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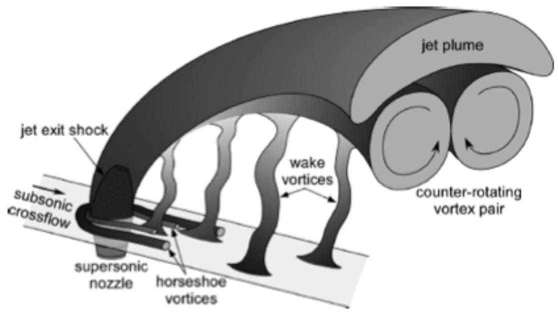

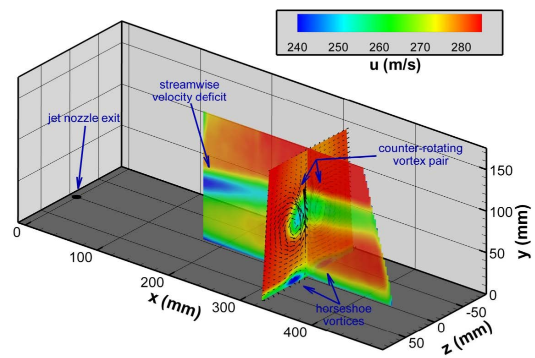

Tuning a RANS k-ε model for jet-in-crossflow simulations

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Introduction

- 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

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

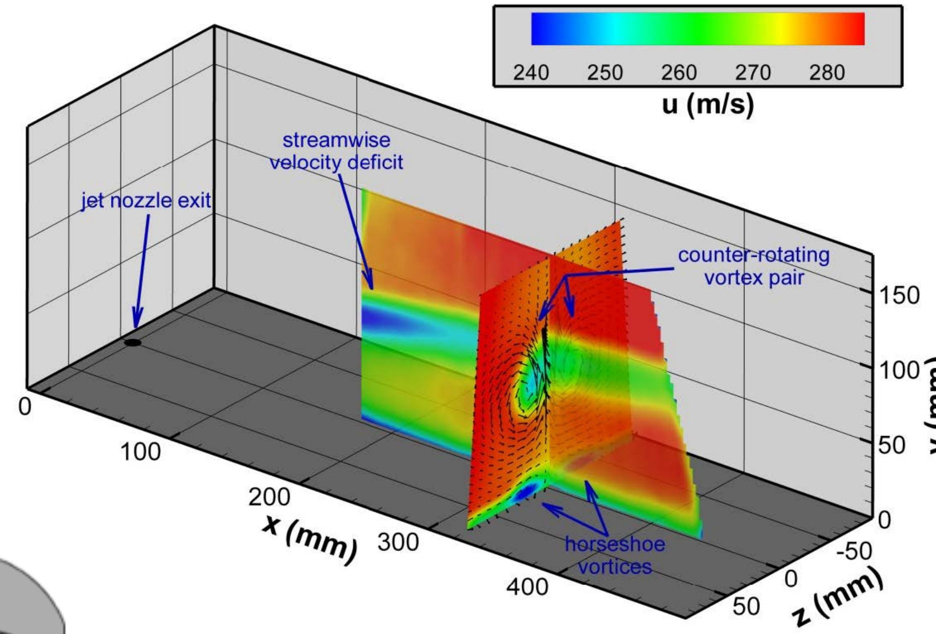
$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_i}\left[\rho u_i \varepsilon - \left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] = \frac{\varepsilon}{k}\left(C_1 f_1 P_k - C_2 f_2 \rho\varepsilon\right) + S_\varepsilon$$

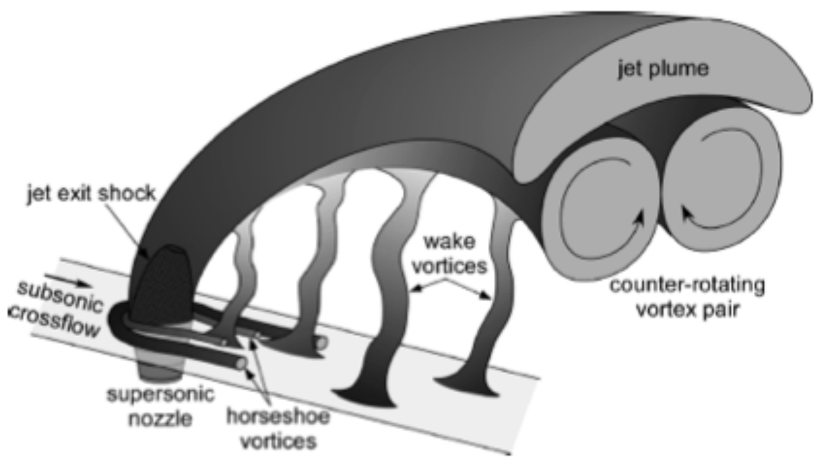
$$\mu_T = C_\mu f_\mu \rho \frac{k^2}{\varepsilon}$$

- 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

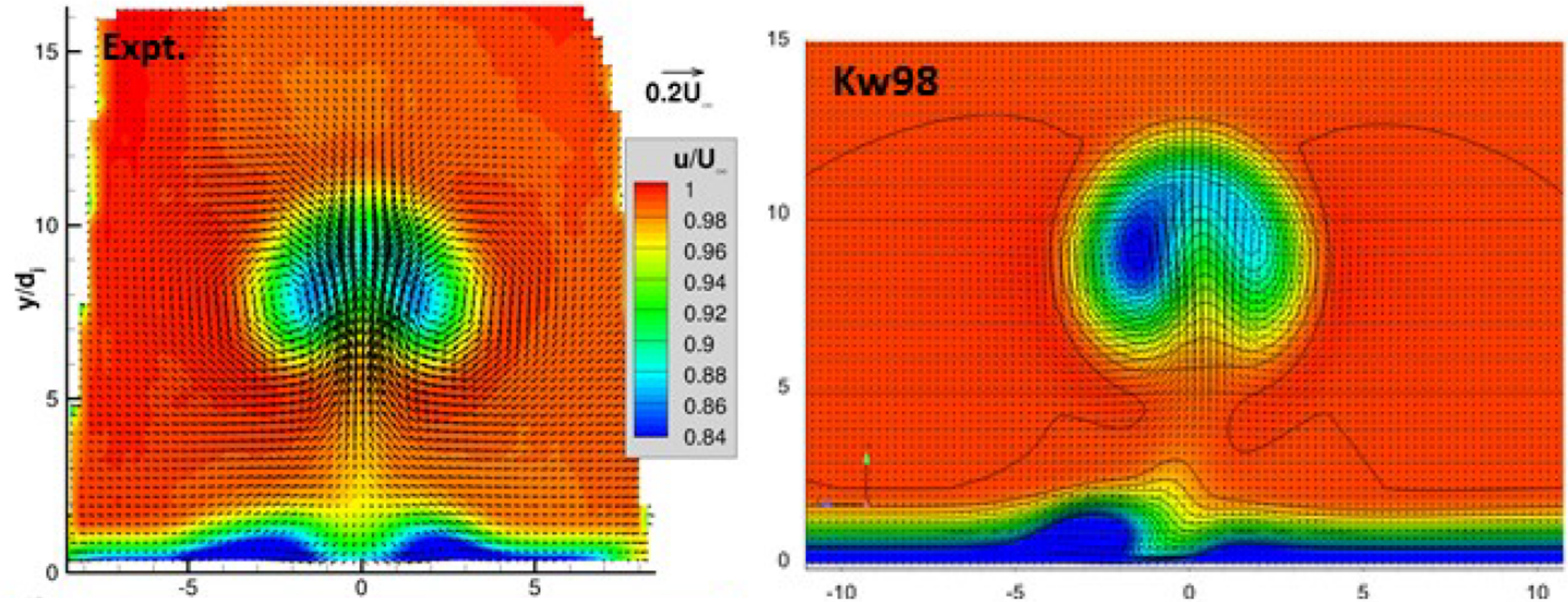
Target problem - jet-in-crossflow

- 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



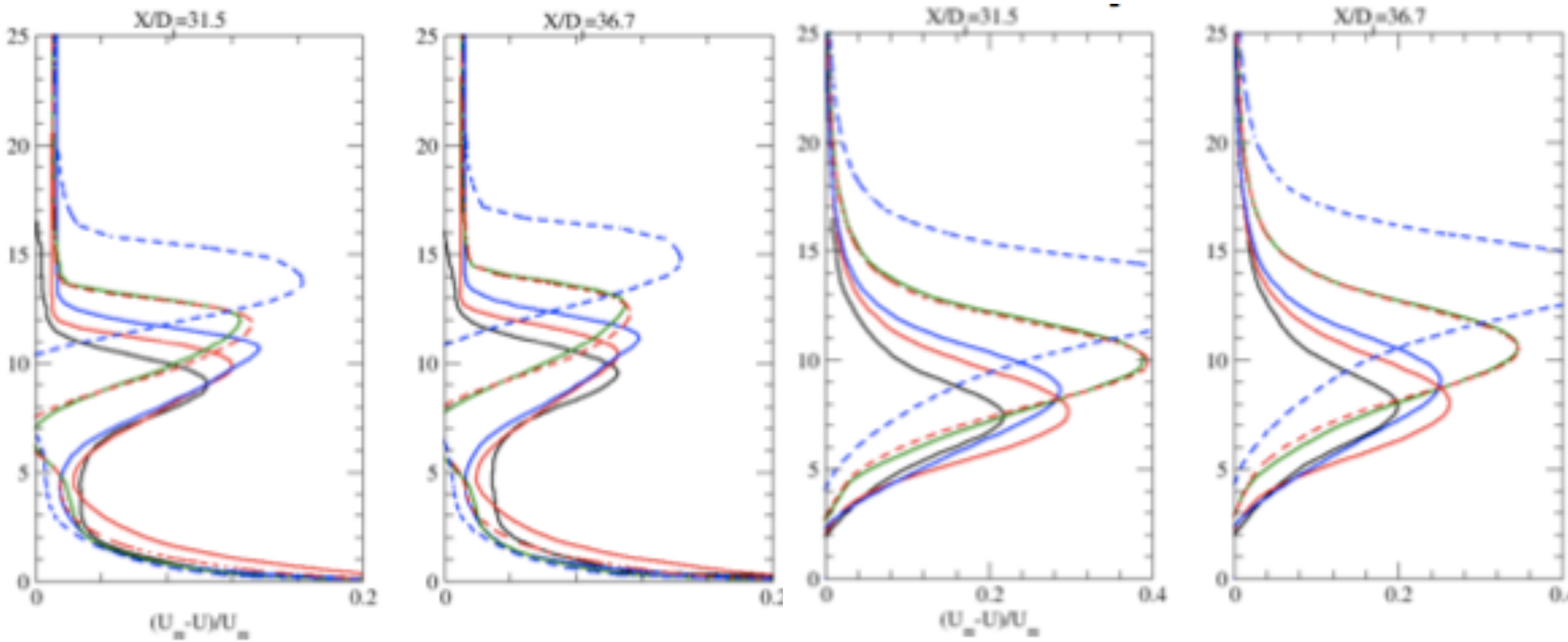


RANS (k-ω) simulations - crossplane results



- 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

RANS (k-ω) simulations – midplane results



U-defect

W - velocity

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

The desired outcome

- Summary
  - The velocity distribution from RANS at the crossplane is pretty terrible
  - At the mid-plane, the jet sits too high; the vertical velocity is too high indicating a very strong vortex
- Aims of the calibration
  - Get the crossplane vorticity distribution right
    - Correct circulation, position and size of the CVP
  - Match the midplane velocity profiles
- Procedure
  - Use experimental data from a flow-over-square-cylinder experiment
    - Observations of Reynolds stress in the wake behind the cylinder
  - Construct a computationally inexpensive surrogate for the RANS model / predictions of Reynolds stress
  - Use the surrogate for Bayesian calibration of the 3 parameters

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
- Calibration: Make a map of η to (C_μ, C_2, C_1)
  - Use a statistical (surrogate) model
  - Make a RANS training set using 2744 samples from the (C_μ, C_2, C_1) space
  - Save $\eta = u'v'$ at the 96 probes for each run

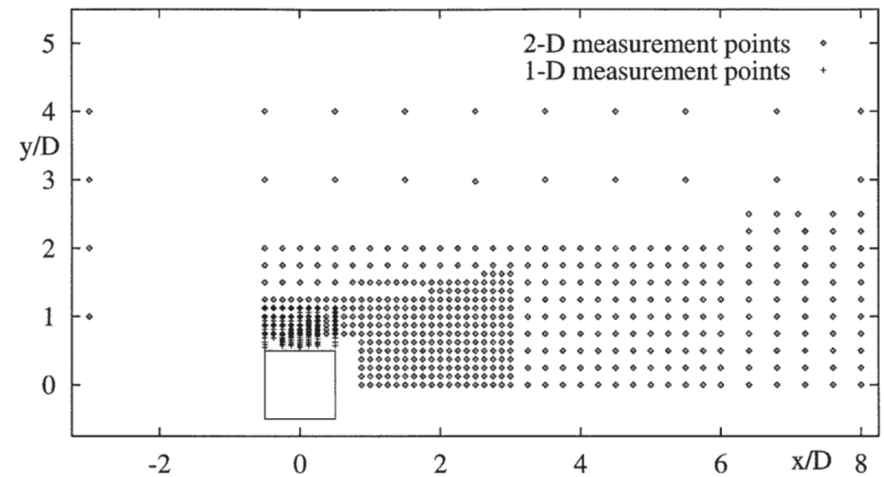


Figure 1: Coordinate system and location of measurement points.

Experimental data and setup from Lyn & Rodi, JFM, 1994

Surrogate models

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

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

  - 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 $(a_0, a_1, \ldots.)$ 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; a 10% error threshold was used to select models for the probes

Calibration – in earnest

- Basic idea:
  - Choose 55/96 probes at x/D = 2 ... 8
  - Measured u'v', u' and v'
  - minimize $||h_{ex} - h_{trend}||_2$ by finding 'good' values of (C_m, C_2, C_1)
  - Bayesian calibration: Find $P(C_m, C_2, C_1 \mid h_{expt})$

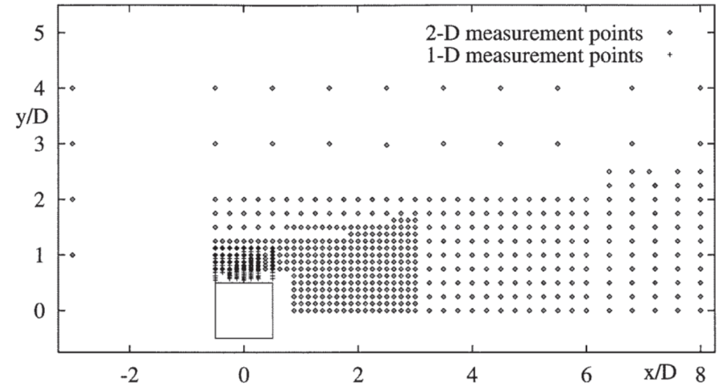


Figure 1: Coordinate system and location of measurement points.

- RANS does not even provide a very good prediction for the wake
  - $(\eta_{ex} - \eta_{trend})$ can be large for many probes
- Choose a set of 'calibration' probes
  - $0.25 < \eta_{ex} / \eta_{trend}(\mathbf{C}_{nominal}) < 4$
- We end up with 28 / 96 probes which we can use for calibration
  - We call this set of 28 probes $\mathcal{P}$

The Bayesian calibration problem

- Model experimental values at probe p as $\eta^{(p)}_{ex} = \eta^{(p)}_{trend}(\mathbf{C}) + \varepsilon^{(p)}$, $\varepsilon^{(p)} \sim N(0, \sigma^2)$

$$\Lambda\left(\eta_{\mathrm{ex}}^{(p)} \mid C\right) \propto \prod_{p \in \mathcal{P}} \exp\left(-\frac{\left(\eta_{ex}^{(p)} - \eta_{trend}^{(p)}(C)\right)^2}{2\sigma^2} \right)$$

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

$$P(C,\sigma \mid \eta_{ex}^{(p)}) \propto \Lambda(\eta_{ex}^{(p)} \mid C,\sigma)\, \pi_\mu(C_\mu)\, \pi_2(C_2)\, \pi_1(C_1) \pi_\sigma(\sigma)$$

- P(**C**|η_{ex}) is a complicated distribution that has to be described/ visualized by drawing samples from it
- This is done by MCMC

What is MCMC?

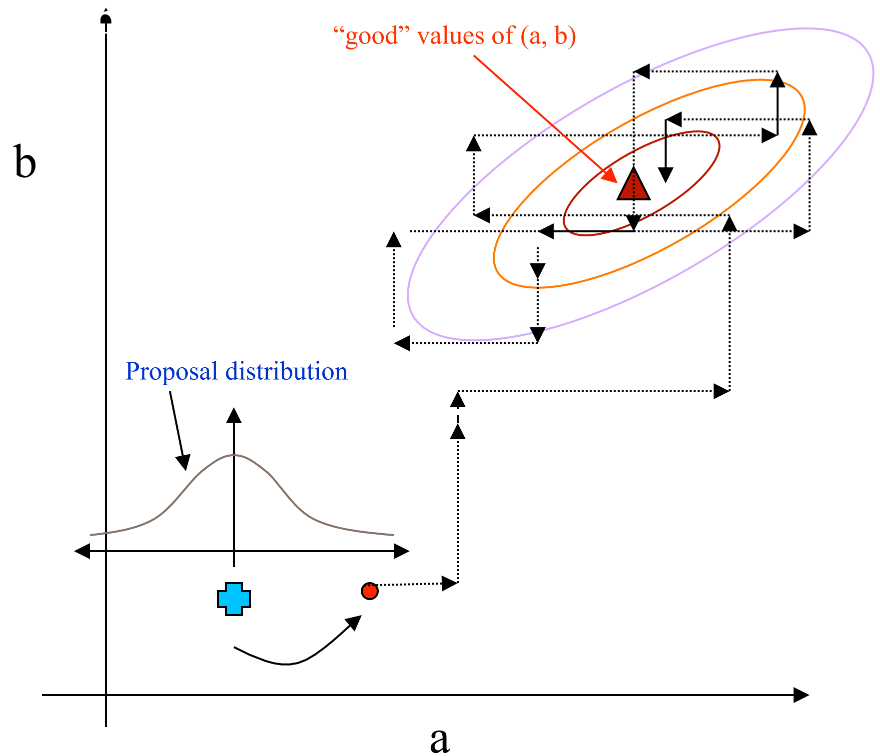
- A way of sampling from an arbitrary distribution
  - The samples, if histogrammed, recover the distribution
- Efficient and adaptive
  - Given a starting point (1 sample), the MCMC chain will sequentially find the peaks and valleys in the distribution and sample proportionally
- Ergodic
  - Guaranteed that samples will be taken from the entire range of the distribution
- Drawback
  - Generating each sample requires one to evaluate the expression for the density π
  - Not a good idea if π involves evaluating a computationally expensive model

An example, using MCMC

- Given: (Y^{obs}, X), a bunch of n observations
- Believed: $y = ax + b$
- Model: $y_i^{obs} = ax_i + b_i + \varepsilon_i$, $\varepsilon \sim \mathcal{N}(0, \sigma)$
- We also know a range where a, b and σ might lie
  - i.e. we will use uniform distributions as prior beliefs for a, b, σ
- For a given value of (a, b, σ), compute "error" $\varepsilon_i = y_i^{obs} - (ax_i + b_i)$
  - Probability of the set (a, b, σ) = $\Pi \exp(- \varepsilon_i^2/\sigma^2)$
- Solution: π (a, b, σ | Y^{obs}, X) = $\Pi \exp(- \varepsilon_i^2/\sigma^2)$ * (bunch of uniform priors)
- Solution method:
  - Sample from π (a, b, σ | Y^{obs}, X) using MCMC; save them
  - Generate a "3D histogram" from the samples to determine which region in the (a, b, σ) space gives best fit
  - Histogram values of a, b and σ, to get individual PDFs for them
  - Estimation of model parameters, with confidence intervals!

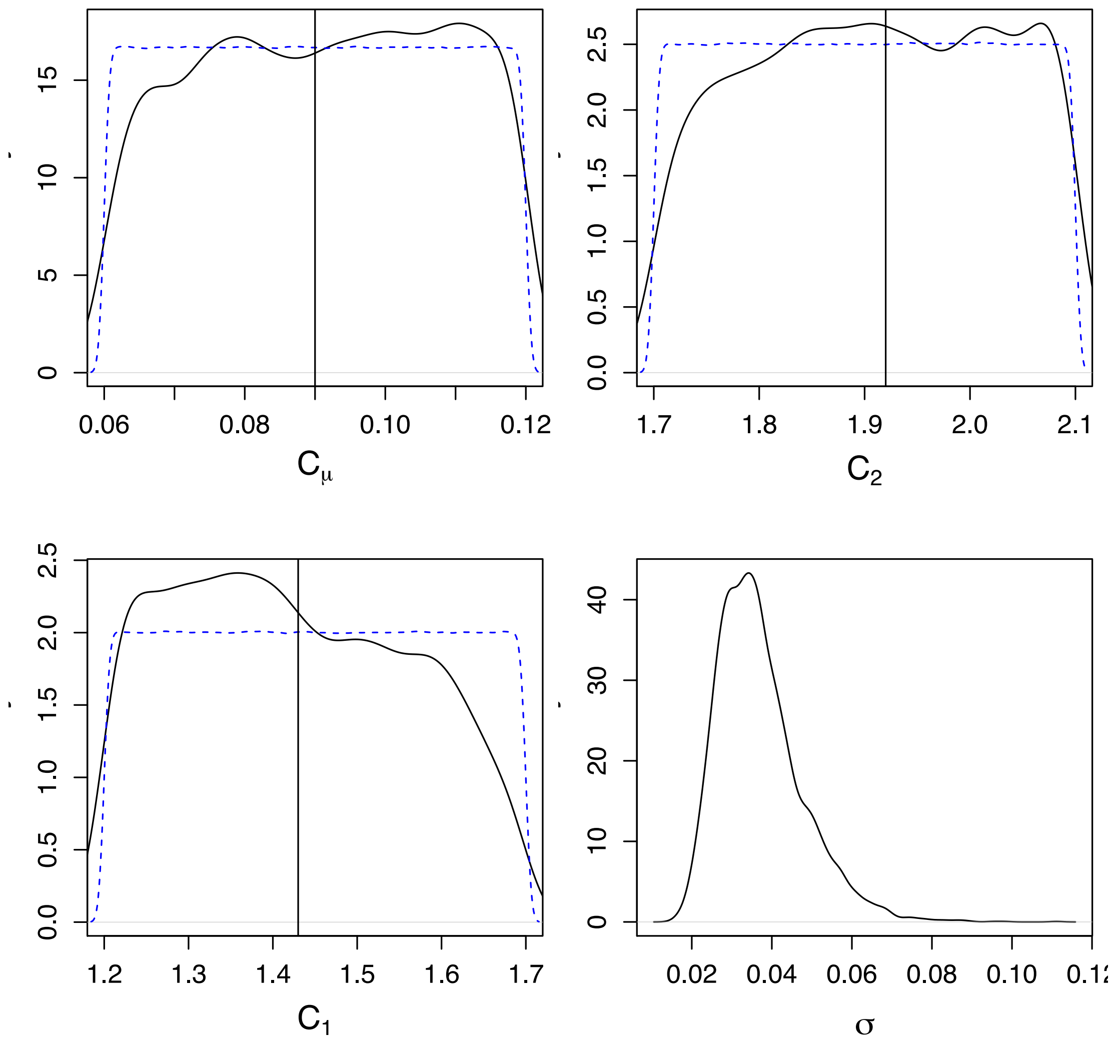
MCMC, pictorially

- Choose a starting point, $P^n = (a_{curr}, b_{curr})$
- Propose a new a, $a_{prop} \sim \mathcal{N}(a_{curr}, \sigma_a)$
- Evaluate $\pi\, (\, a_{prop}, b_{curr} \mid \ldots) \,/\, \pi\, (\, a_{curr}, b_{curr} \mid \ldots\,) = m$
- Accept a_{prop} (i.e. $a_{curr} \leftarrow a_{prop}$) with probability $\min(1, m)$
- Repeat with b
- Loop over till you have enough samples



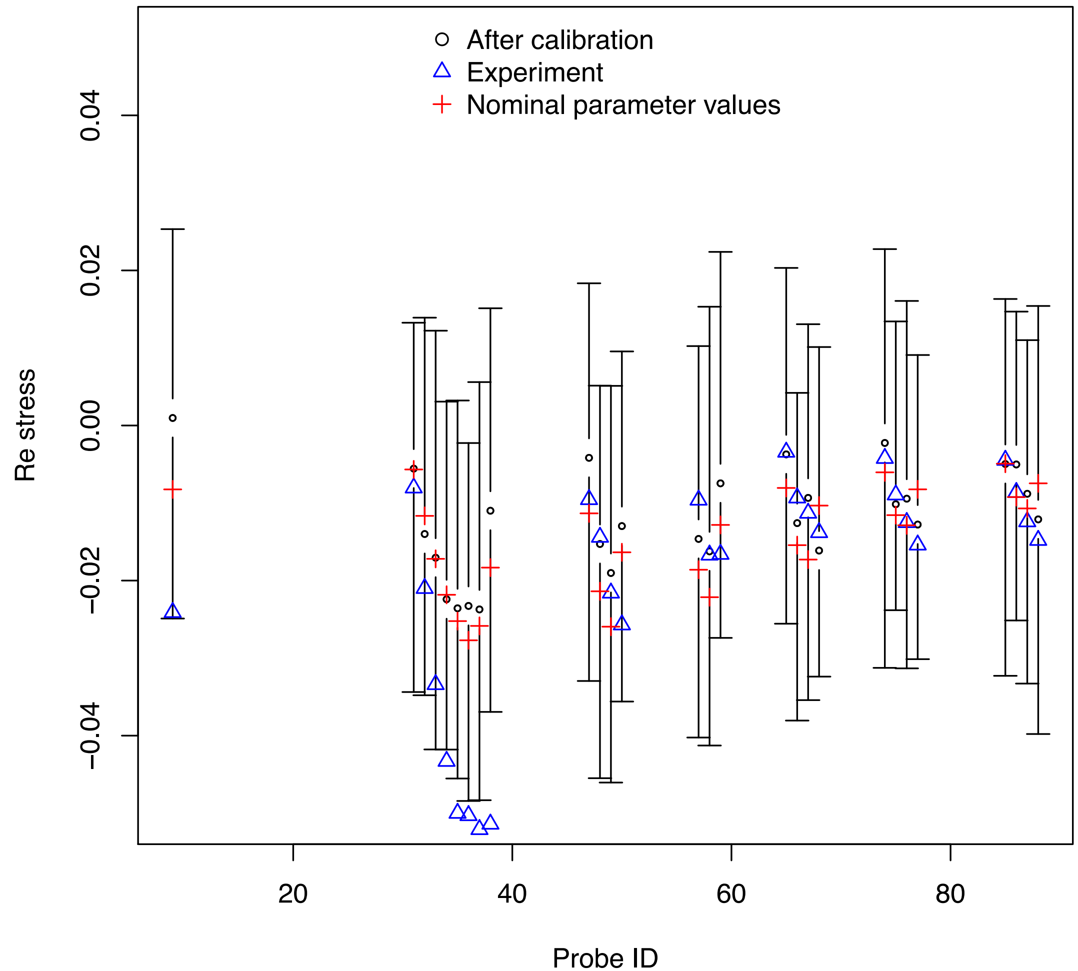
MCMC solution for (C_μ, C_2, C_1)

- 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



Recreating expt. observations

- Post-calibration, we choose 100 **C** samples from the PDF
  - Run the ensemble of 100 RANS runs and plot results at $\mathcal{P}$
- Median predictions close to experimental values
- Error bars capture all measurements



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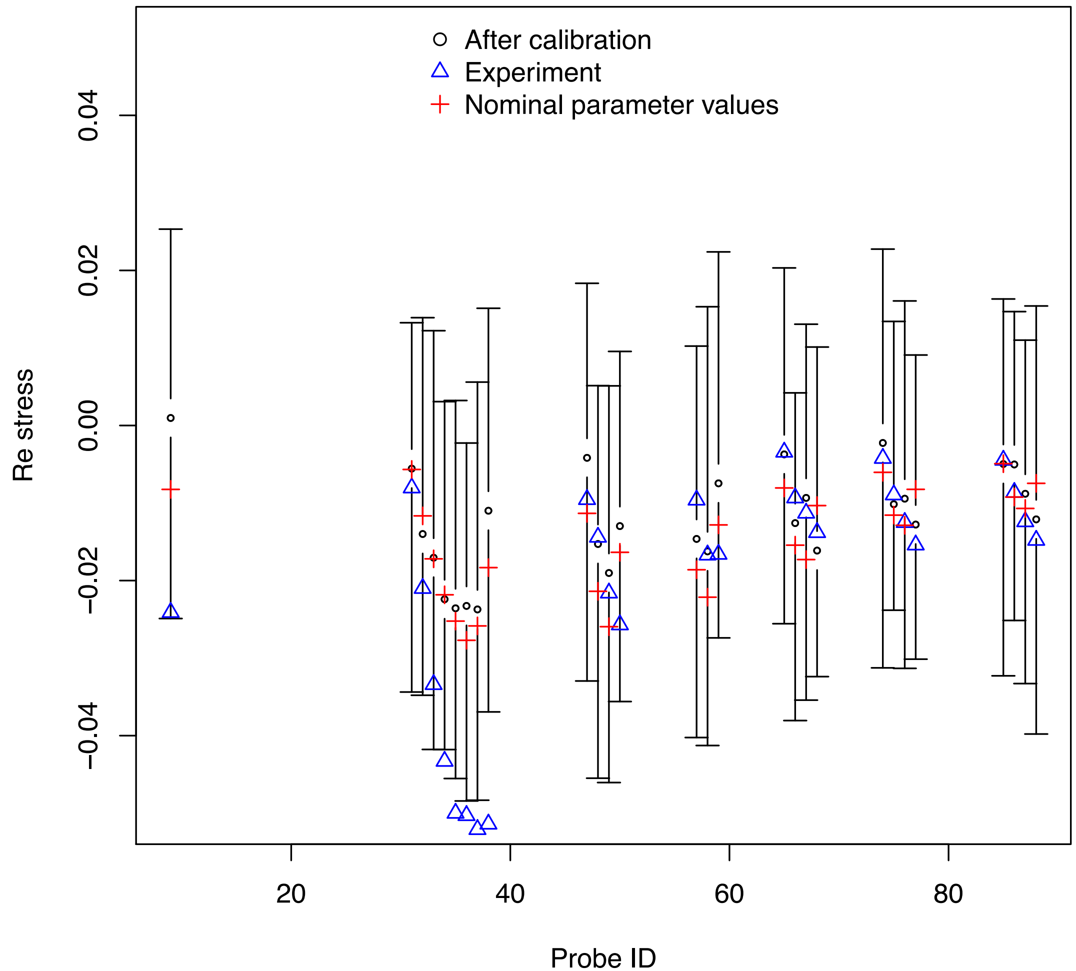
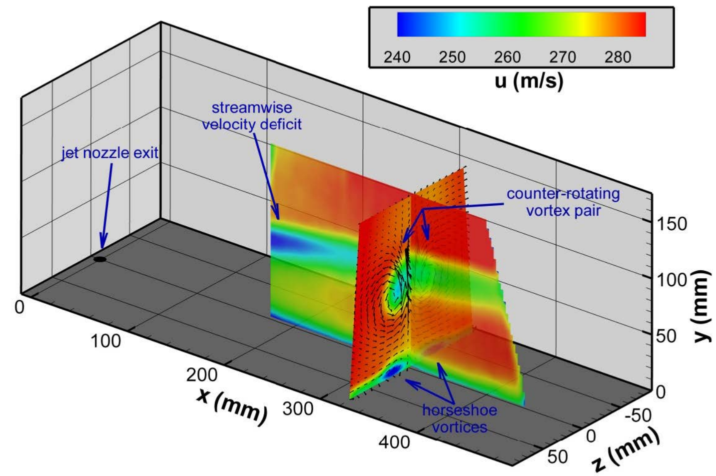
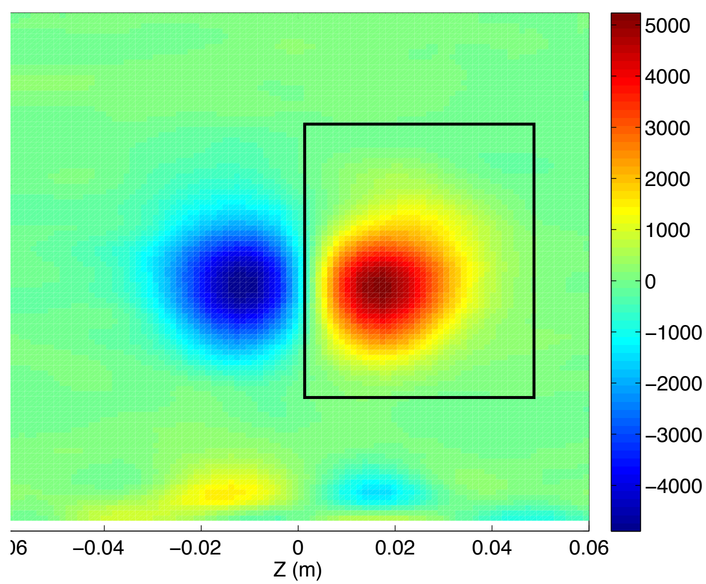


Is the PDF predictive for jet-in-crossflow?

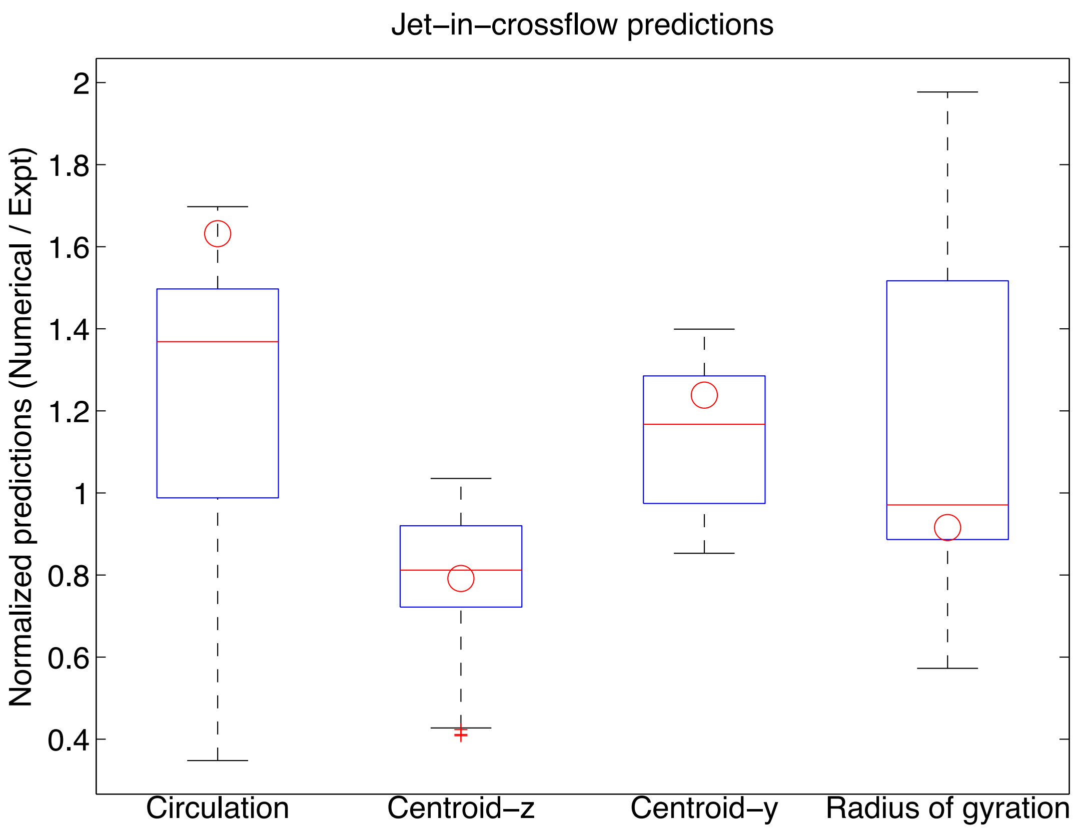
- Pick 100 C samples from the PDF
- Simulate jet-in-crossflow
- In the crossplane, quantify
  - Circulation
  - Centroid of vorticity
  - Radius of gyration
- From the ensemble, calculate median, quartiles etc
- Compare with experimental values



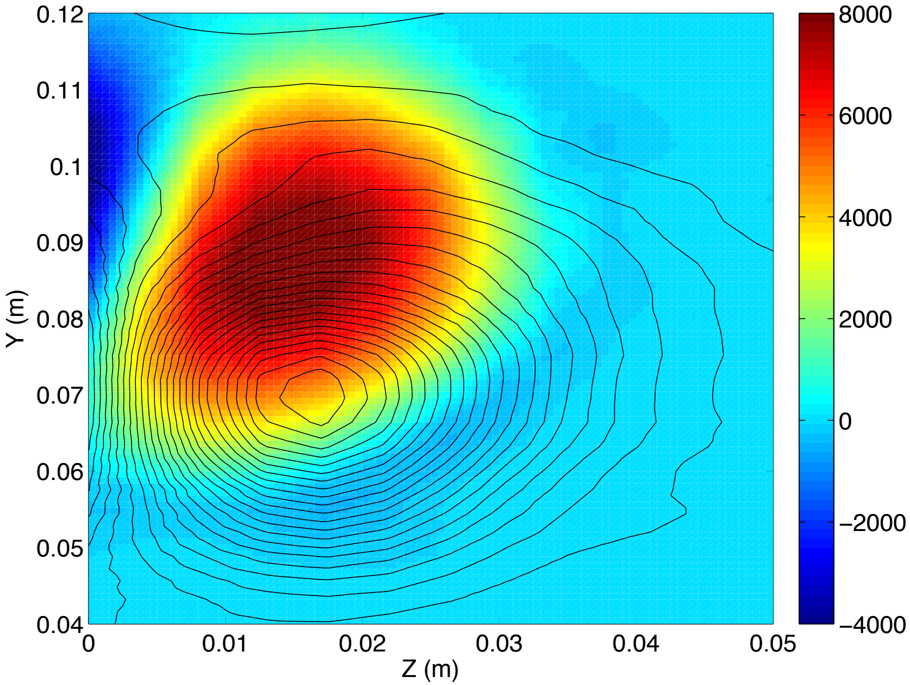


Comparison of predictions and experiments

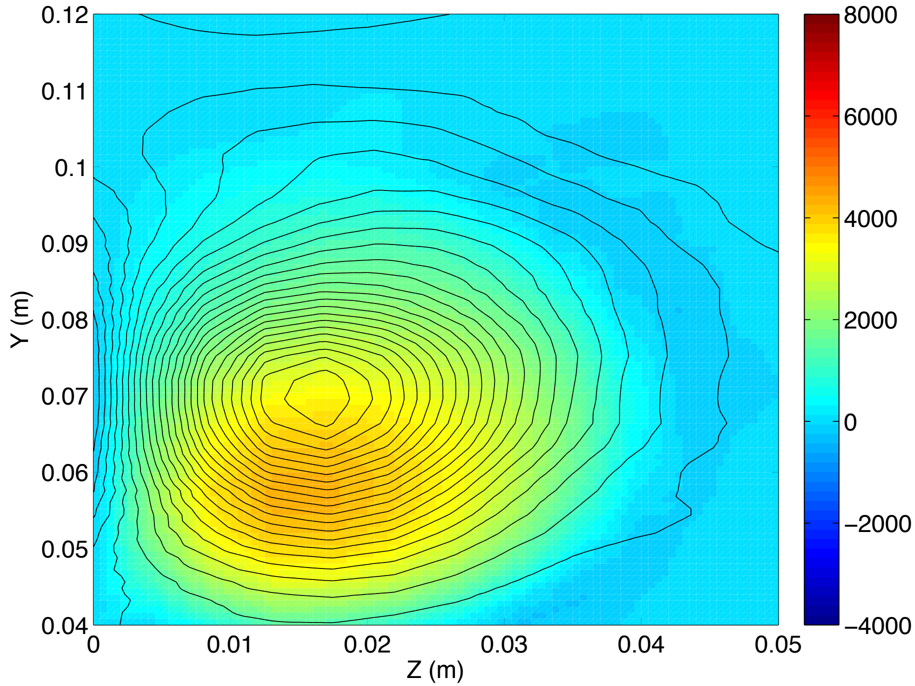
- Plotting Predictions / Experimental values
- We overpredict circulation
- Location is somewhat off
- Size is somewhat larger
- Big improvements over nominal value
- Also search the 100 ensemble members for best prediction
  - "Optimal" ensemble member



Optimal ensemble member – vorticity



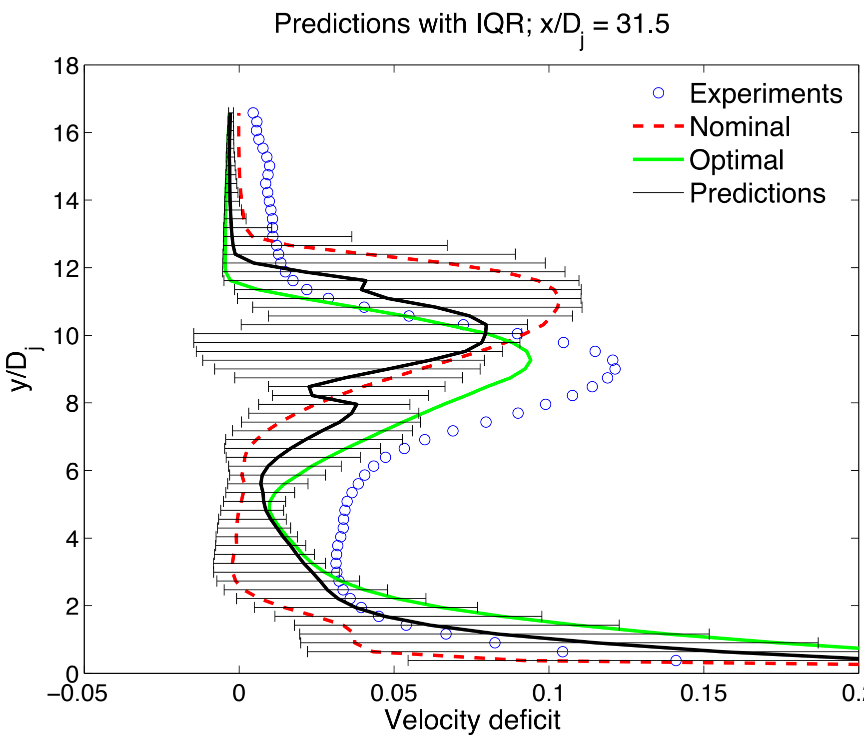
With nominal **C**



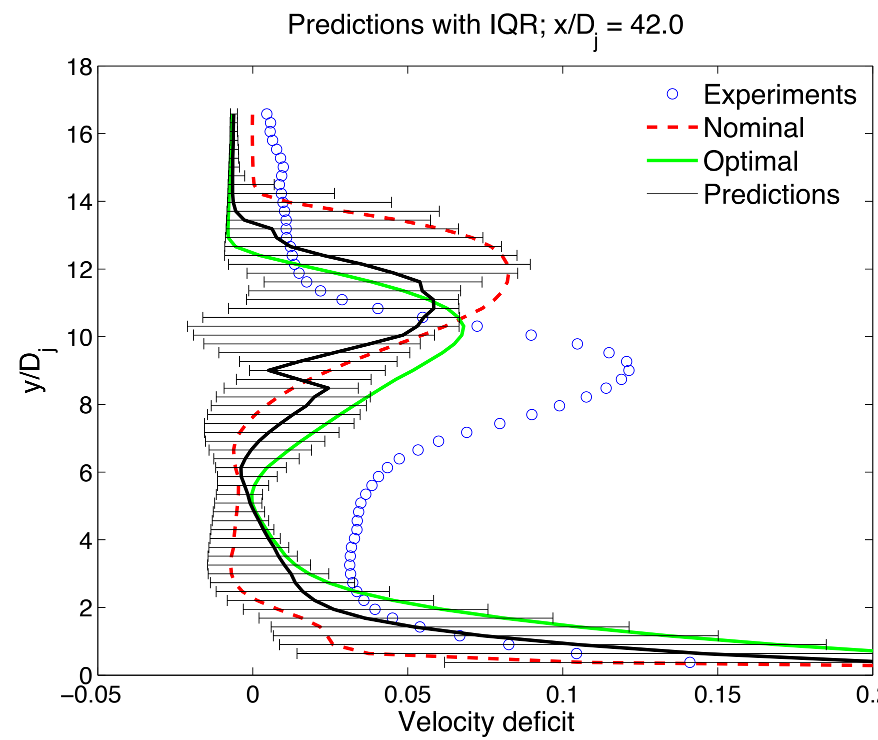
With best **C**

- 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 – u deficit



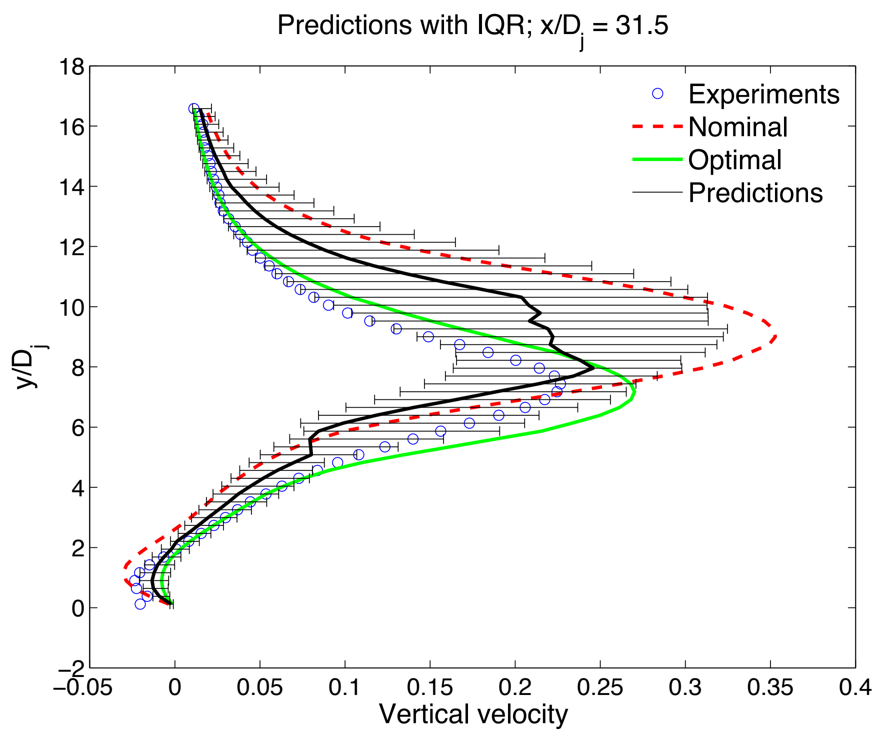
x/D = 31.6



x/D = 42.0

- Improvement over $\mathbf{C}_{\mathbf{nominal}}$, but u-deficit error is significant

Optimal ensemble member: w velocity



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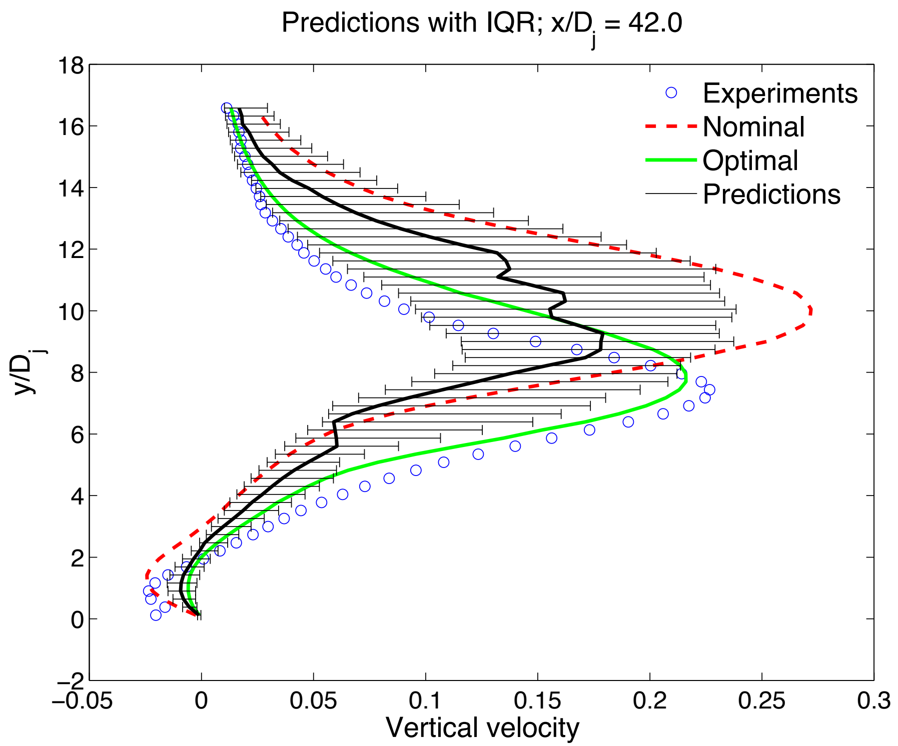

x/D = 42.0

- Improvement over $\mathbf{C}_{\mathbf{nominal}}$
- 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*