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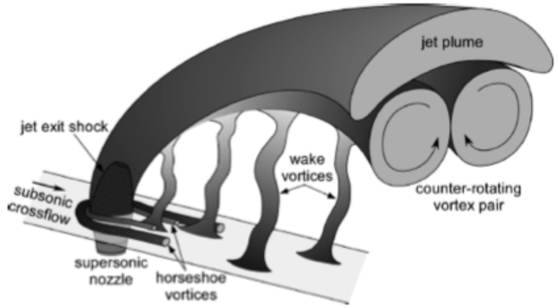

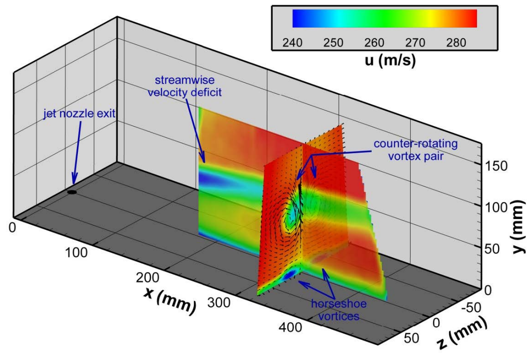

Tuning a RANS k-ε model for jet-in-crossflow simulations

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U.S. DEPARTMENT OF ENERGY

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Introduction

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- Aim: Develop a predictive RANS model for transonic jet-in-crossflow simulations
  - A strongly vortical flow, often with weak shocks
- Drawback: RANS simulations are simply not predictive
  - They have "model-form" error i.e., missing physics
  - The numerical constants/parameters in the k-ε model are usually derived from canonical flows – incompressible flow over plates, channel etc.
- Hypothesis
  - One can calibrate RANS on flow over a square cylinder (strongly vortical) to obtain better parameter estimates
  - Due to model-form error and limited square-cylinder experimental measurements, the parameter estimates will be approximate
    - We will estimate parameters as probability density functions (PDF)

The problem

- The model
  - Devising a method to calibrate 3 k-ε parameters **C** = {C_μ, C_2, C_1} from expt. data

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

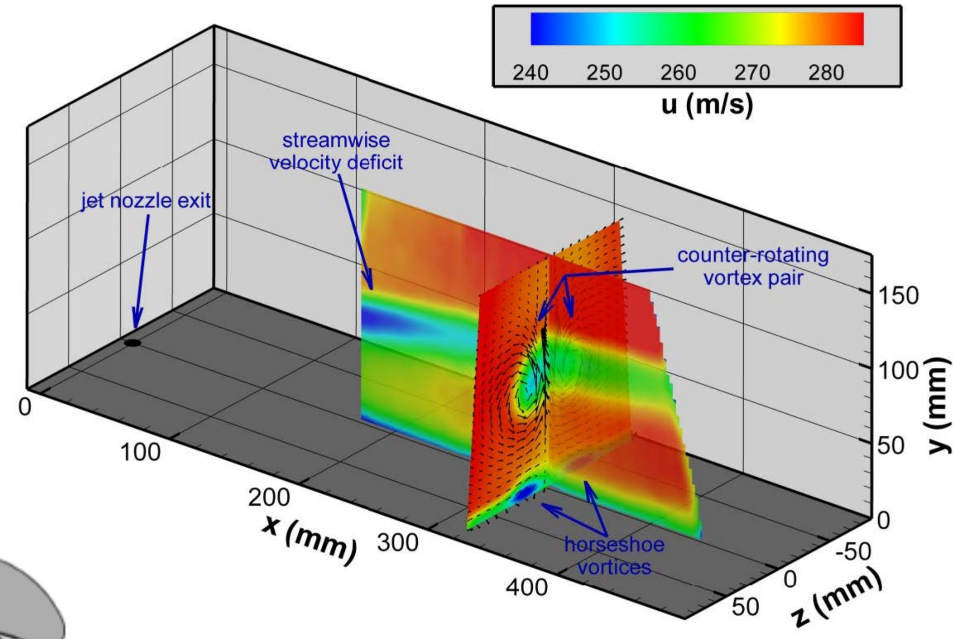
$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_i}\left[\rho u_i \varepsilon - \left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] = \frac{\varepsilon}{k}\left(C_1 f_1 P_k - C_2 f_2 \rho\varepsilon\right) + S_\varepsilon$$

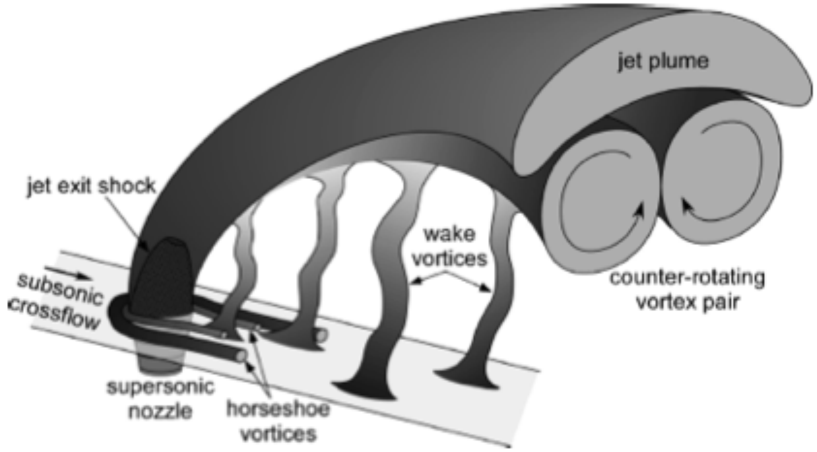
$$\mu_T = C_\mu f_\mu \rho \frac{k^2}{\varepsilon}$$

- Calibration parameters
  - C_μ: affects turbulent viscosity; C_1 & C_2: affects dissipation of TKE
- Calibration method
  - Pose a statistical inverse problem using experimental data for flow-over-a-square-cylinder
  - Estimate parameters using Markov chain Monte Carlo
  - Construct a polynomial surrogate for square-cylinder RANS simulations

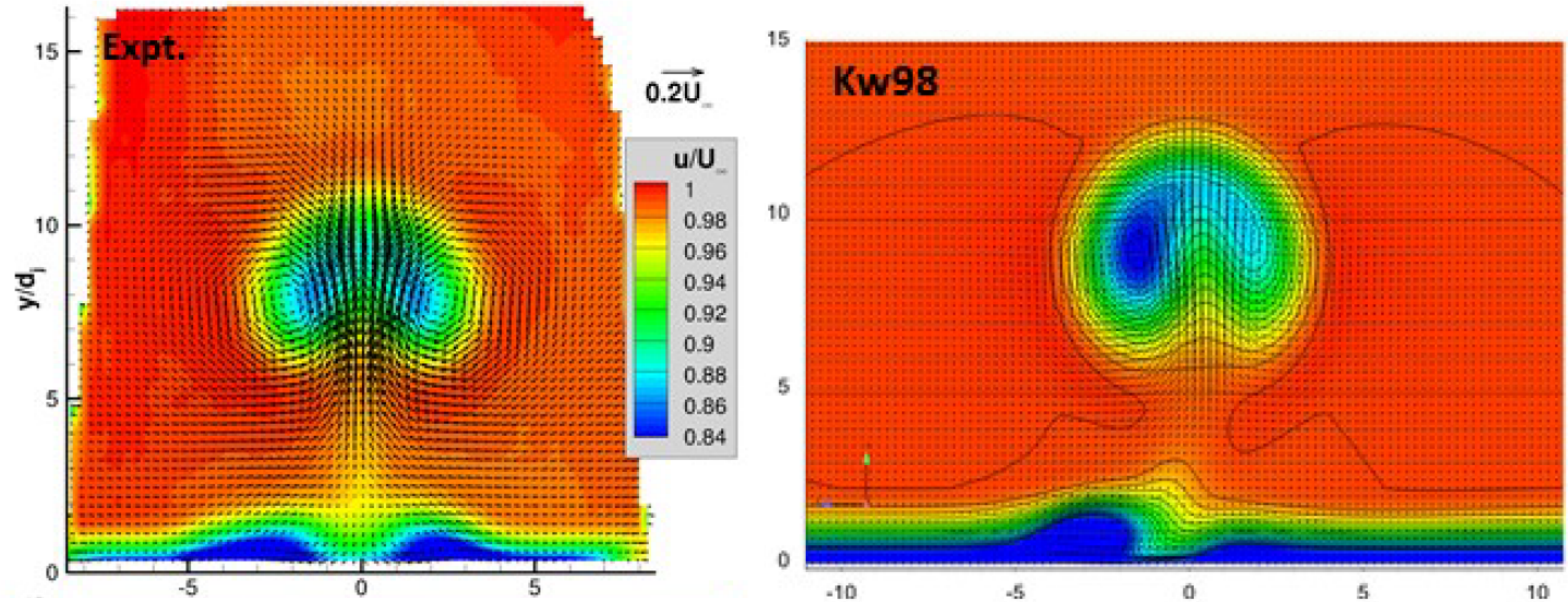
Target problem - jet-in-crossflow

- A canonical problem for spin-rocket maneuvering, fuel-air mixing etc.
- We have experimental data (PIV measurements) and corresponding RANS simulations
- The RANS simulations have stability problems





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

Flow over a square cylinder

- Experimental data
  - Water tunnel, 39 cm X 56 cm cross-section
    - Square-cylinder 4 cm per side
  - 96 probes in the wake where $\eta = u'v'$ are measured
- Making the RANS training set
  - Take 2744 (14^3) samples from the (C_μ, C_2, C_1) space
  - Save $\eta = u'v'$ at the 96 probes for each run

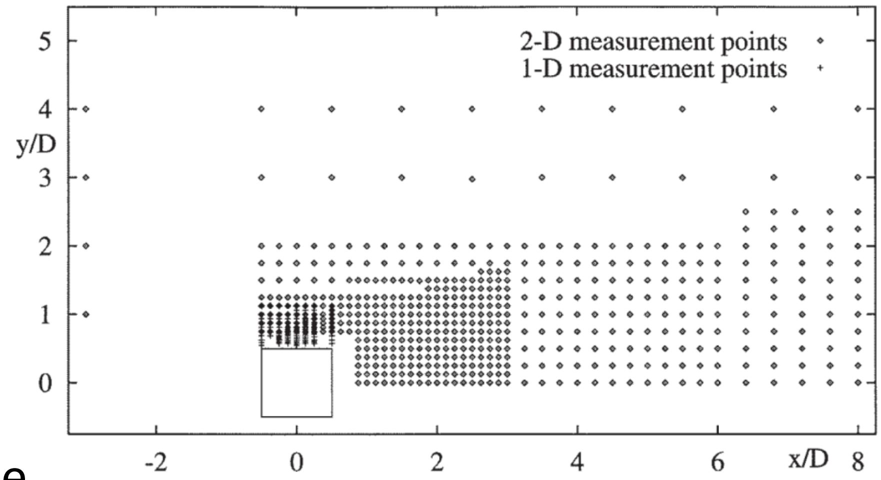


Figure 1: Coordinate system and location of measurement points.

Surrogate models

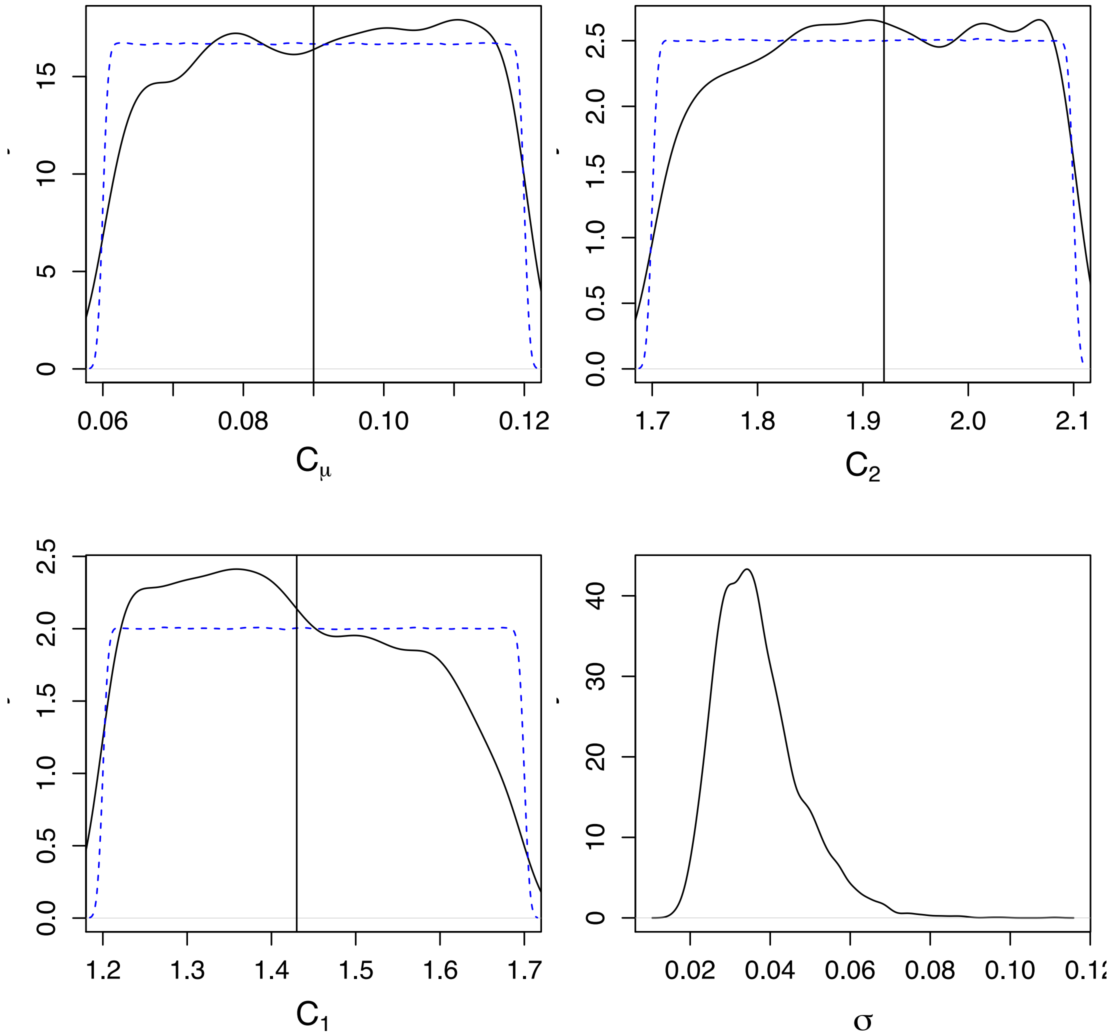
- Model η as a function of **C** i.e. $\eta = \eta(\mathbf{C})$
  - Approximate this dependence with a polynomial

$$\eta \cong \eta_{trend} = a_0 + a_1 C_\mu + a_2 C_2 + a_3 C_1 + a_4 C_\mu C_2 + a_5 C_\mu C_1 + a_6 C_2 C_1 + ...$$

  - Given η_{exp} at a bunch of probe locations, it should be possible to estimate $\{C_\mu, C_2, C_1\}$ by fitting the polynomial model to data
- But how to get $(a_0, a_1, ...)$ for each of the probe locations to complete the surrogate model for each probe?
  - Divide training data in a Learning Set and Testing Set
  - Fit a full quadratic model for η to the Learning Set via least-squares regression; sparsify using AIC
  - Estimate prediction RMSE for Learning & Testing sets; should be equal
- Final model tested using 100-fold cross-validation

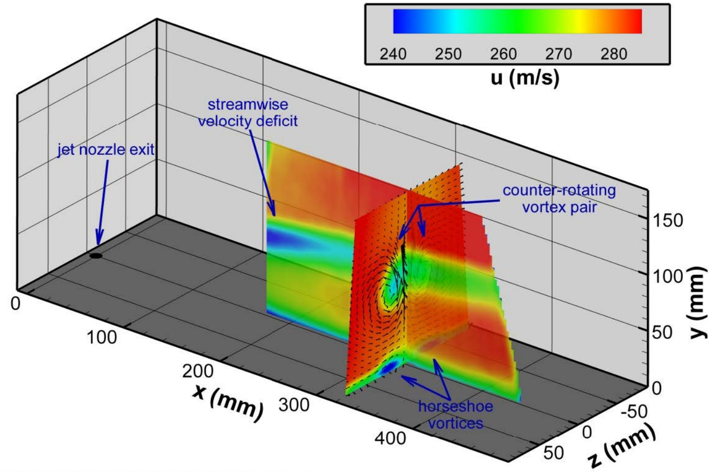
MCMC solution for (C_μ, C_2, C_1)

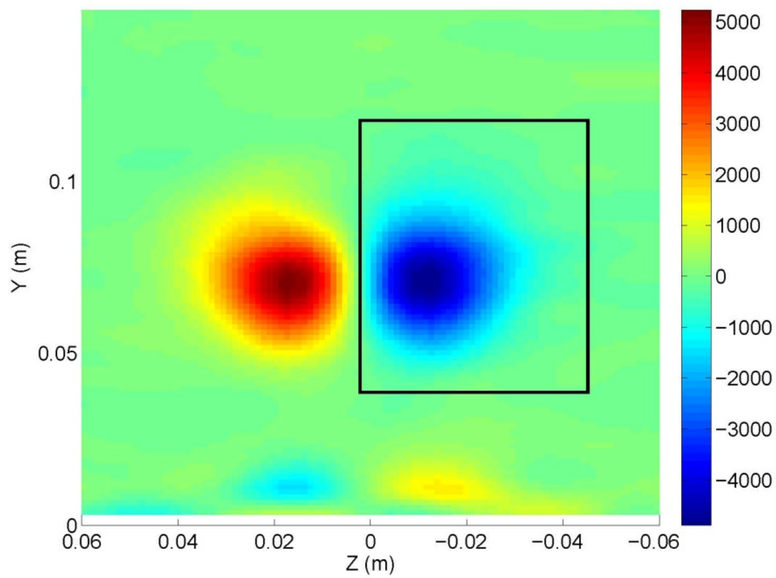
- Computed using an adaptive MCMC method (DRAM)
- These are marginals – the distribution is 4D
- Nominal values are vertical lines
- Blue dashed lines are prior beliefs
- The model error σ is large



Is the PDF predictive for jet-in-crossflow?

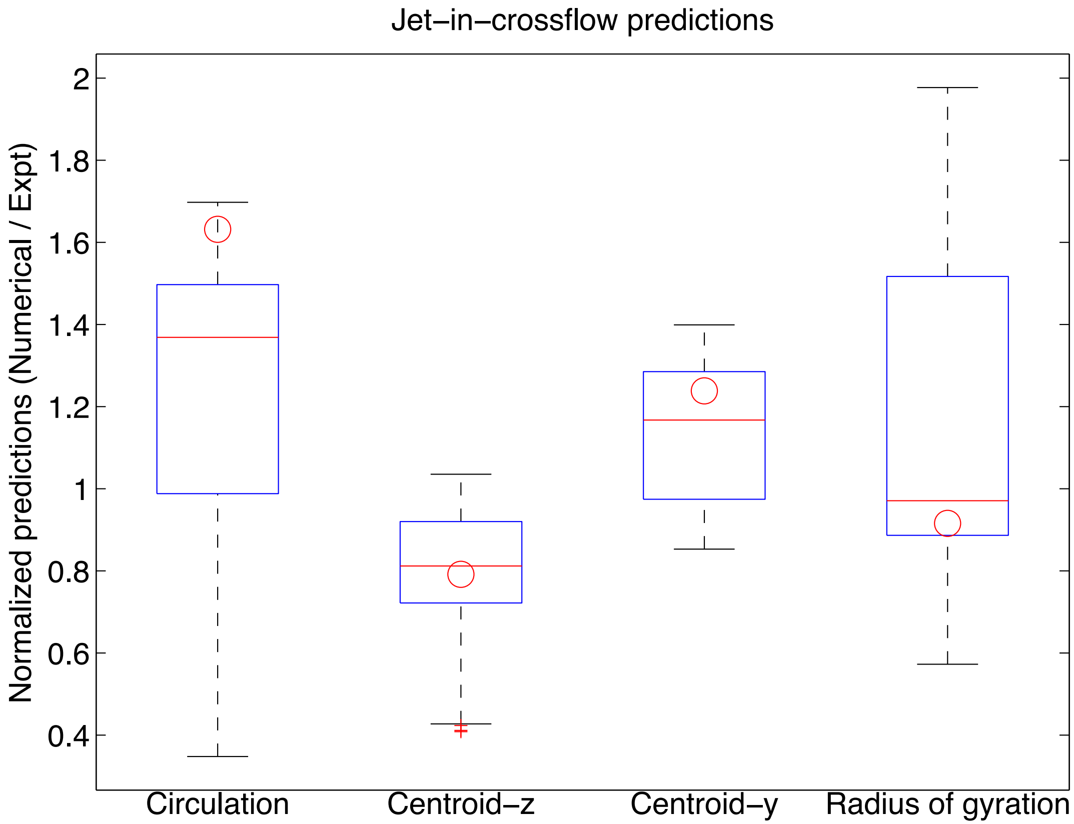
- Pick 100 C samples from the PDF
- Simulate jet-in-crossflow
- In the crossplane, quantify
  - Circulation
  - Centroid of vorticity
  - Radius of gyration
- From the ensemble, calculate median, quartiles etc
- Compare with experimental values



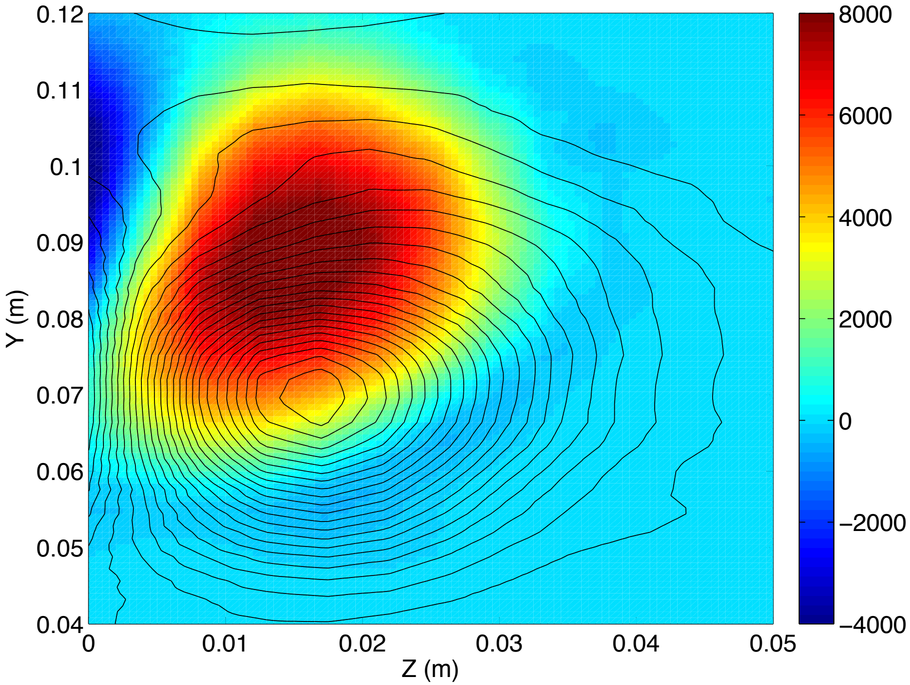


Comparison of predictions and experiments

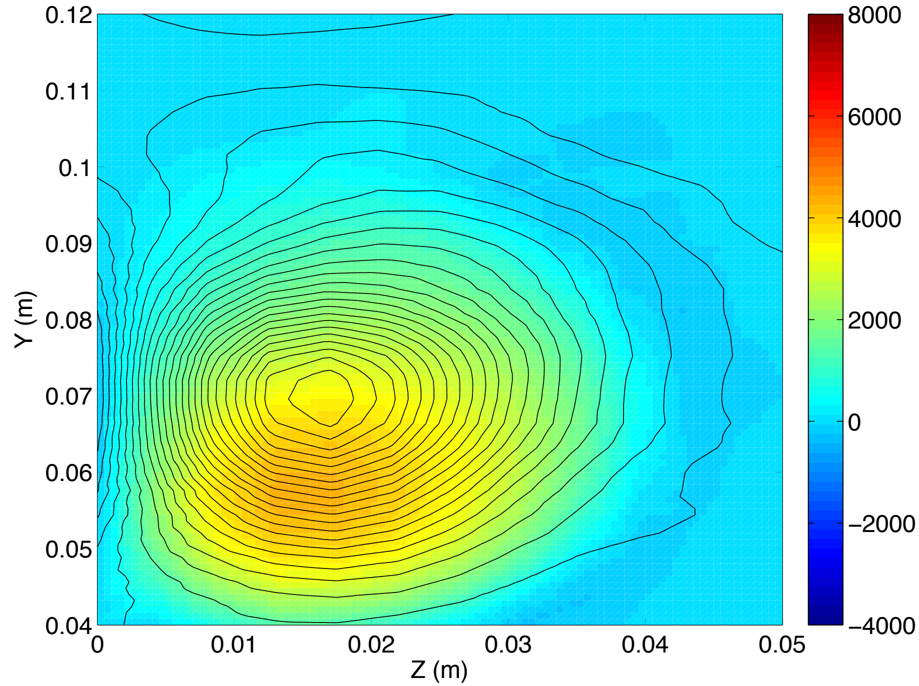
- Plotting Predictions / Experimental values
- We overpredict circulation
- Location is somewhat off
- Size is somewhat larger
- Big improvements over nominal value
- Also search the 100 ensemble members for best prediction
  - “Optimal” ensemble member



Optimal ensemble member – vorticity



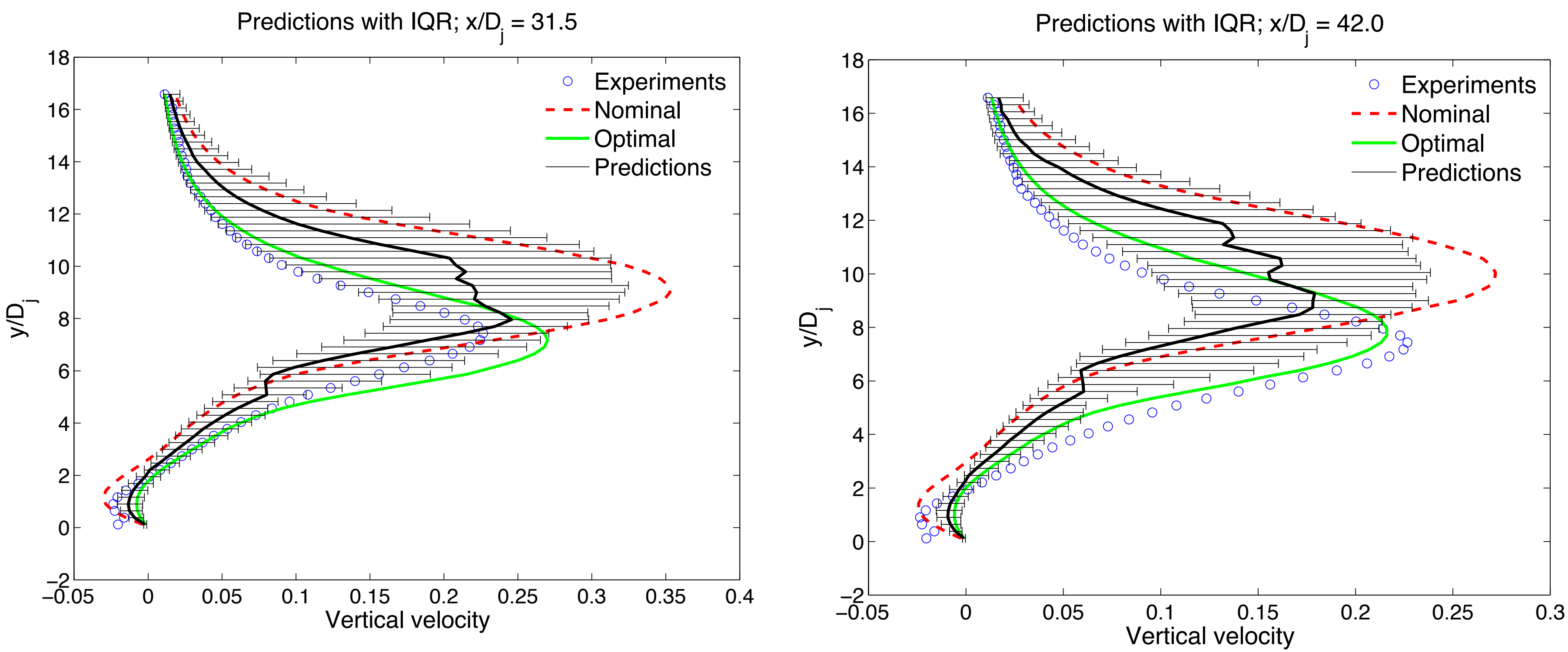
With nominal **C**



With best **C**

- Experimental vorticity as contours
- Calibration positions the vortex better; also gets its strength right
- The circulation, position and size are +/- 15% from experiments

Optimal ensemble member: w velocity



x/D = 31.6 **x/D = 42.0**

- Improvement over $\mathbf{C_{nominal}}$
- Nearly nailed the experiment

Conclusions

- Our hypothesis of calibrating to a simple vortical flow for predictive jet-in-crossflow proved correct
- Even simple, polynomial surrogates were sufficiently accurate to allow us to calibrate RANS models
  - More elaborate models, with the deficit would probably do somewhat better
  - With surrogates come Bayesian calibration and PDFs of calibrated parameters
- Being able to get a PDF for (C_μ, C_2, C_1) proved to be very convenient
  - Ensemble predictions provide error bars on predictions
  - They allow us to test various (C_μ, C_2, C_1) combinations for predictive power
- *Details: S. Lefantzi, J. Ray, S. Arunajatesan and L. Dechant, "Tuning a RANS k-ε model for jet-in-crossflow simulations", Sandia Technical Report, SAND2013-8158*