j)}_3 C_1 + a^{(j)}_4 C\mu C_2 + a^{(j)}_5 C\mu C_1 + \ldots$
- Making surrogates
  - Generate ~5000 ($C\mu$, C_2, C_1) samples (bounds are known); run RANS
  - For the rest, OLS fitting for $a^{(j)}_i$
    - Simplify using AIC
  - If within 10% of RANS, accept surrogate as being "accurate enough"
- Usually left with ~50 / 315 probes where we can make sufficiently good surrogates



All probes. Those with surrogates are in red and track the jet

Solution of the inverse problem

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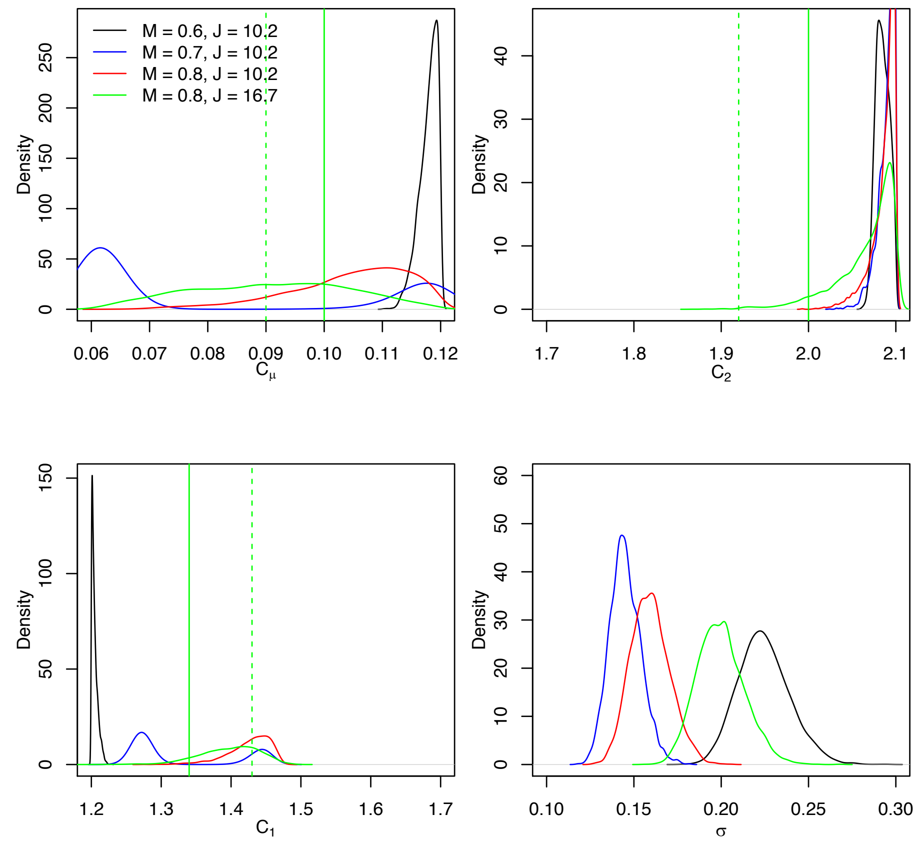
- We estimated **C** = (C_μ, C_2, C_1) for 4 (M, J) cases
  - M = [0.6, 0.7], J = 10.2
  - M = 0.8, J = [10.2, 16.7]
- A few commonalities
  - C_2 is higher than nominal
  - C_1 (nominal) is probably OK
  - Cμ ?? – probably does not affect mean flow much and is not constrained by it
- σ show that
  - M = 0.7 case probably best fit
  - M = 0.6 case worst fit

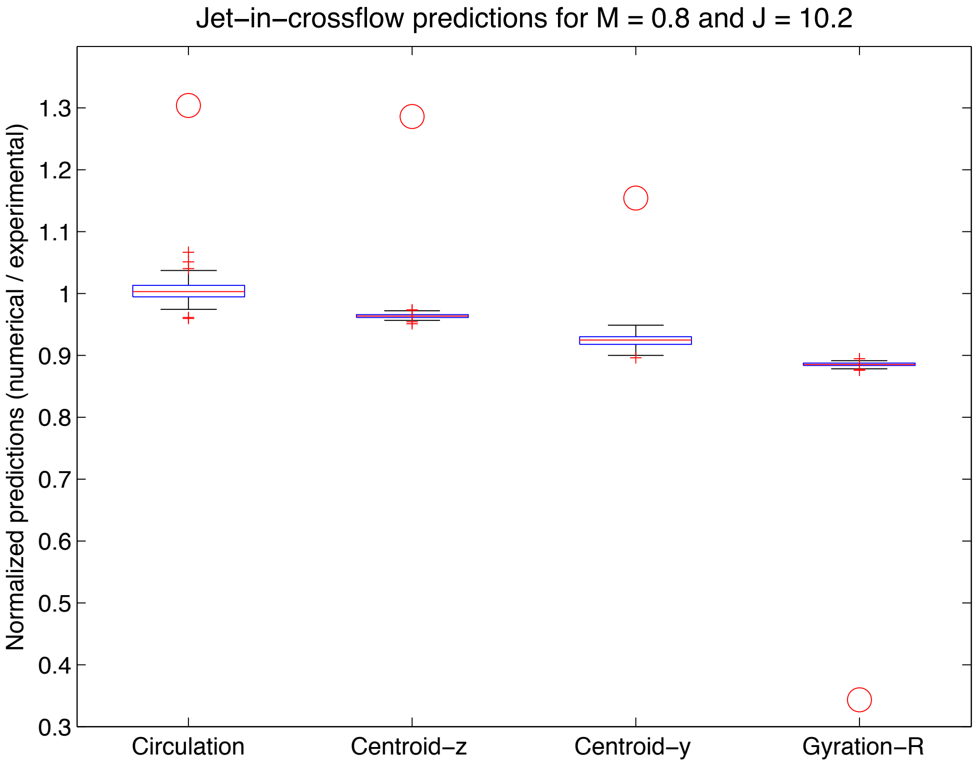


Vertical green lines:

- Dashed: nominal value
- Solid: Analytical model's estimate

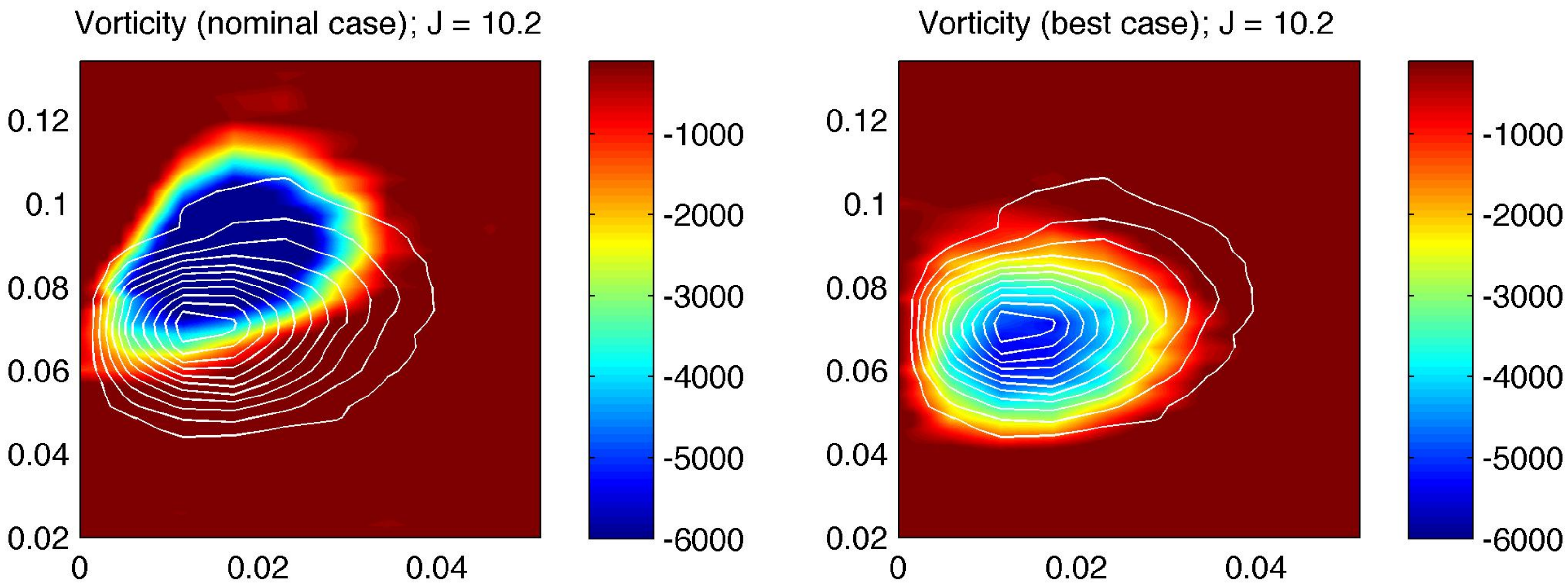
Check # 1 – point vortex summary

- 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 $\mathbf{C}_{opt}$ = {0.1025, 2.09, 1.42} that provides the best predictions



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

Check # 2 – the vorticity field

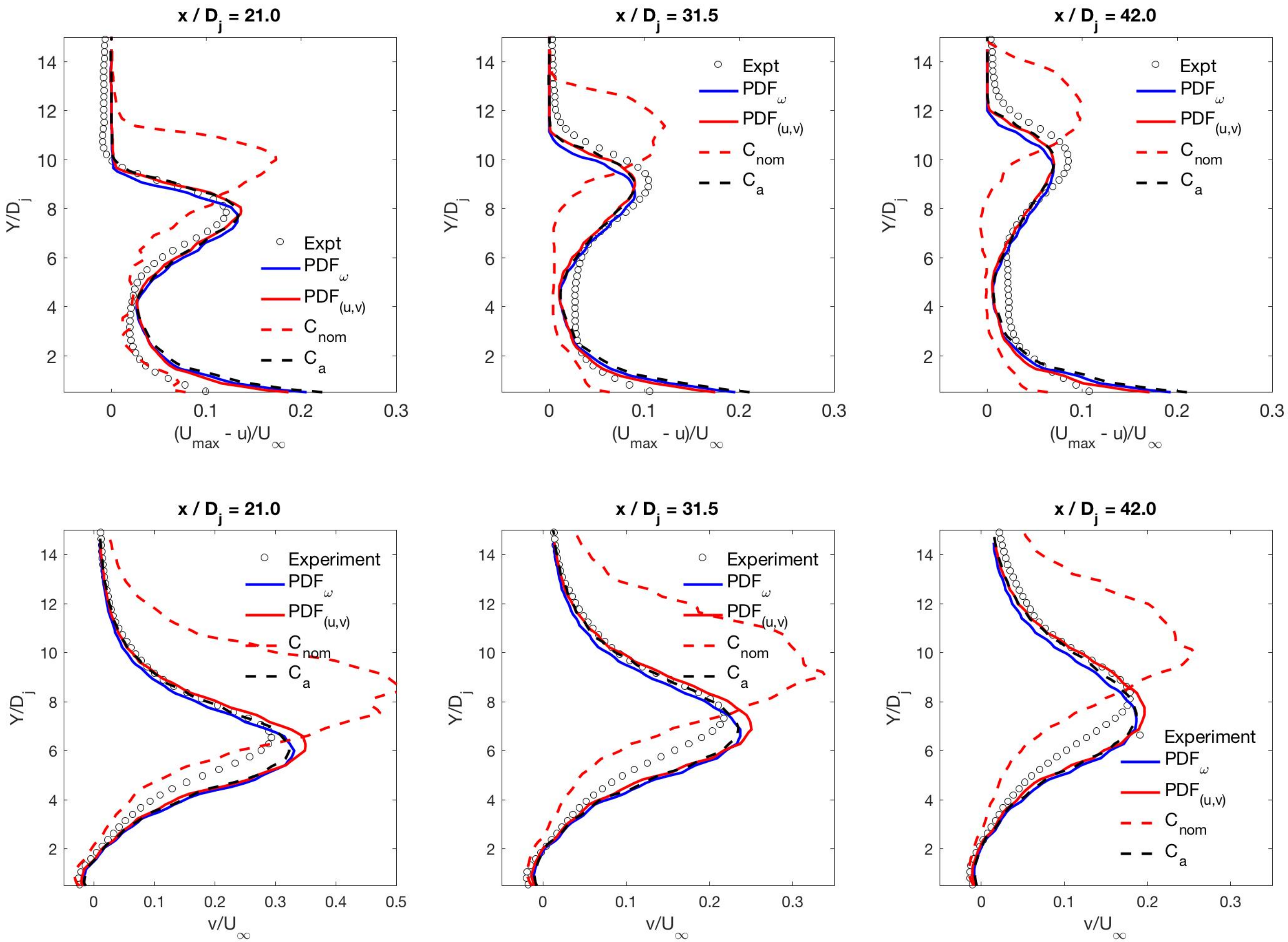


RANS predictions with $\mathbf{C}_{nom}$

RANS predictions with $\mathbf{C}_{opt}$

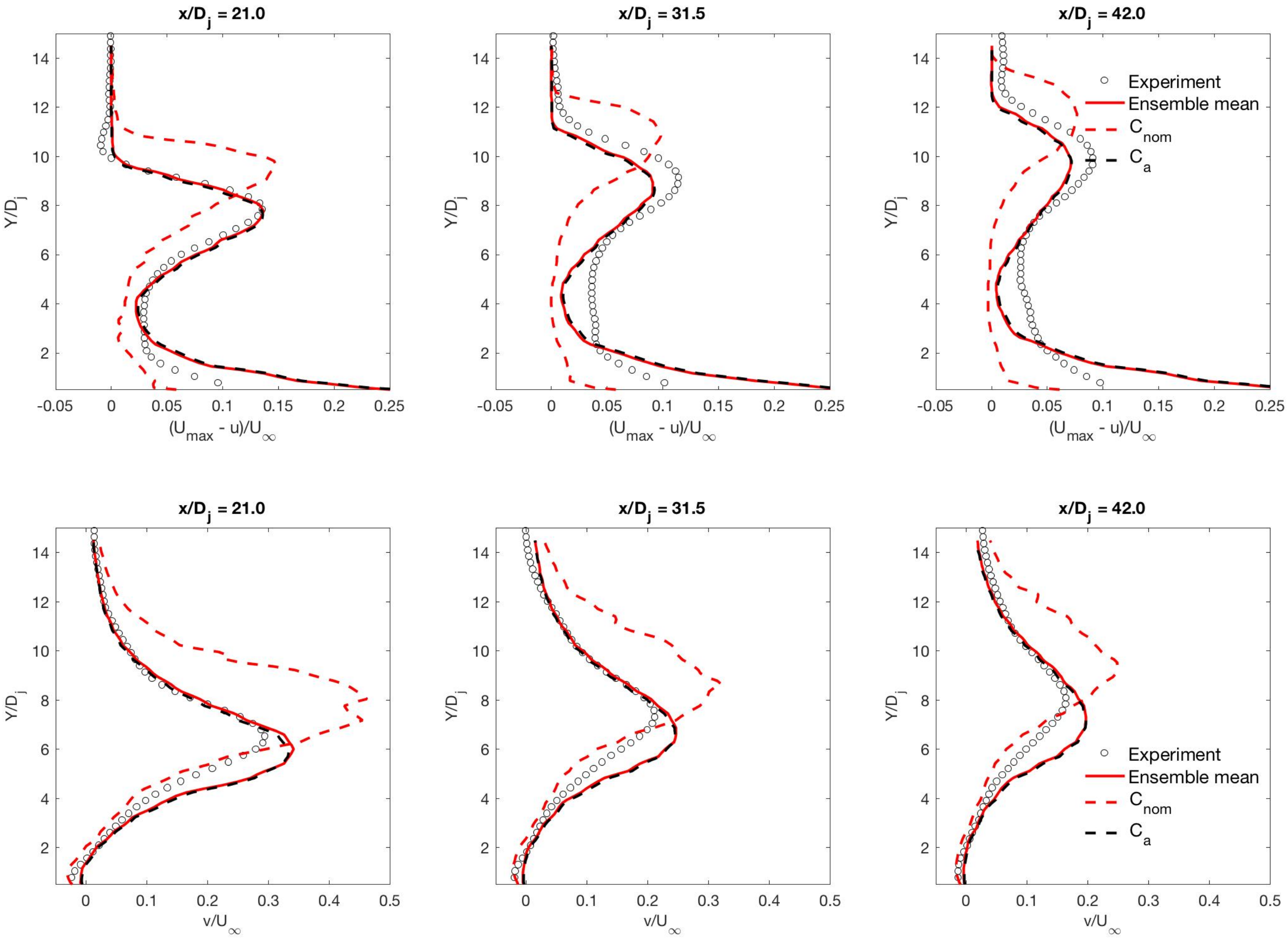
- Contours are plotted using the experimental measurements
- The improvement is significant

Check # 3 – mid-plane comparisons



- M = 0.8, J = 10.2, case

Check # 4 – M = 0.7 case

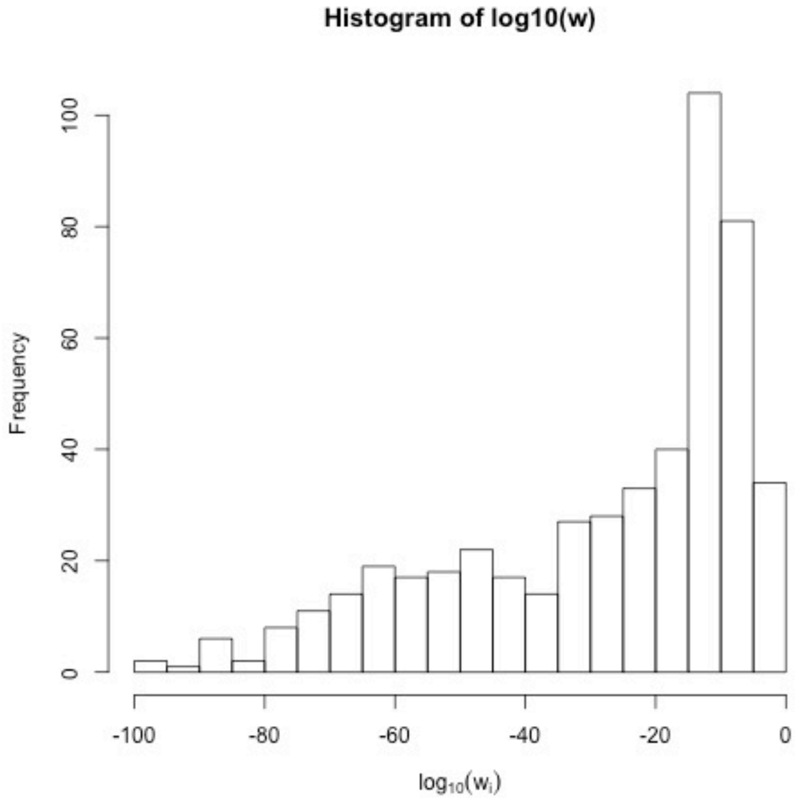


- M = 0.7, J = 10.2

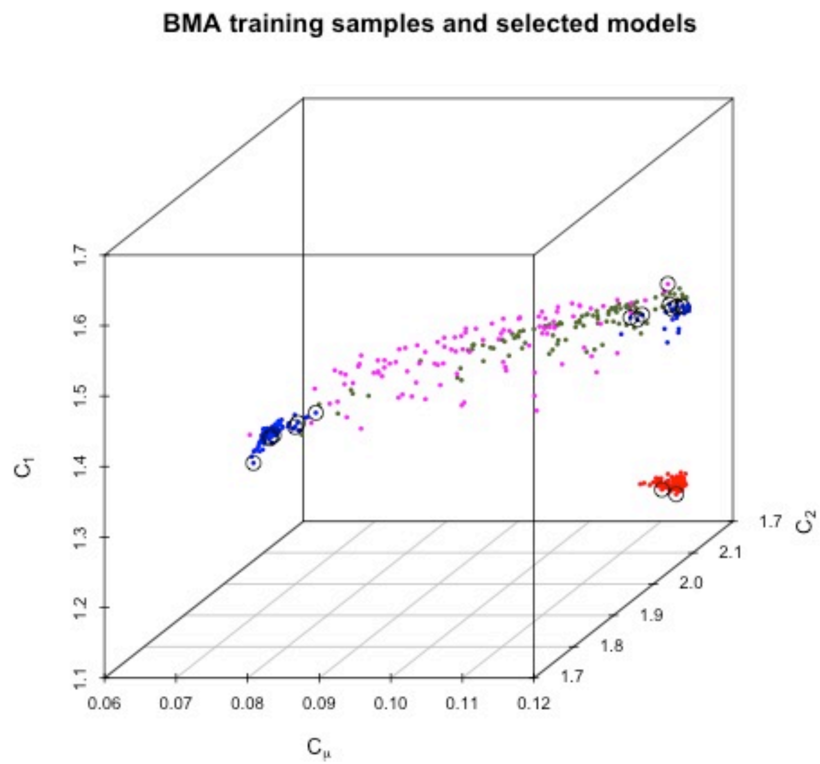
Combining PDFs

- The 4 PDFs have overlaps
  - Could (C_μ, 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_μ, 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_μ, 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



Histogram of model weights



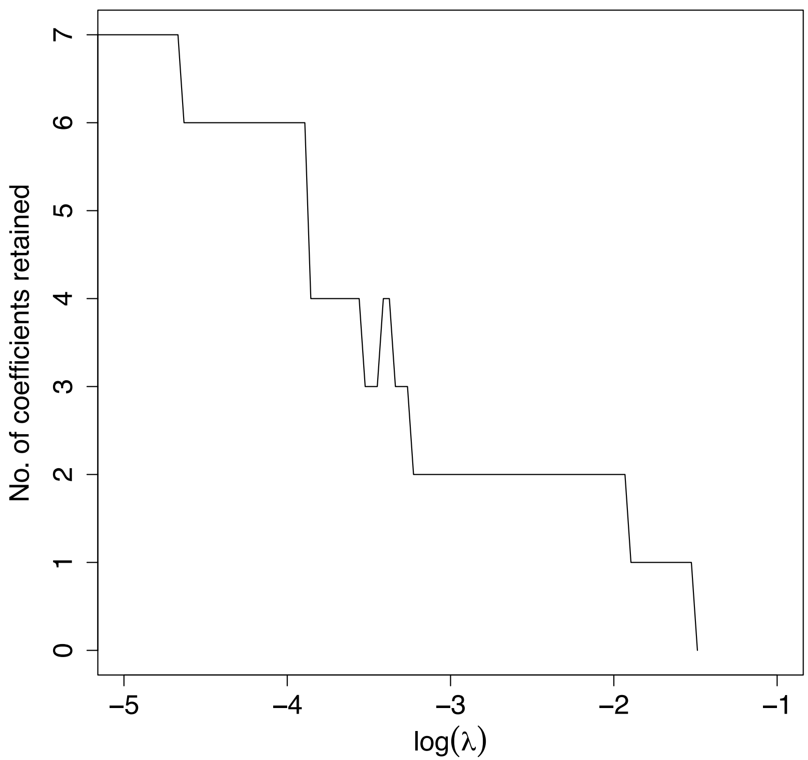
400 **C** samples, colored by the PDF they were drawn from

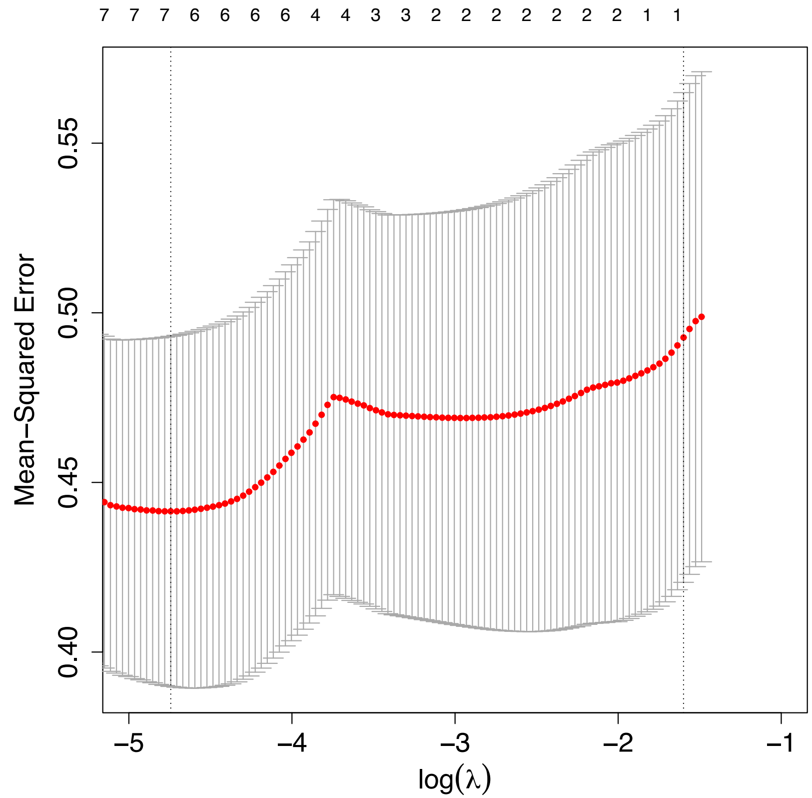
- 22/400 account for 99.9% of the probability mass
- They don't cluster. Failed!

Model-form error

- Hypothesis: The simple form of the EVM is responsible for lack of predictive skill
  - Can enriching it fix the problem?
  - $-\tau_{ij} = -\overline{u_i'u_j'} = \frac{2}{3}\mathrm{k}\delta_{ij} - \nu_T S_{ij} + \nu_T \frac{k}{\epsilon}\sum_{l=1}^{3} c_l f_l(S,\omega) + \nu_T \left(\frac{k}{\epsilon}\right)^2 \sum_{l=4}^{7} c_l f_l(S,\omega)$
  - We do have estimates of c_l 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, ω and τ_{ij} on the midplane; no ε
  - Approximate ε as Production = destruction
  - $\min_{\mathbf{c}} \left\| \tau_{ij} - \mathbf{A}(k,\epsilon,S,\omega)\mathbf{c} \right\|_2^2 + \lambda \|\mathbf{c}\|_1$
  - This will retain only those c_l that are supported by observations
- Note that the values of c_l so obtained are not trustworthy

Model-form error results

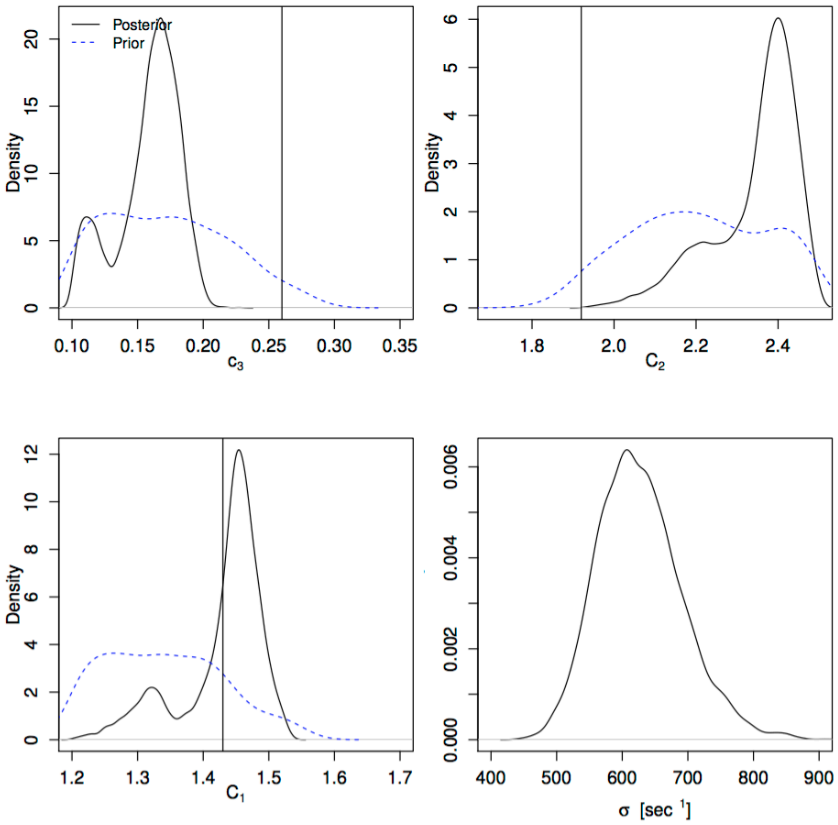




- Good value of λ obtained via 7-fold cross-validation
- Final chosen value of λ retains one extra quadratic term (ω^2) in the EVM

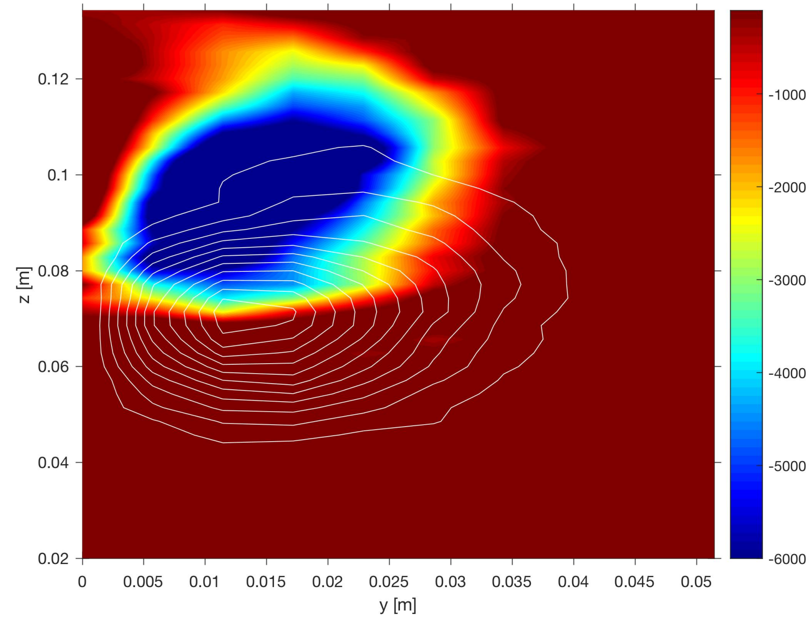
Calibrating QEVM

- 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"

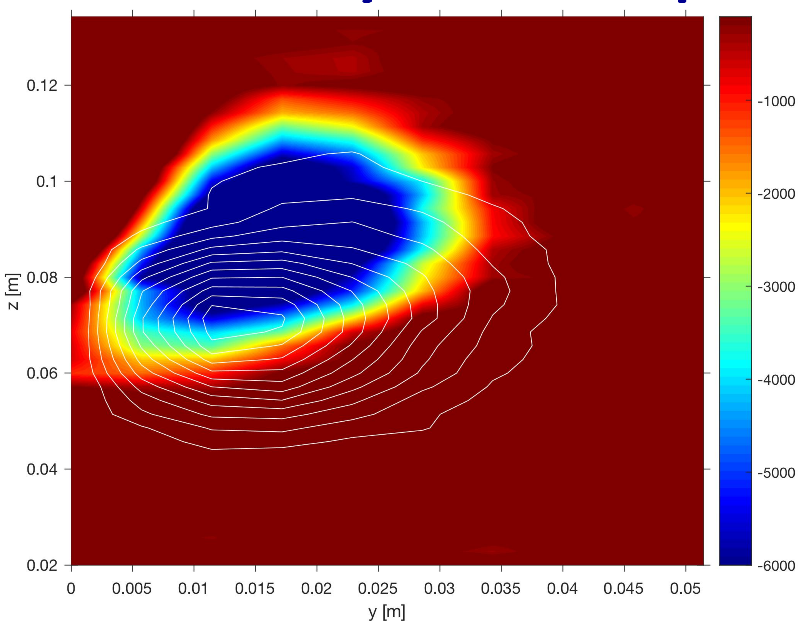


Vorticity, crossplane

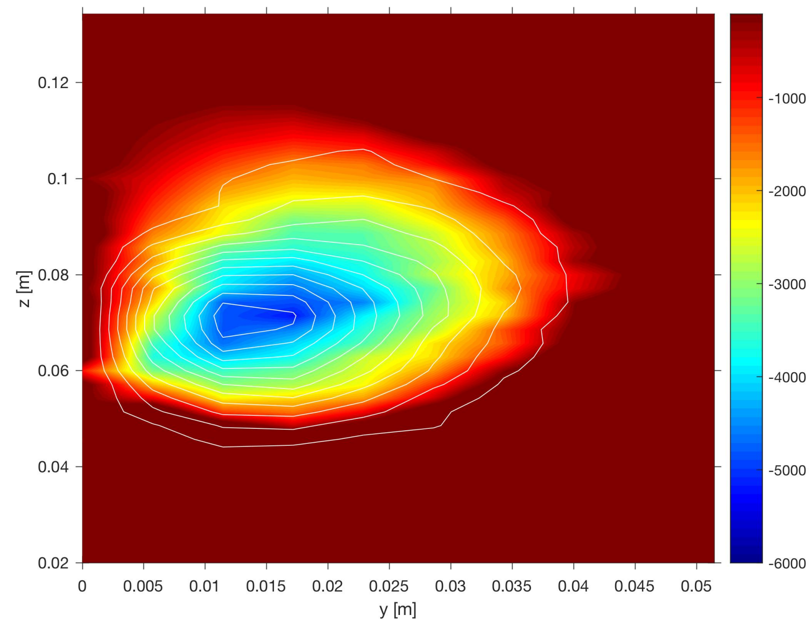
Uncalibrated, CEVM



Uncalibrated, LEVM



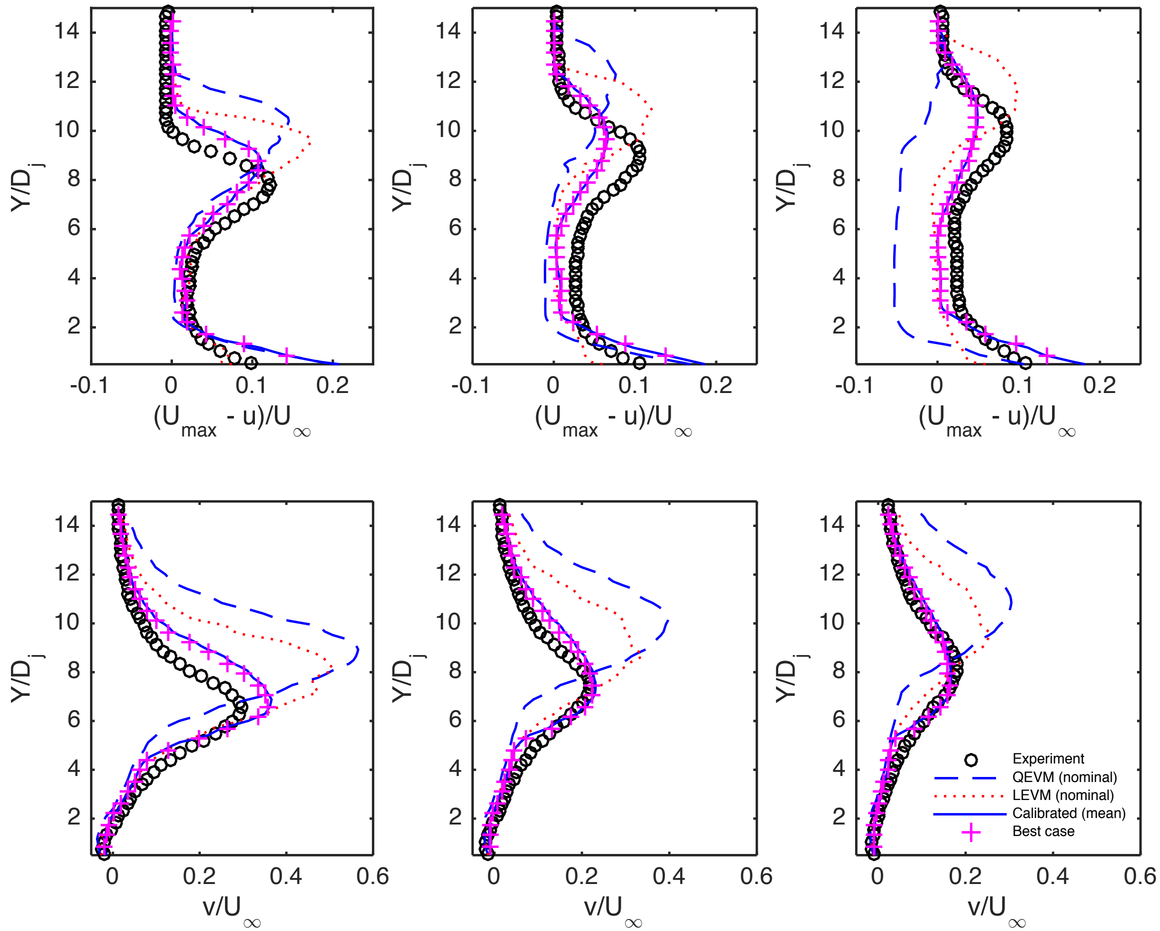
Calibrated, QEVM



- Experiments: Contours
- Significant improvement

Velocities, midplane

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



Discussion

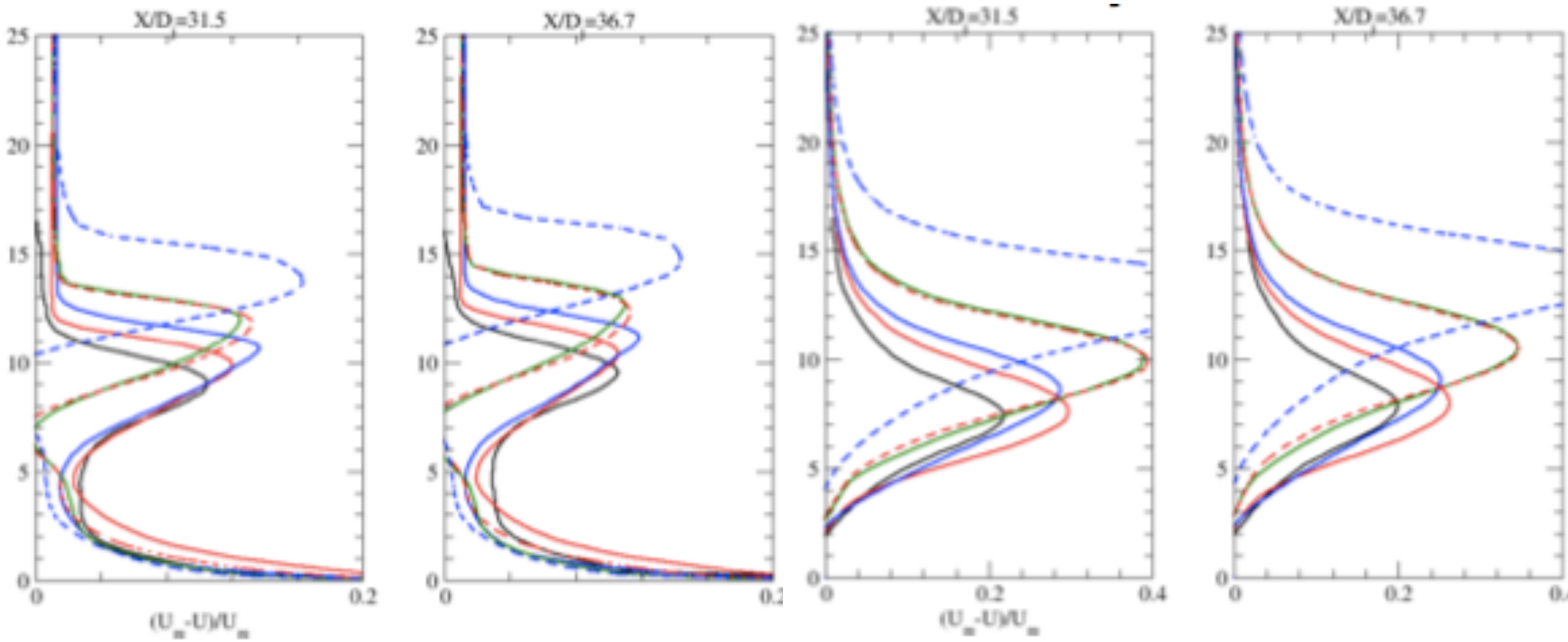
- We have shown how Bayesian calibration improves predictive skill
  - New (C_μ, C_2, C_1) could be a mere artefact to fitting to data; may have no physical significance
  - But analytical model predictions very close to predictions with C_{opt}
    - Next talk: $C_{opt} \sim C_{analytical}$
  - Our 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-ω) simulations – midplane results



U-defect

V - velocity

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