SAND2022-10081C

Sandia National Laboratories

Exceptional service in the national interest

Data-Driven Calibration of RANS Closure Models with PIV

Nathan E. Miller, Steven J. Beresh, Eric J. Parish, Jaideep Ray, and Matthew F. Barone

2022 Symposium on Turbulence Modeling

July 27-29, 2022

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

RANS Performance

Jet-in-crossflow (JIC)

- CVP, HSV, shear layer, etc.

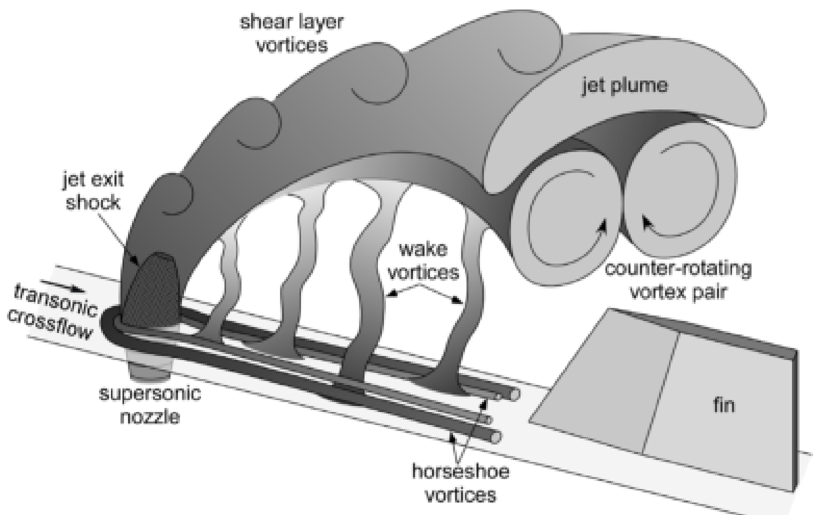
S. Arunajatesan *AIAA* (2012):

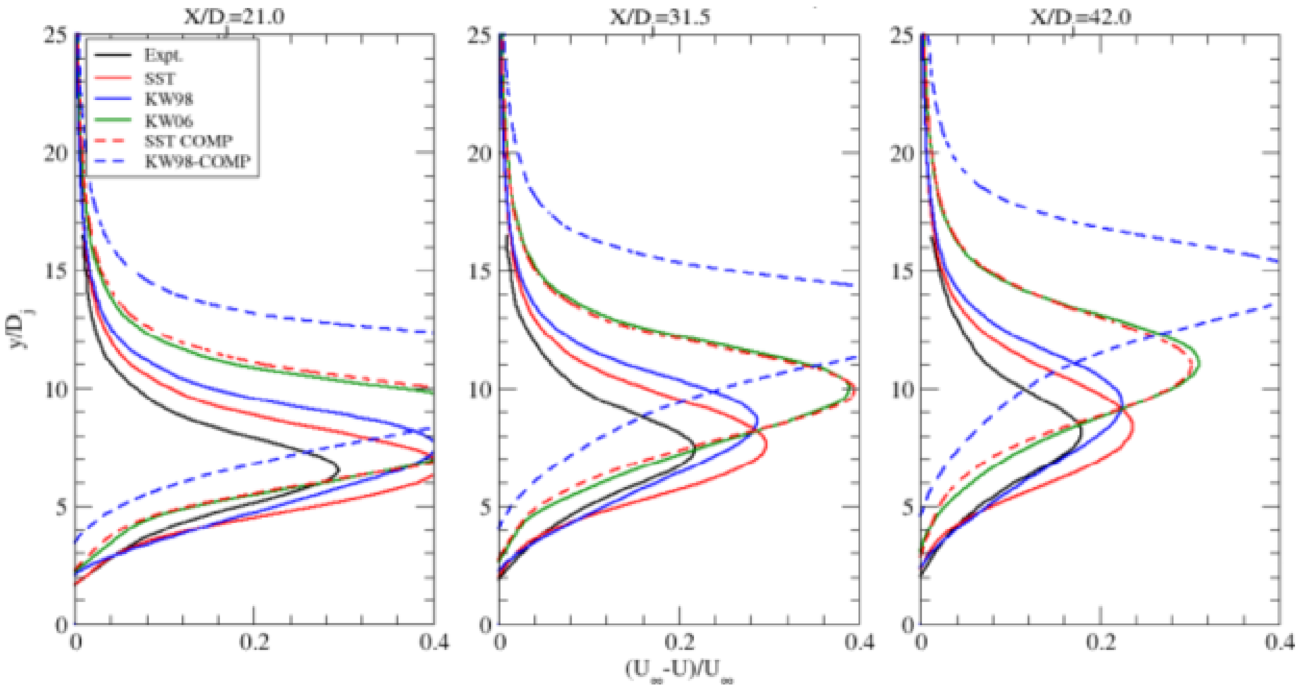
"[T]he predictive capabilities of the family of models examined here for the jet-in-crossflow problem are marginal at best."

- overpredicted velocity deficit
- overpredicted CVP strength, wrong location
- poor Reynolds stress predictions

Two causes:

1. Model-form error → Missing physics
2. Inadequate coefficient calibration



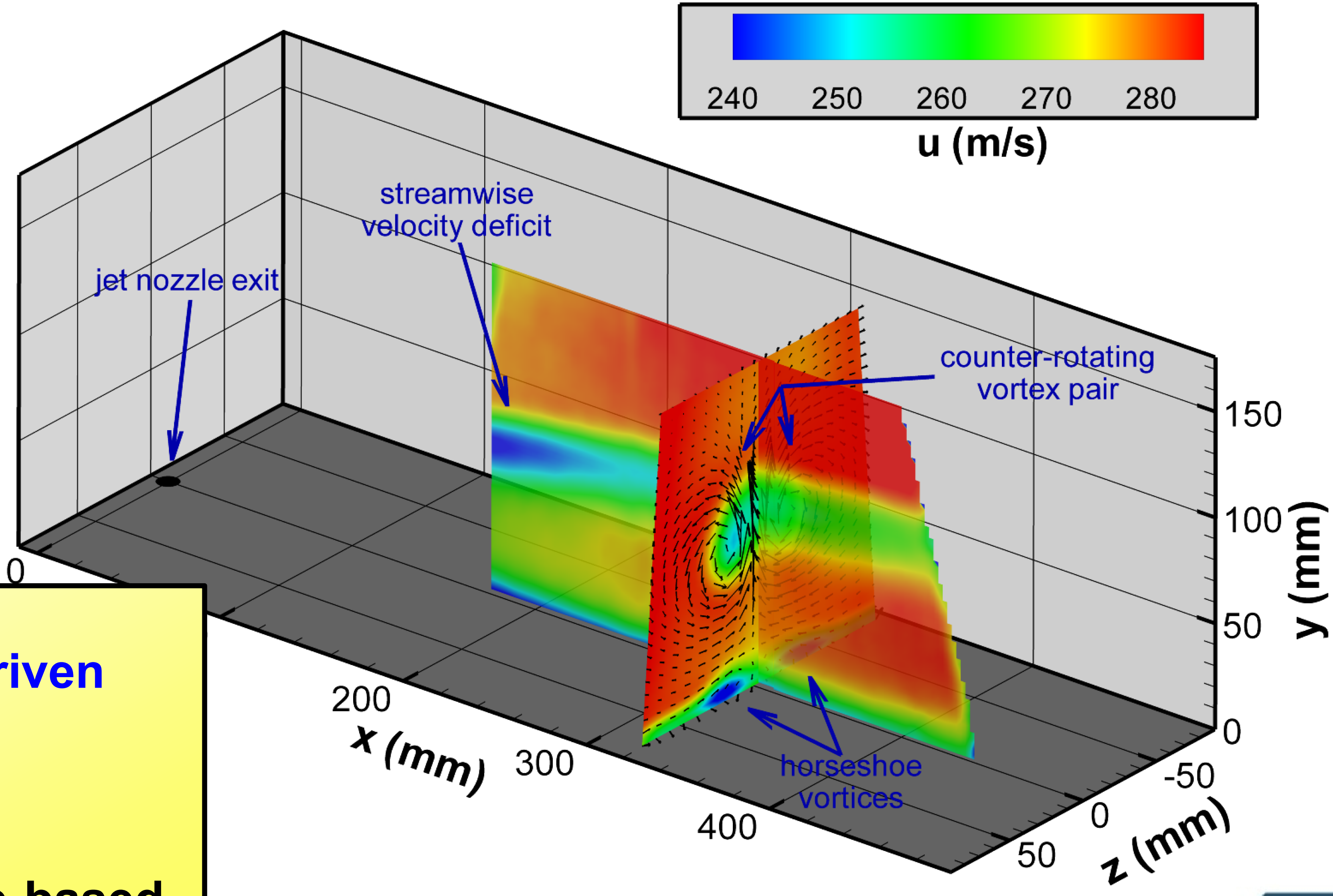


Top: Beresh *et al.* *JSR* (2018), Bottom: Arunajatesan *AIAA* (2012)

Application: Supersonic jet in transonic crossflow

PIV data from Sandia experiments circa 2005.

Beresh et al. AIAA Journal, 43:2, 2005
Beresh et al. JPP, 23:2, 2007
etc.

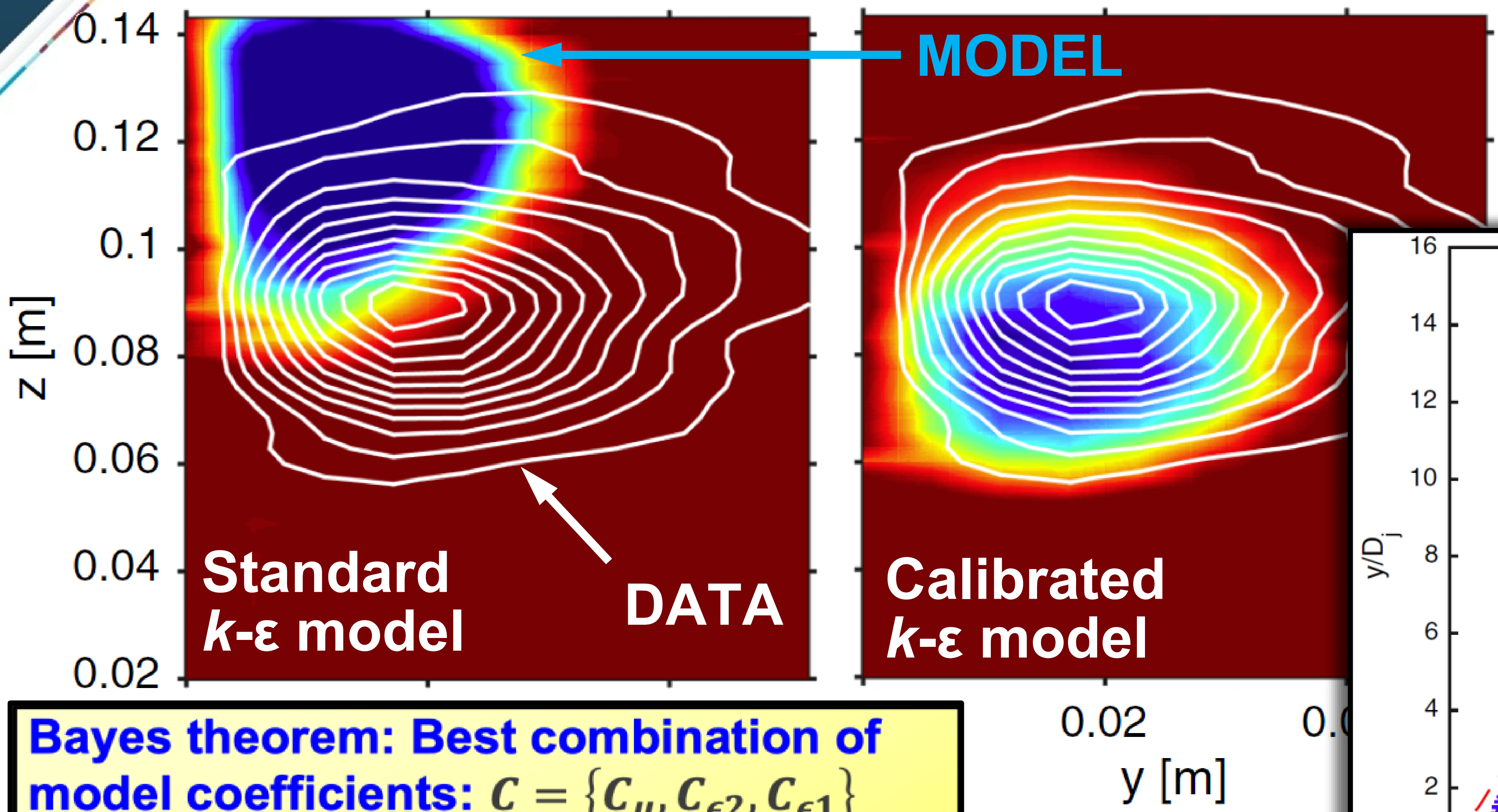


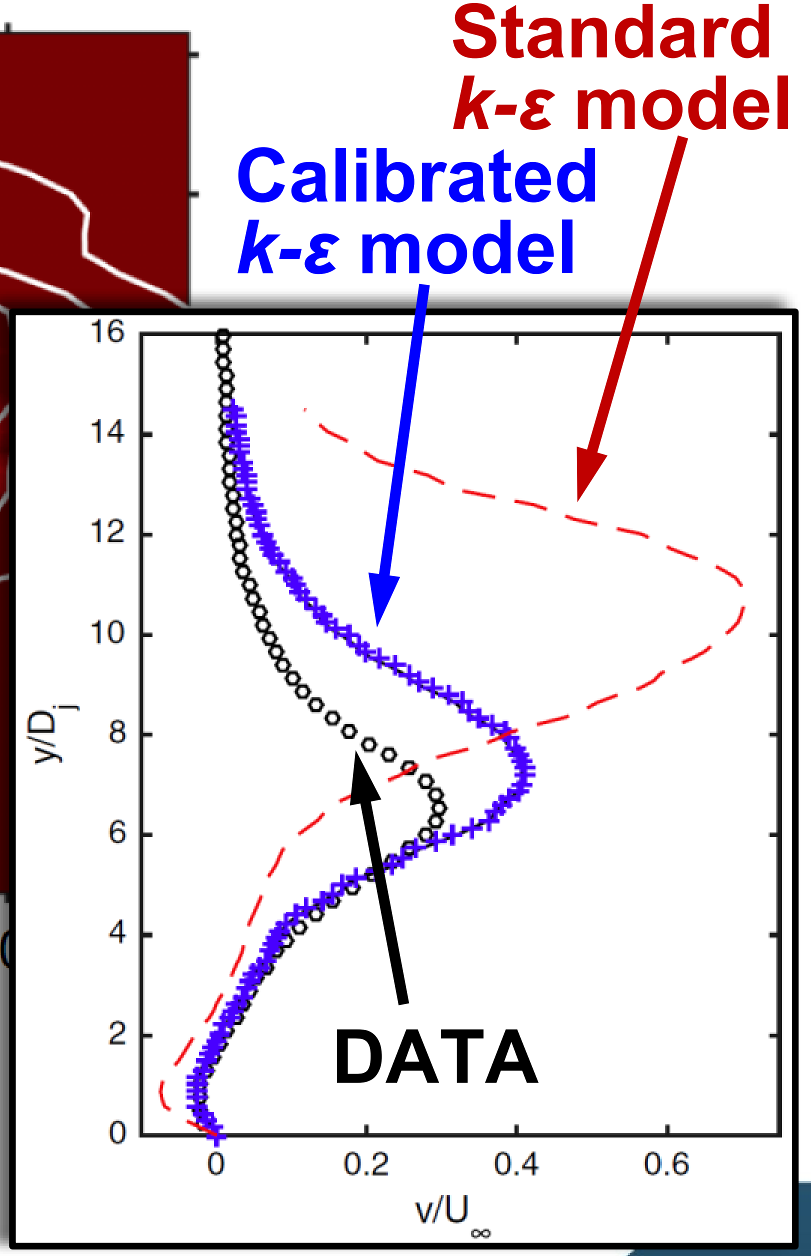
Redefine RANS model coefficients via a data-driven calibration.

Two approaches:
1. Best scalar
2. Spatially-varying state-based

Approach #1: Calibrate Model Coefficients via PIV

Calibrate RANS based on PIV data





Bayes theorem: Best combination of model coefficients: $C = \{C_\mu, C_{\epsilon 2}, C_{\epsilon 1}\}$

$$C_{nom} = \{0.09, 1.90, 1.43\}$$

$$C_{opt} = \{0.1025, 2.099, 1.416\}$$

Figures from Ray *et al*, *AIAAJ, 54:8*, 2016.
See also AIAAJ, 56:12, 2018.

The jet interaction data set

Calibrated based on only four PIV planes:

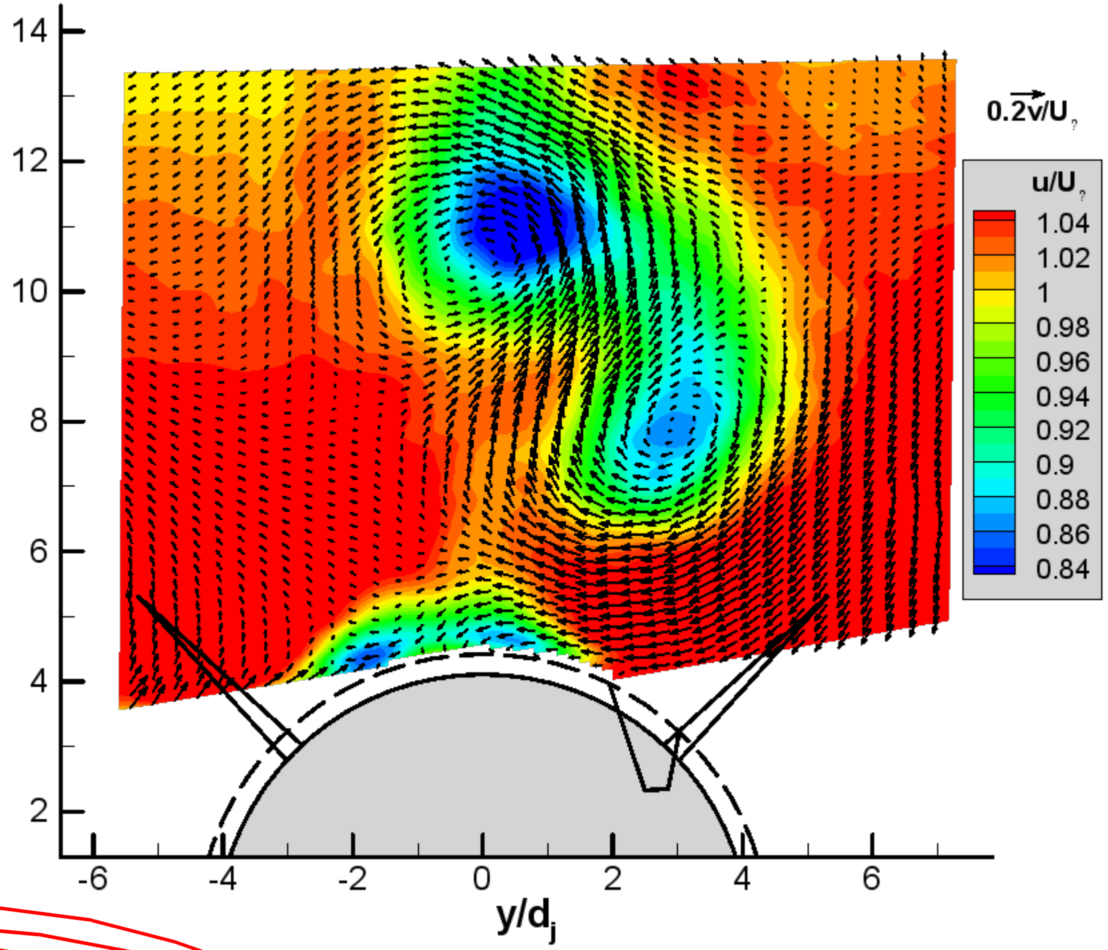
Transverse jet of varying strength.

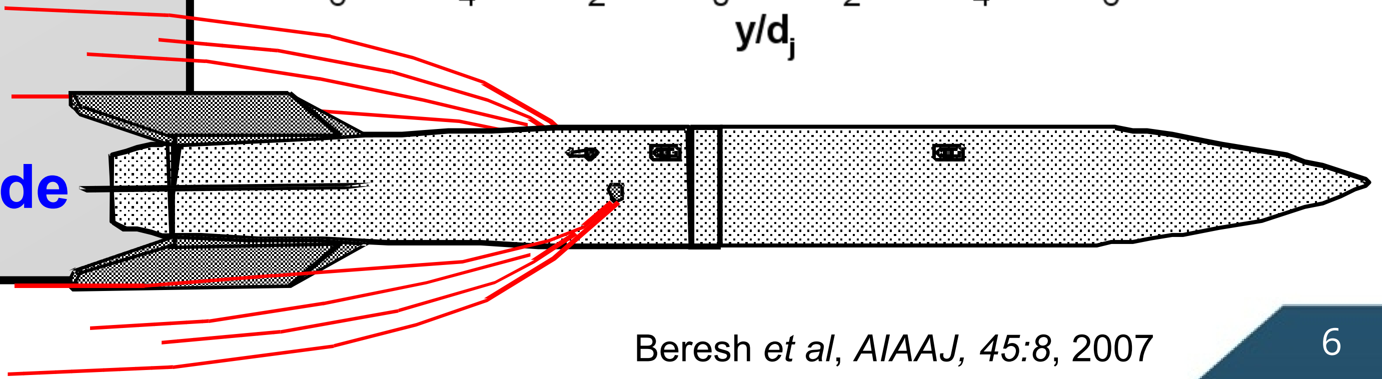
The full data set contains 48 test cases, varying:

- **Jet strength**
- **Nozzle inclination**
- **Measurement station**

Also, PIV test case on a full-scale vehicle with spin rockets.

RANS run using SIERRA Aero CFD Code



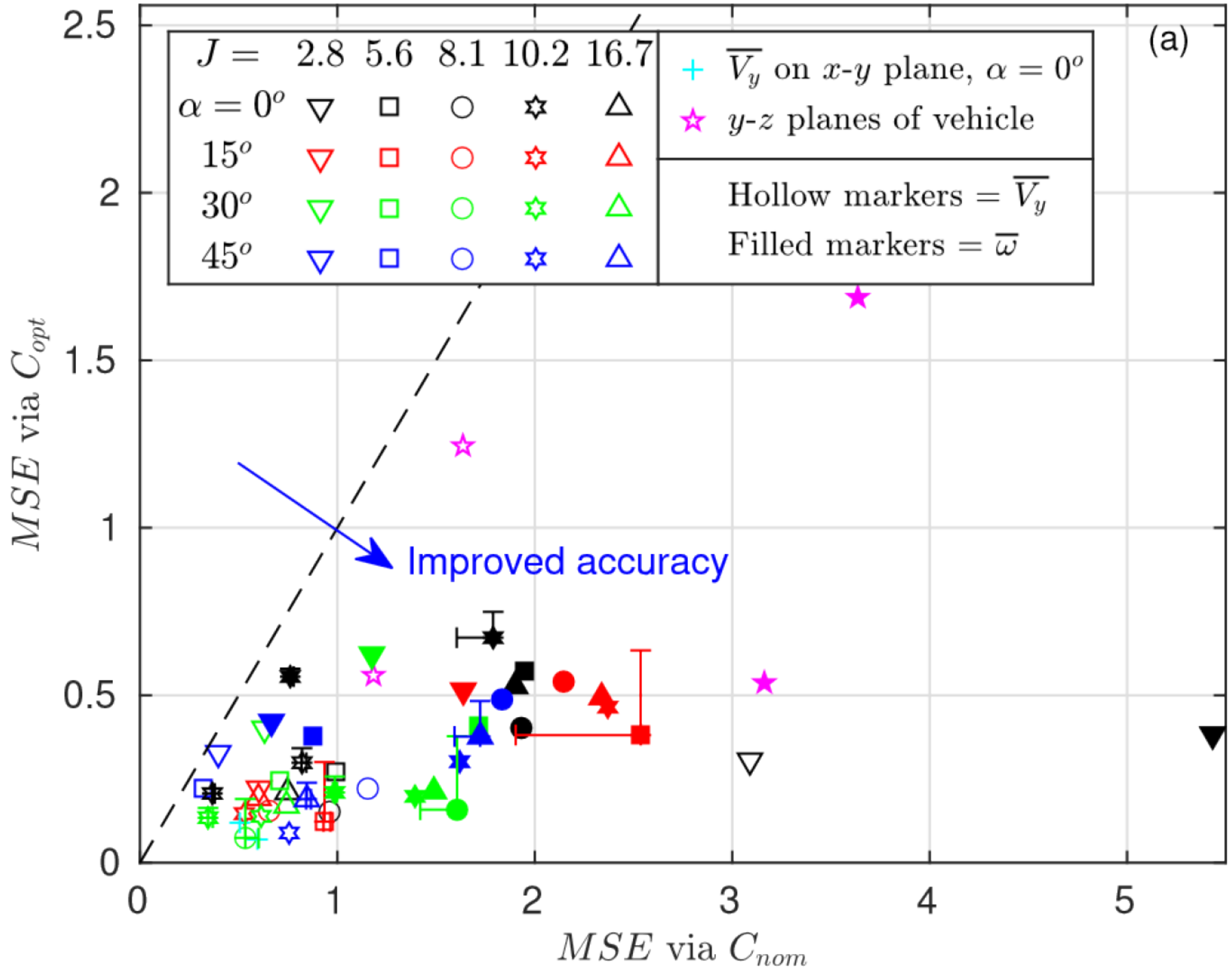


Beresh *et al*, *AIAAJ, 45:8*, 2007

Validating the calibrated C_μ model

We examined 6 quality metrics on $\overline{V}$ and $\overline{\omega}$ (Miller et al. 2022)

Here's one:



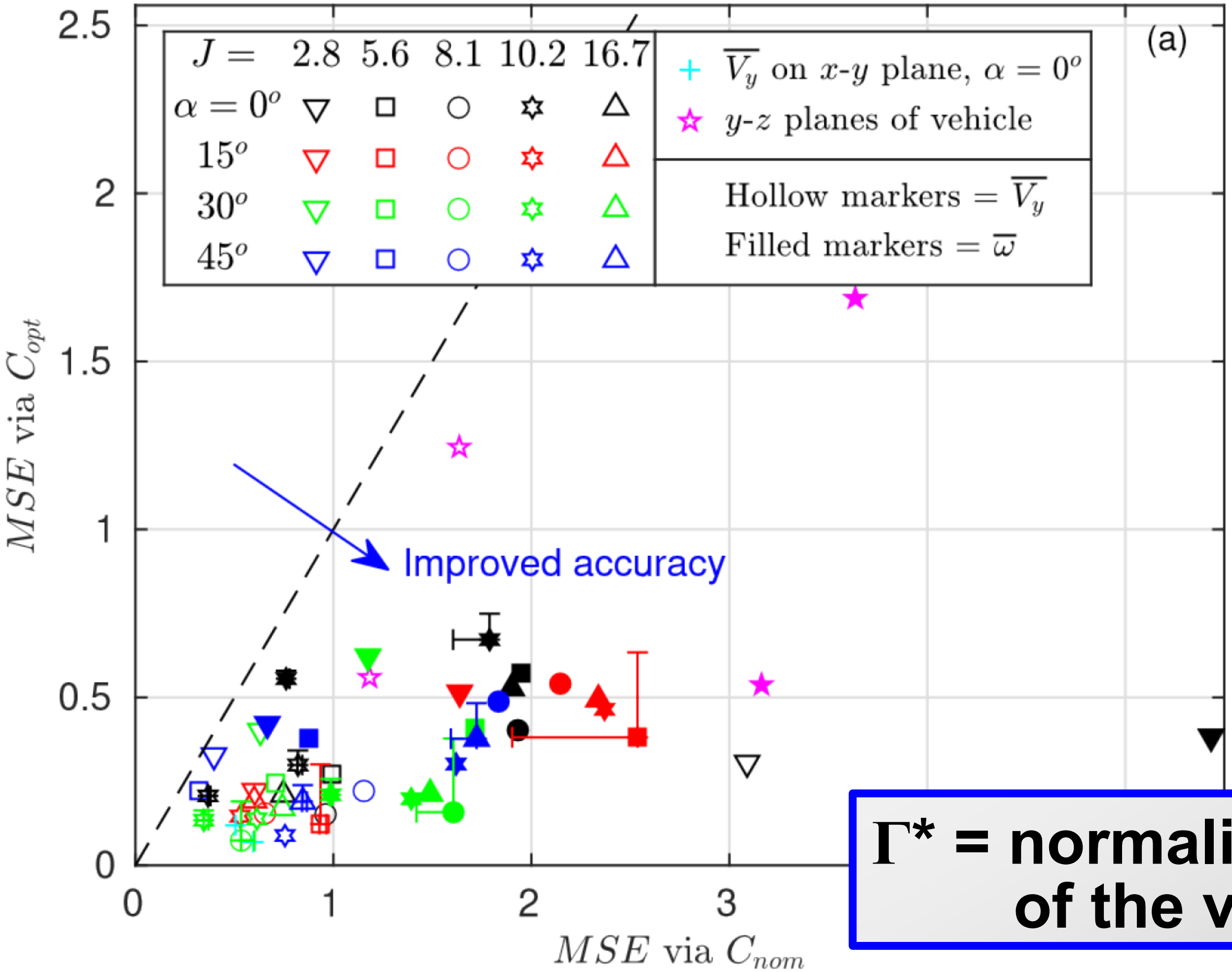
MSE = mean square error

Overall picture of the error of the CFD w.r.t. the PIV.

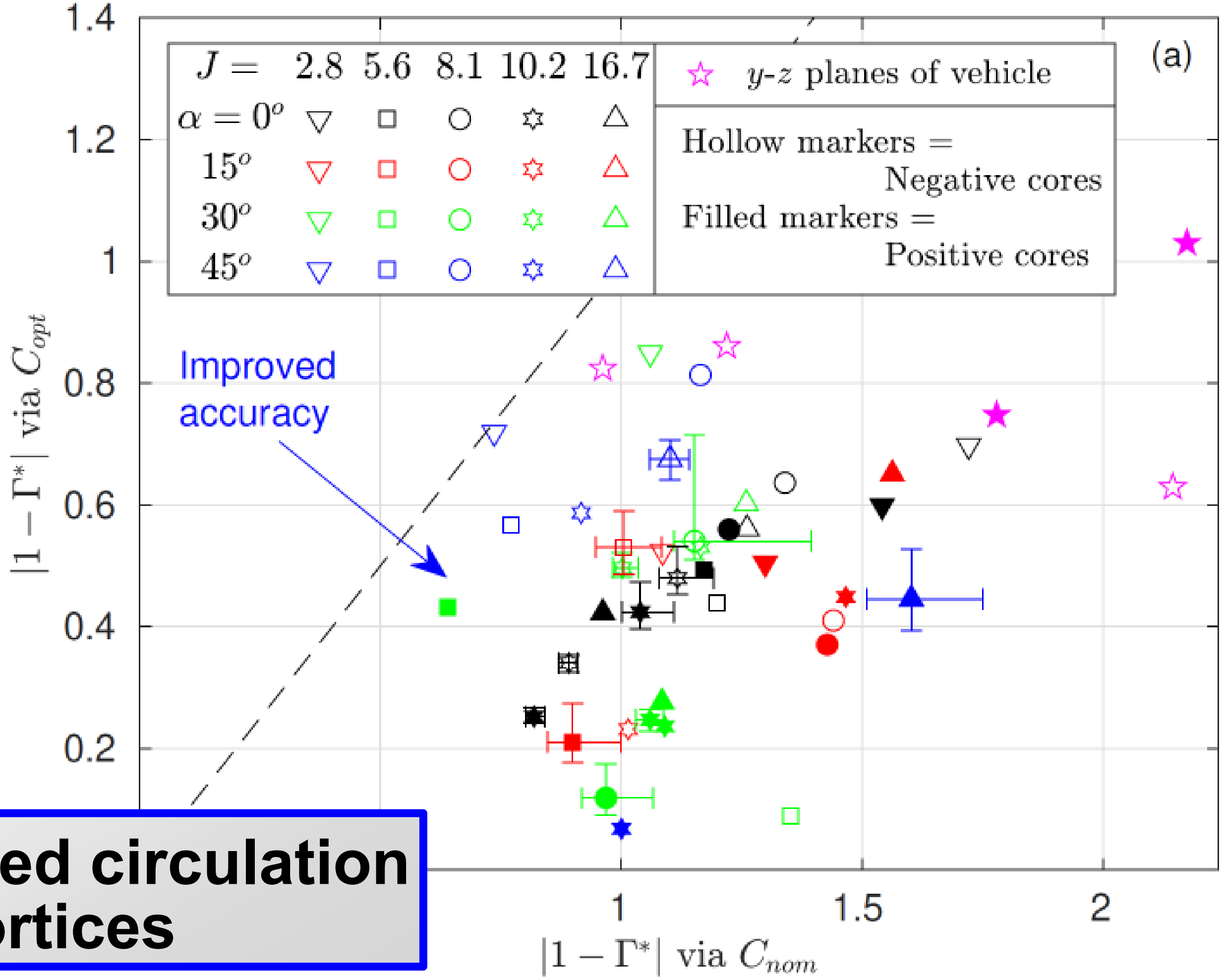
Validating the calibrated C_μ model

We examined six quality metrics (Miller et al. 2022)

Here's one:



Here's another:

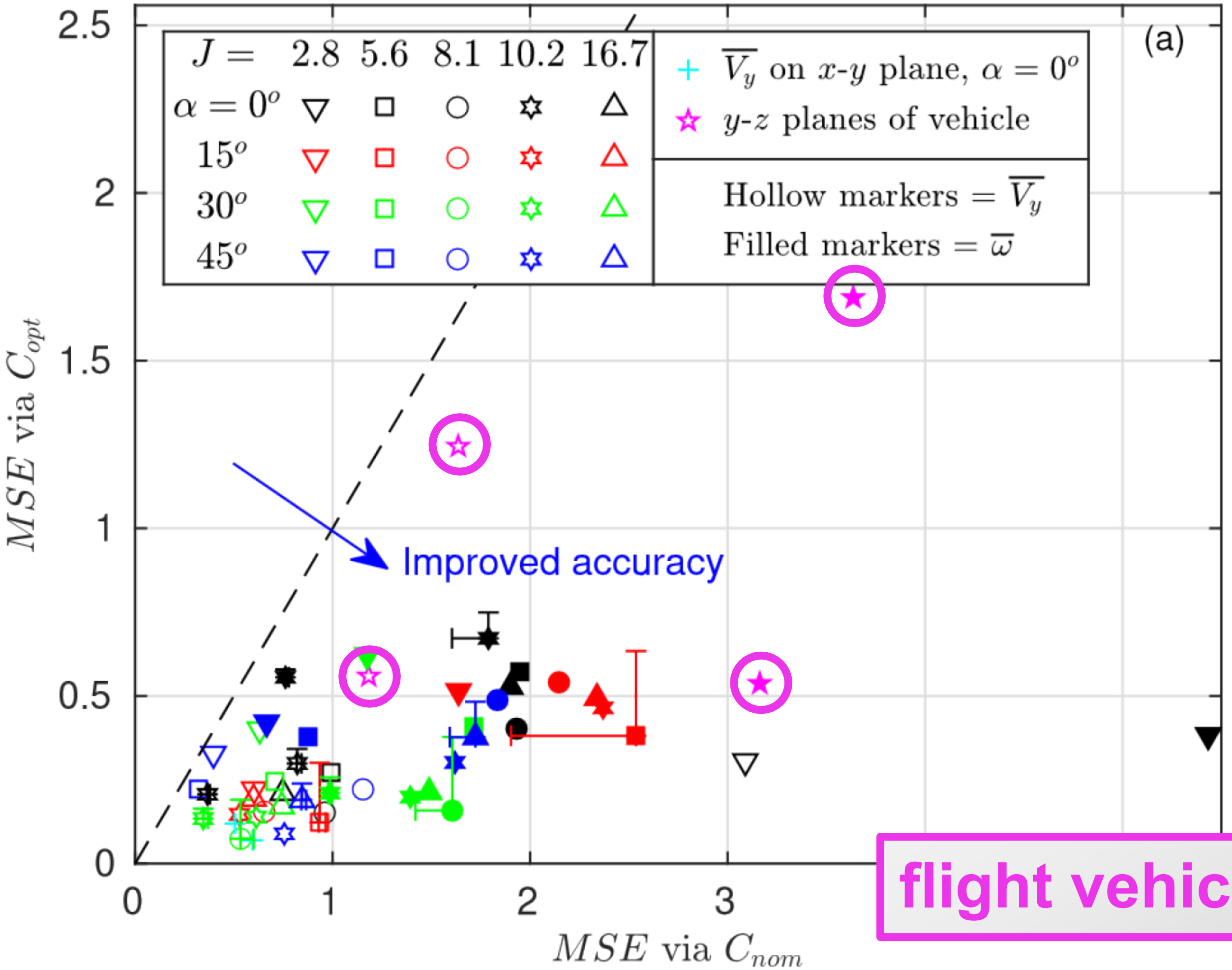


Γ^* = normalized circulation of the vortices

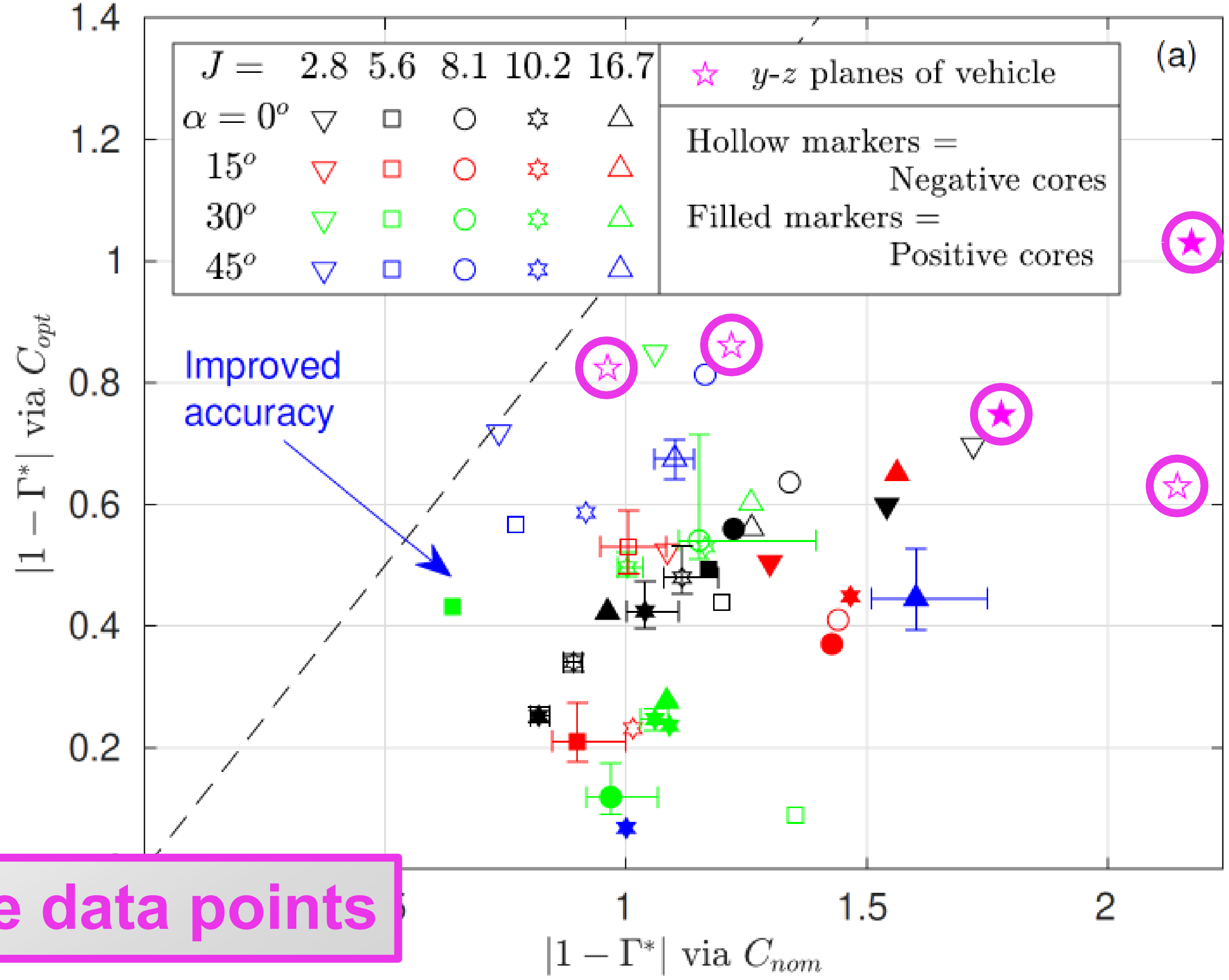
Validating the calibrated C_μ model

We examined six quality metrics (Miller et al. 2022)

Here's one:



Here's another:

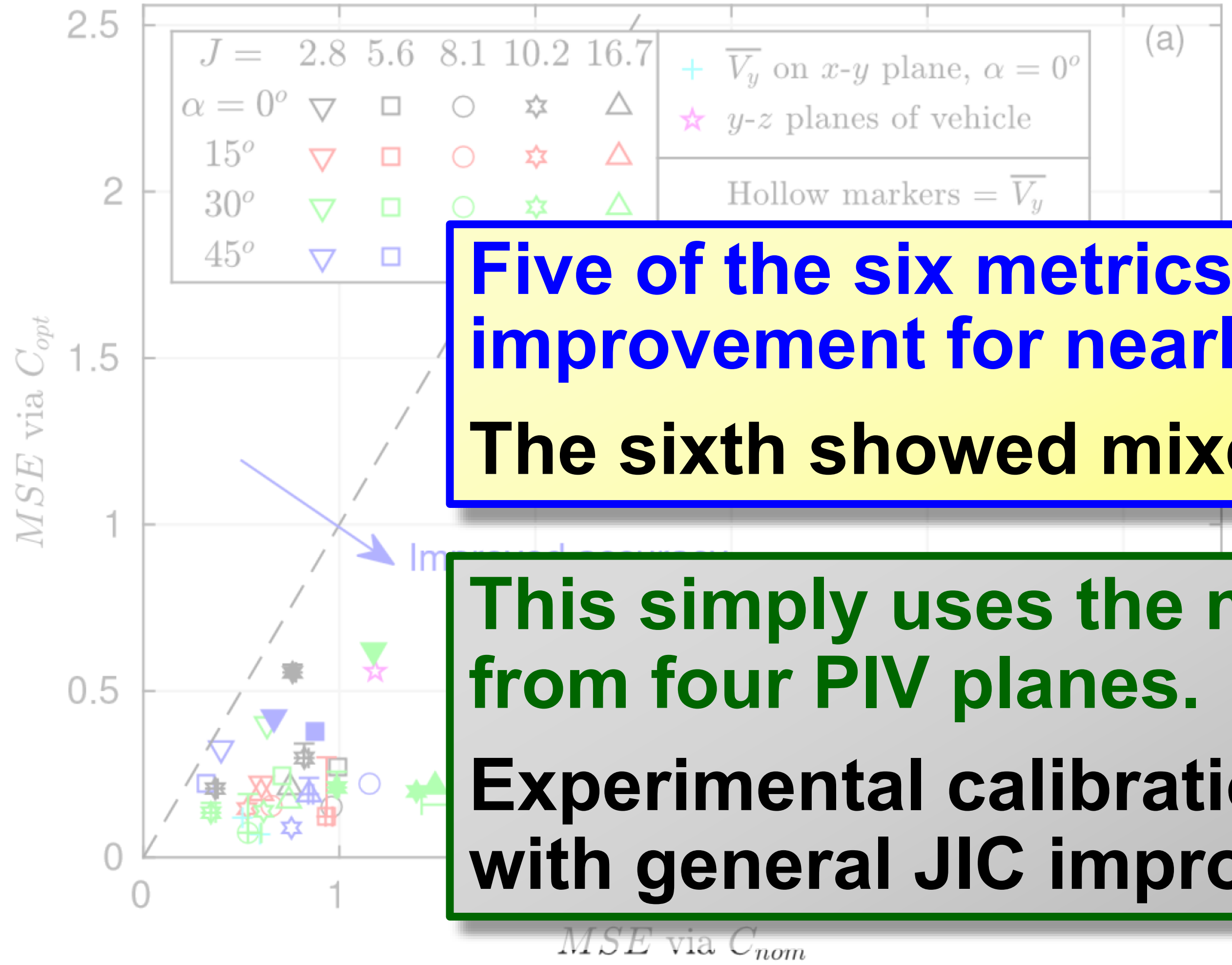


flight vehicle data points

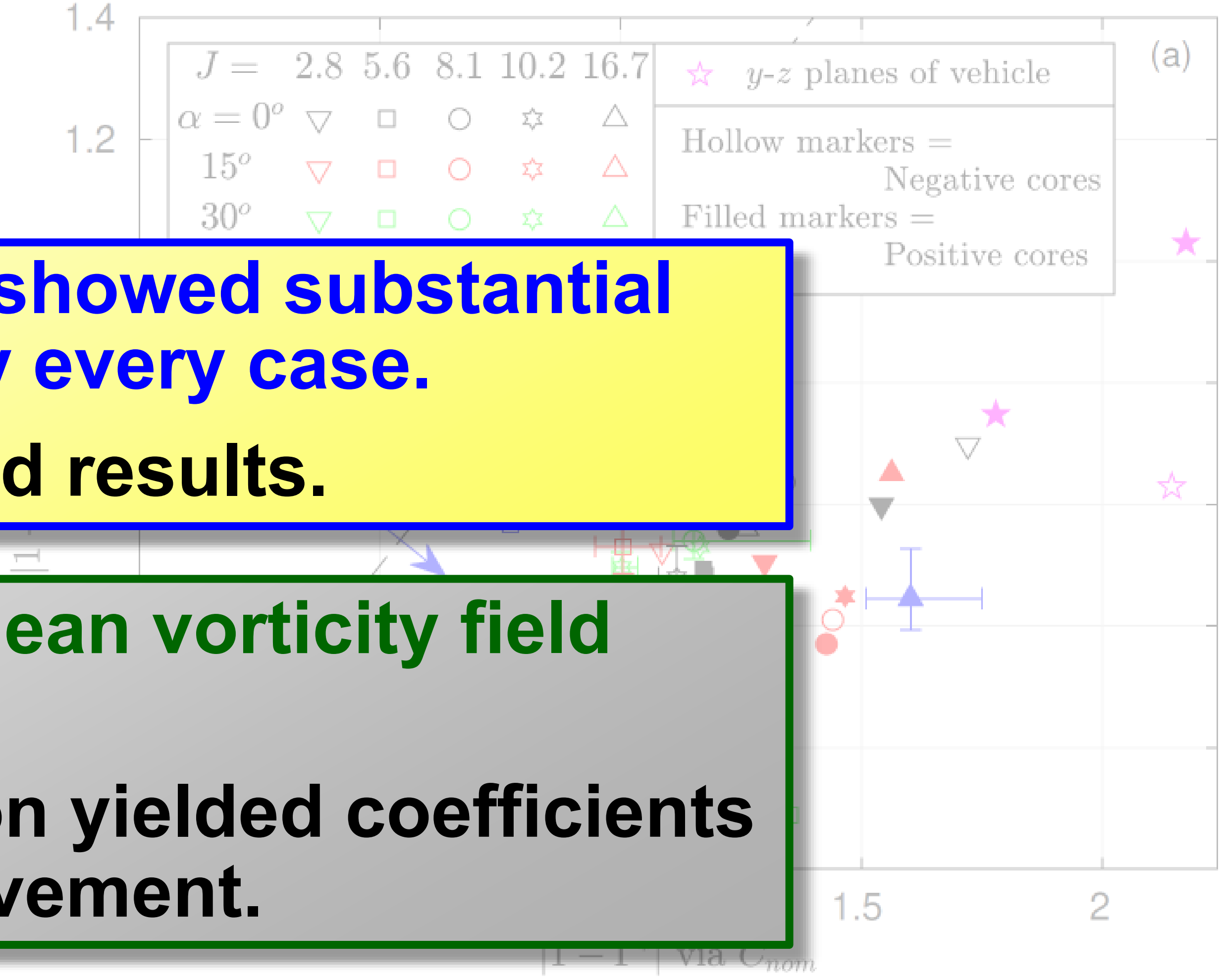
Validating the calibrated C_μ model

We examined six quality metrics (Miller et al. 2022)

Here's one:



Here's another:



Five of the six metrics showed substantial improvement for nearly every case.

The sixth showed mixed results.

This simply uses the mean vorticity field from four PIV planes.

Experimental calibration yielded coefficients with general JIC improvement.

Approach #2: Spatially-variable C_μ based on PIV

A look inside a turbulence closure model

Turbulent eddy viscosity:

Linear Boussinesq:

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

Ordinary Least Squares:

$$\nu_t = \frac{\overline{a_{ij}}\,\overline{S_{ij}}}{-2\overline{S_{kl}}\,\overline{S_{kl}}}$$

In a *k*-*ε* model:

$$\nu_t = \frac{C_\mu k^2}{\varepsilon}$$

model constant

t.k.e.

$k = \frac{1}{2}\overline{u_i'u_i'}$

dissipation rate

How realistic? Consistency issue?

<u>We can calculate all of these terms directly from PIV!</u>

A simple computation based on the above equations will not suffice.

The full story: see Miller and Beresh, *AIAA Journal*, 2021.

Move to a spatially-variable C_μ model

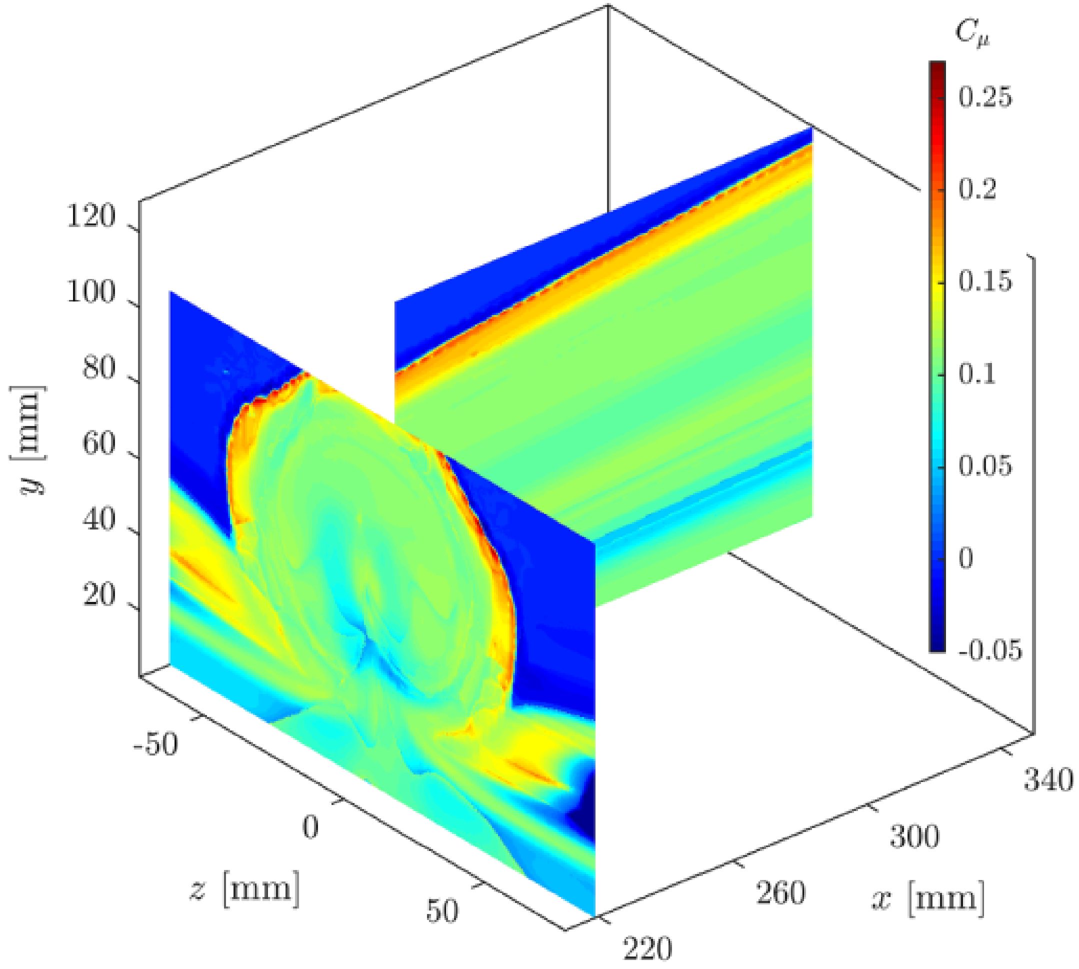
New approach:
C_μ is allowed to vary spatially **based on wind tunnel PIV data, rather than assuming a fixed constant.**

We need C_μ over the entire computational domain.

The PIV provides C_μ in only two planes.

Machine learning of C_μ from the PIV data…

$$C_\mu = f\left(\hat{S}_{ij}, \hat{\Omega}_{ij}\right)$$



Move to a spatially-variable C_μ model

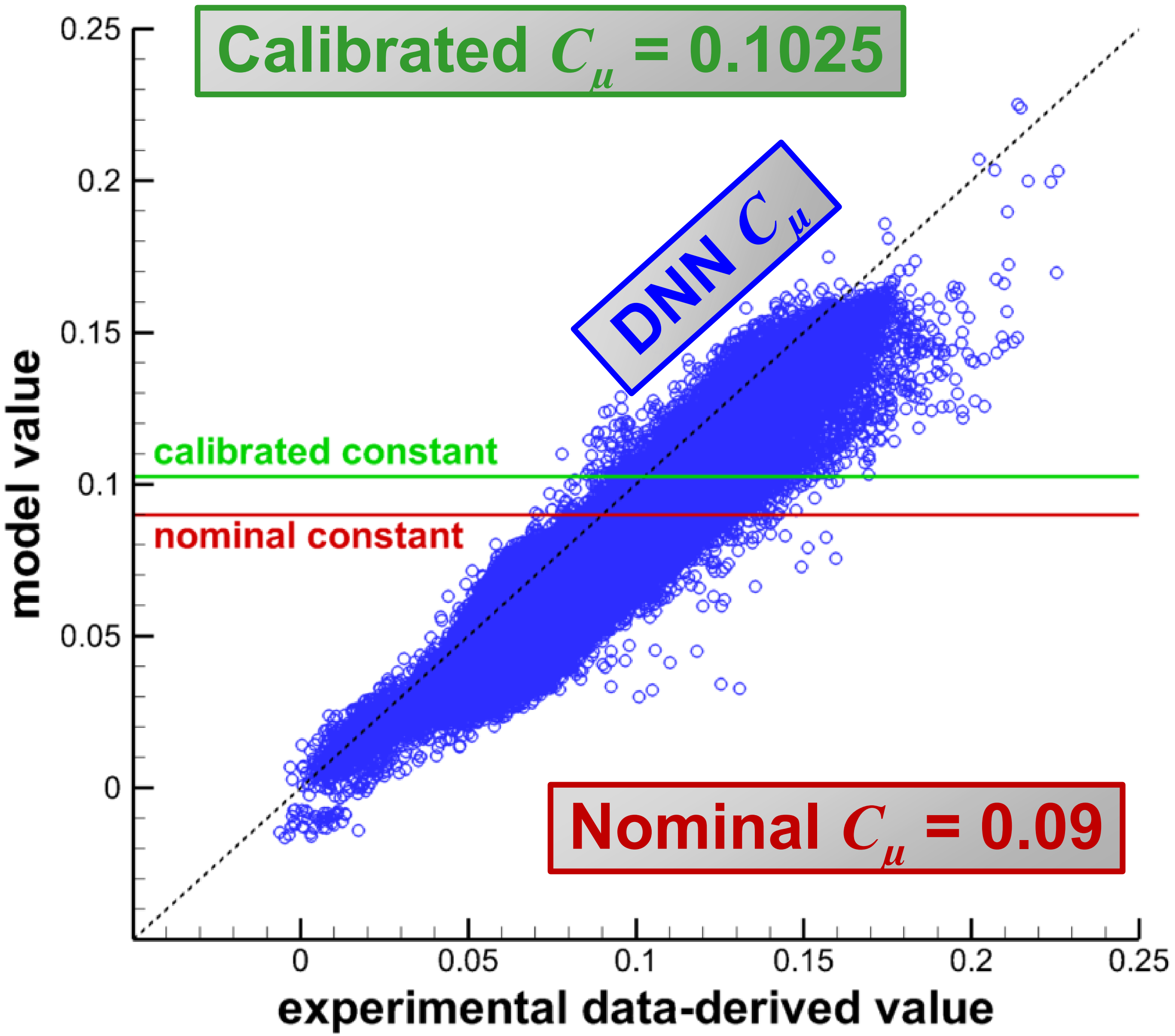
New approach:
C_μ is allowed to vary spatially
based on wind tunnel PIV data, rather than assuming a fixed constant.

- **Deep Learning of PIV-derived C_μ values**

$$C_\mu = f(\lambda_{1-5})$$

$$\lambda_1 = \{\hat{\mathbf{S}}^2\},\ \lambda_2 = \{\hat{\mathbf{\Omega}}^2\},$$
$$\lambda_3 = \{\hat{\mathbf{S}}^3\},\ \lambda_4 = \{\hat{\mathbf{S}}\,\hat{\mathbf{\Omega}}^2\},\ \lambda_5 = \{\hat{\mathbf{S}}^2\hat{\mathbf{\Omega}}^2\}$$

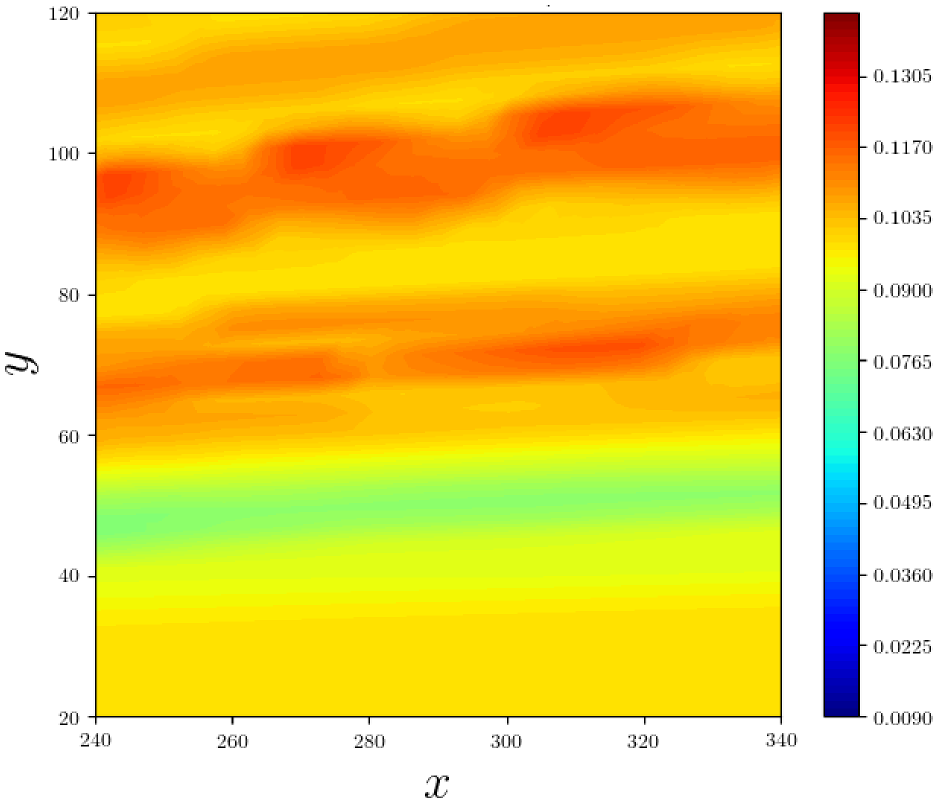
- Deep Neural Network (DNN)
  - Multiple (3) hidden layers
    - 18, 9, 3 nodes per layer
  - ReLU activation function
  - Ensembles of networks

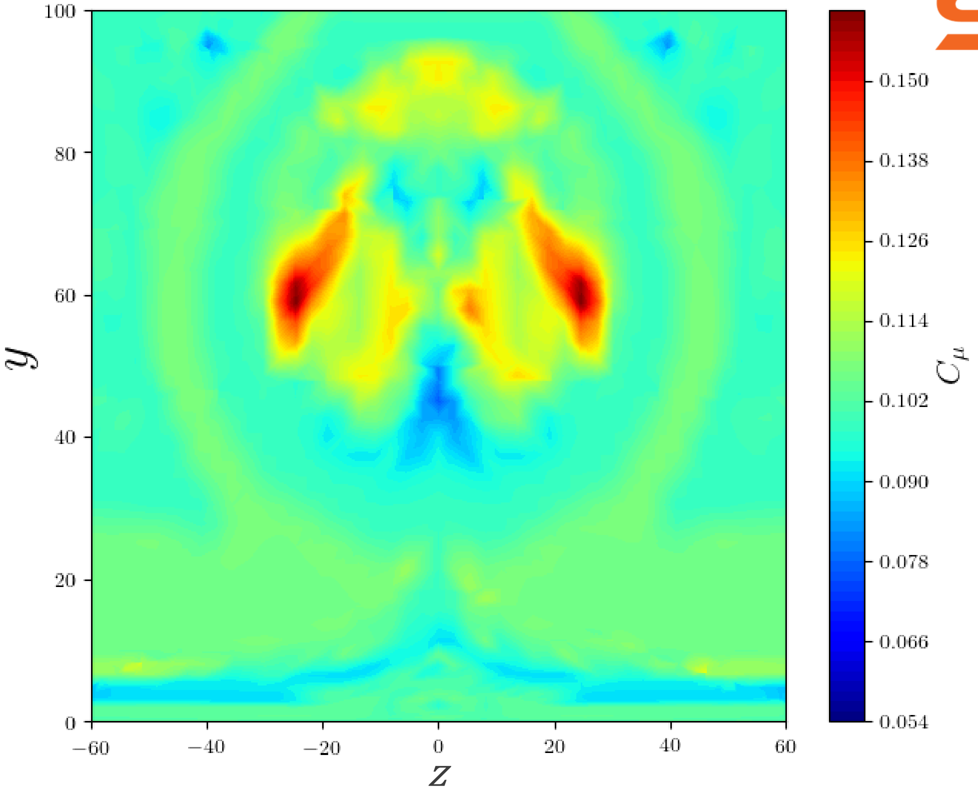


Implementation

Sandia Parallel Aero Reentry Code (SPARC)

- **Nominal, Calibrated, & Variable C_μ models**
  - Variable C_μ model queries ensemble of networks trained on 2 planes of PIV data



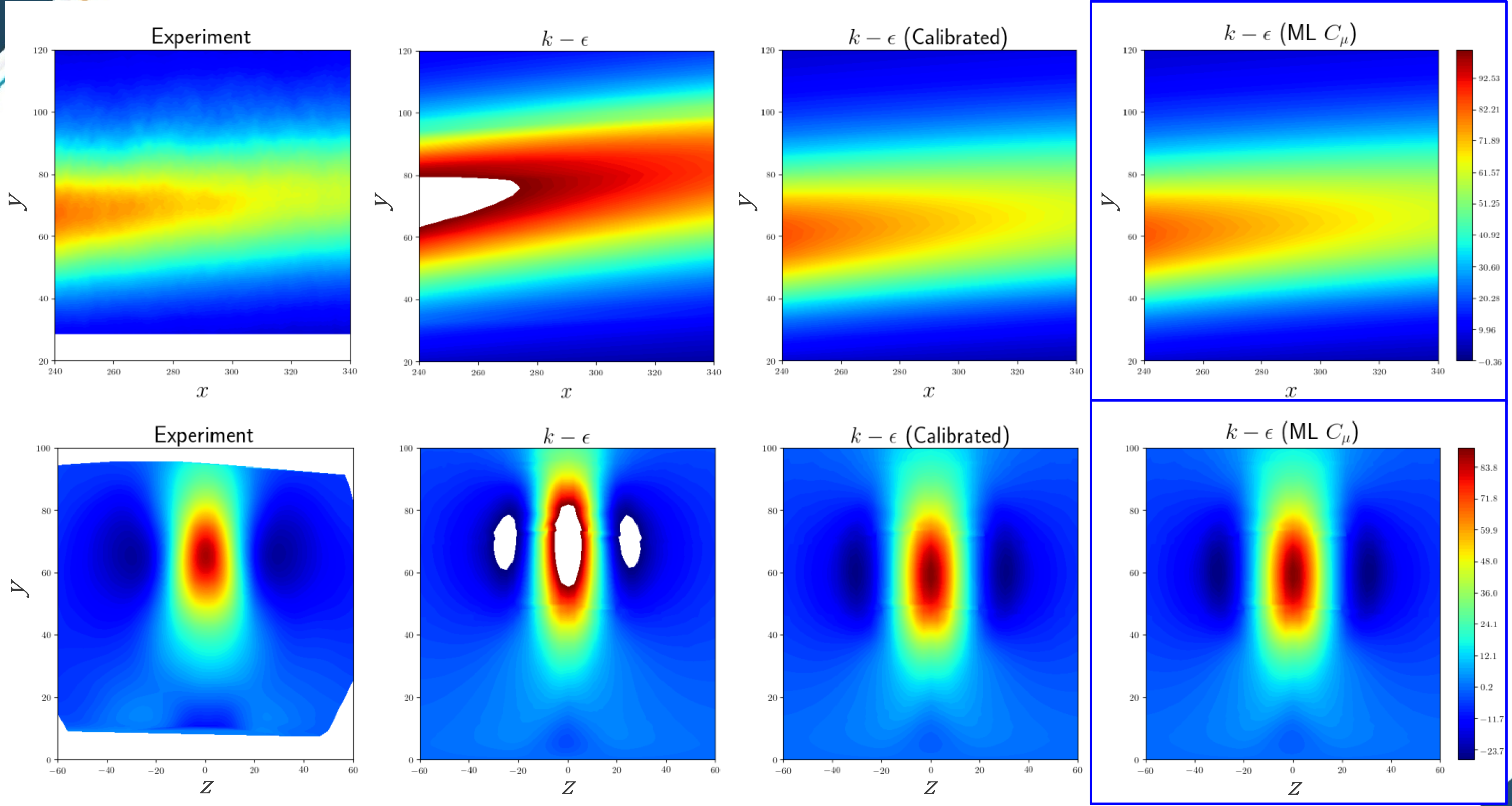


SPARC

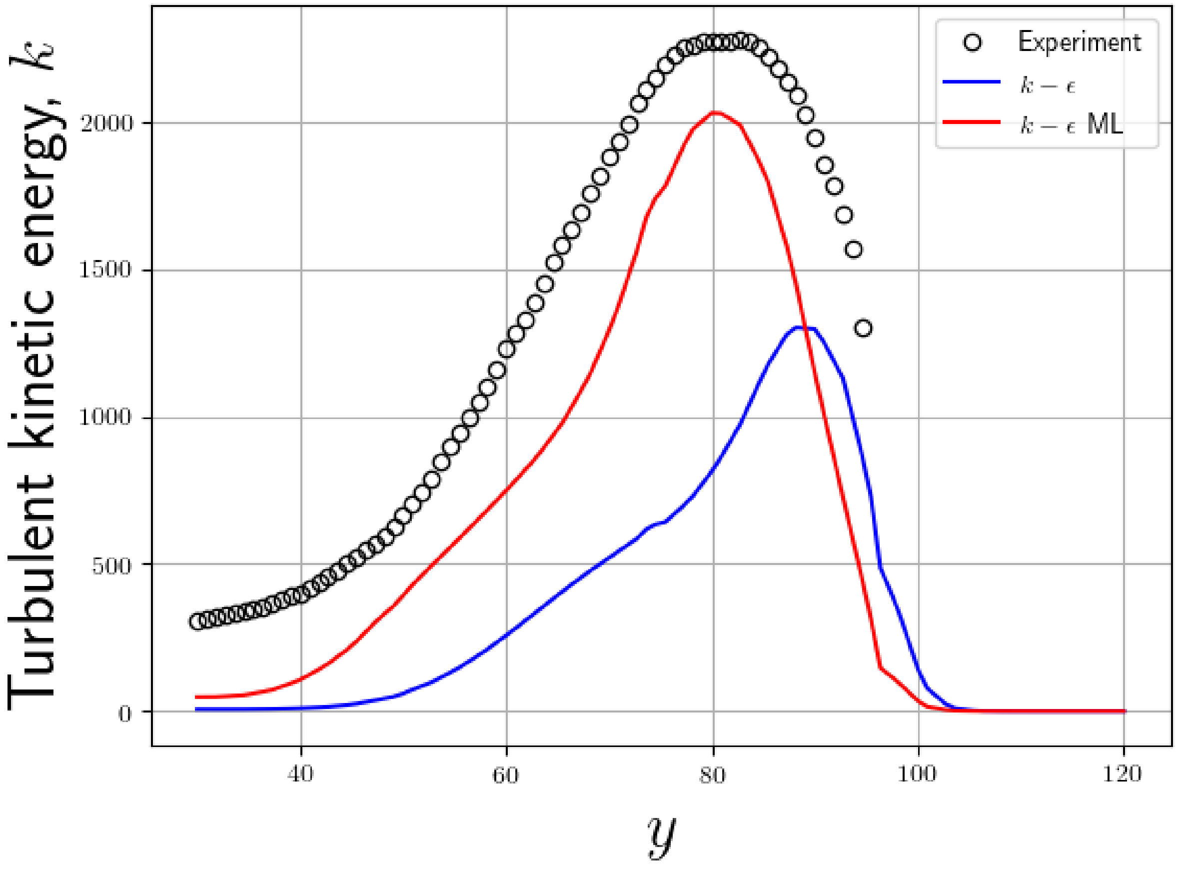
Variable C_μ across the JIC domain

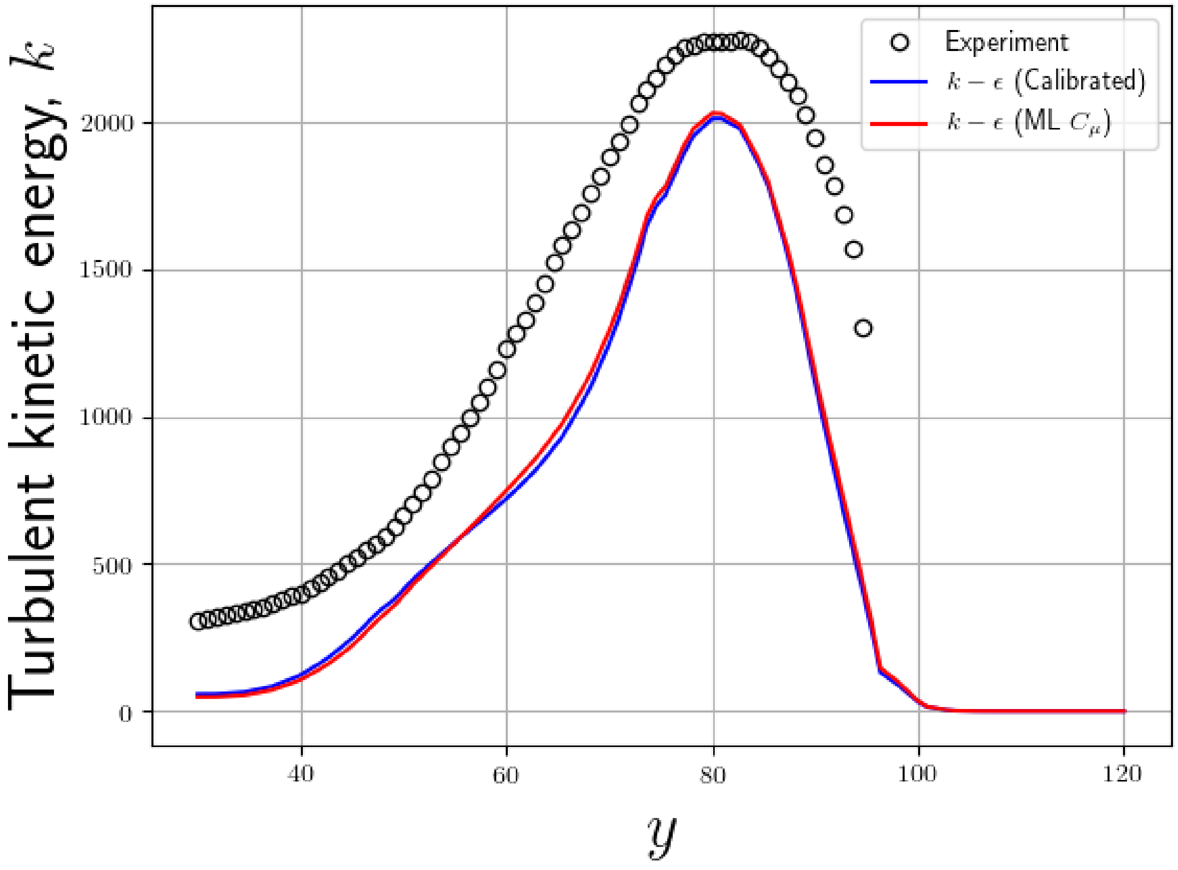
Defaults back to C_μ = 0.1025

How well does this work?



How well does this work?





Significant improvement over nominal

But we already knew that….

Slight improvement over Calibrated?

What's going on?

Default C_μ to 0.1025
Avoid extrapolation or variance

Result: Default C_μ dominates the result

What is C_μ in unmeasured regions?

- **The PIV data miss important physics near the wall and the jet nozzle**

Another issue is *data consistency*

- **C_μ model trained using measured *k* and *ε*, but RANS *k* and *ε* values may be in error**

Conclusions & what's next?

Data-driven CFD trained with PIV-measured physics rather than trained with LES/DNS

Model as implemented may be an improvement over best Calibrated model

Default Calibrated value dominates:
More data needed?

Formalized validation with same 6 metrics ongoing:
Stay tuned

Improve PIV data consistency
Use same data in TBNN: Eric Parish

Citations

- Arunajatesan, S., “Evaluation of Two-Equation RANS Models for Simulation of Jet-in-Crossflow Problems,” AIAA Paper 2012-1199, January 2012

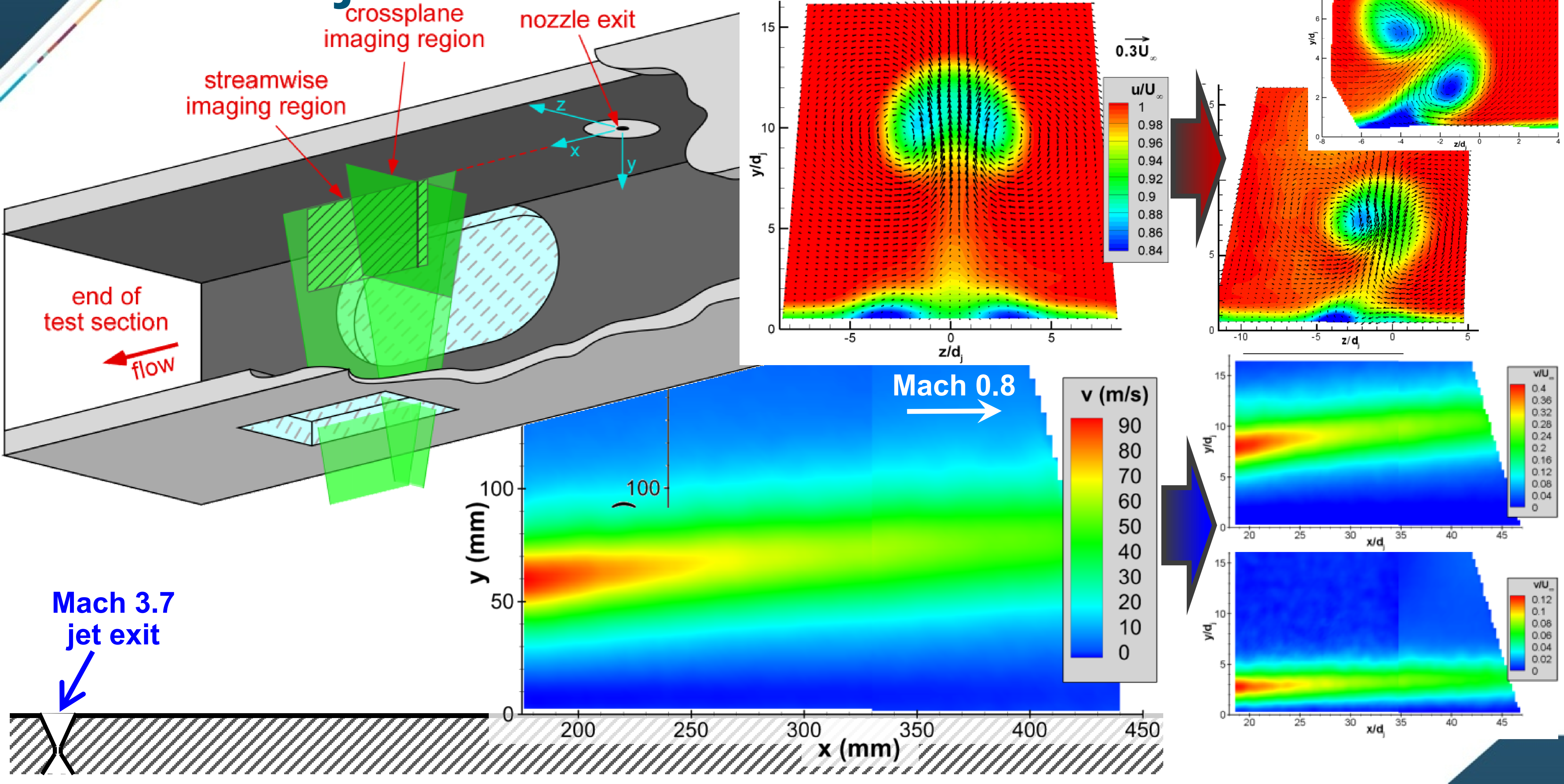
- Beresh, S. J., Henfling, J. F., Erven, R. J., & Spillers, R. W., “Penetration of a Transverse Supersonic Jet into a Subsonic Compressible Crossflow,” AIAA Journal, Vol. 43, No. 2, 2005, pp. 379–389
- Beresh, S. J., Henfling, J. F., Erven, R. J., & Spillers, R. W., “Vortex Structure Produced by a Laterally Inclined Supersonic Jet in Transonic Crossflow,” J. of Prop. and Power, Vol. 23, No. 2, 2007, pp. 353–363
- Beresh, S. J., Heineck, J. T., Walker, S. M., Schairer, E. T., & Yaste, D. M., “Planar Velocimetry of Jet/Fin Interaction on a Full-Scale Flight Vehicle Configuration,” AIAA Journal, Vol. 45, No. 8, 2007, pp. 1827–1840

- Ray, J., Lafantzi, S., Arunajatesan, S., & Dechant, L., “Bayesian Parameter Estimation of a k-ε Model for Accurate Jet-in-Crossflow Simulations,” AIAA Journal, Vol. 54, No. 8, 2016, pp. 2432–2448.
- Ray, J., Dechant, L., Lefantzi, S., Ling, J., & Arunajatesan, S., “Robust Bayesian Calibration of a k-ε Model for Compressible Jet-in-Crossflow Simulations,” AIAA Journal, Vol. 56, No. 12, 2018, pp. 4893–4909.

- Miller, N. E., & Beresh, S. J., “Using Particle Image Velocimetry to Determine Turbulence Model Parameters,” AIAA Journal, Vol. 59, No. 3, 2021, pp. 842–854
- Miller, N. E., Beresh, S. J., & Ray, J., “Validation of calibrated k-ϵ model parameters for jet-in-crossflow,” AIAA Journal, https://doi.org/10.2514/1.J061396

Backup Slides

The jet interaction data set



Metrics

- Quality metrics, predicted (X_{RANS}) vs true (X_{PIV}):

- Mean Squared Error (normalized): 0.0 = perfect
  - Measures peak accuracy

$$MSE = \frac{\langle (X_{PIV} - X_{RANS})^2 \rangle}{\langle X_{PIV}{}^2 \rangle}$$

- Geometric Mean Error (normalized): 0.0 = perfect
  - Measures bulk accuracy

$$GME = \frac{\exp[\langle \ln(|X_{PIV} - X_{RANS}|) \rangle)}{\exp[\langle \ln(|X_{PIV}|) \rangle)}$$

- 2-D Correlation Coefficient: 1.0 = perfect
  - Measures spatial alignment

$$corr = \frac{\sum_i \sum_j (X_{PIV} - \langle X_{PIV} \rangle)\,(X_{RANS} - \langle X_{RANS} \rangle)}{\sqrt{\sum_i \sum_j (X_{PIV} - \langle X_{PIV} \rangle)^2 \sum_i \sum_j (X_{RANS} - \langle X_{RANS} \rangle)^2}}$$

- Vortex Perimeters (normalized): 1.0 = perfect
  - Measures vortex size

$$P^* = \frac{P_{RANS}}{P_{PIV}}$$

- Vortex Circulation (normalized): 1.0 = perfect
  - Measures vortex strength

$$\Gamma^* = \frac{\Gamma_{RANS}}{\Gamma_{PIV}}, \qquad \Gamma = \int \varpi \, dA$$

- Vortex center difference: 0.0 = perfect
  - Measures vortex alignment

$$E^* = \frac{\sqrt{(\overline{y_{PIV}} + \overline{y_{RANS}})^2 + (\overline{z_{PIV}} + \overline{z_{RANS}})^2}}{P_{PIV}}, \quad [\bar{y}, \bar{z}] = \int [y, z]\, \varpi \, dA$$