



Lessons from Data-driven Reynolds Stress and Turbulent Scalar Flux Closures

Roles of anisotropy, auxiliary equations, and
model extrapolation

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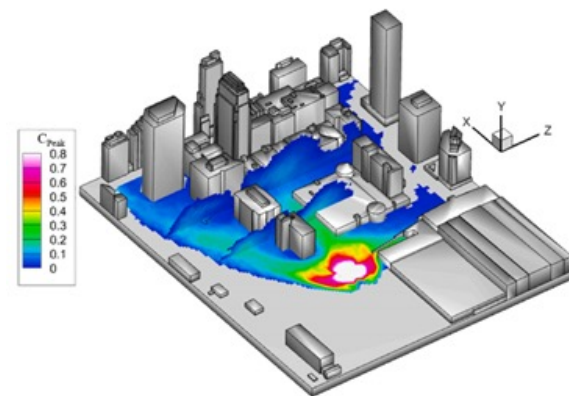
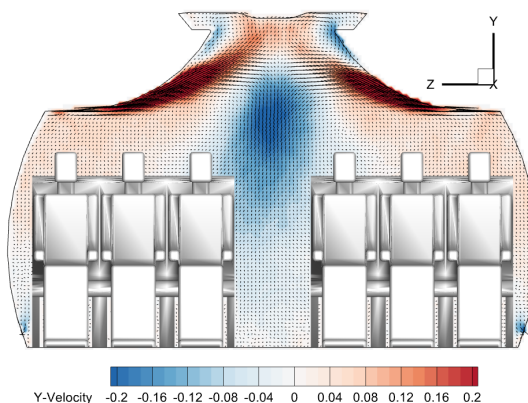
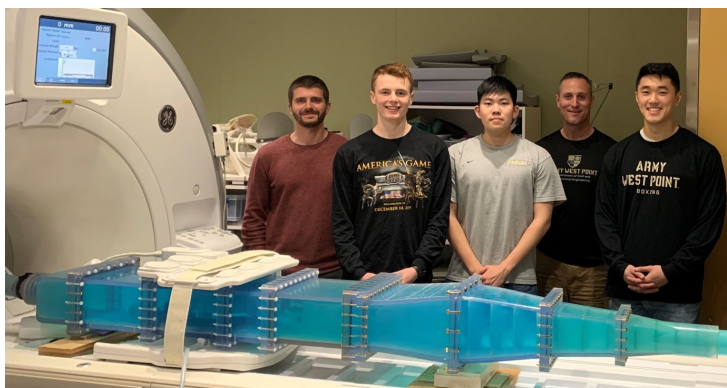
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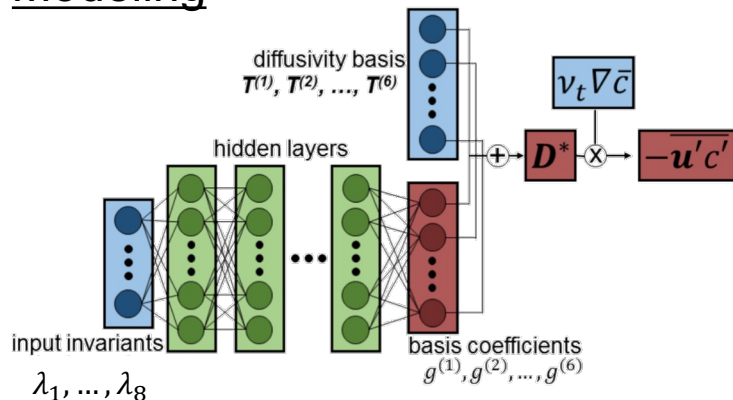


Understanding heat and mass transfer in complex, 3D flows ...

Experiments 3D mean flow measurements using magnetic resonance imaging

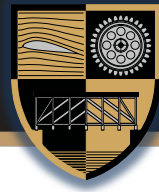


Modeling

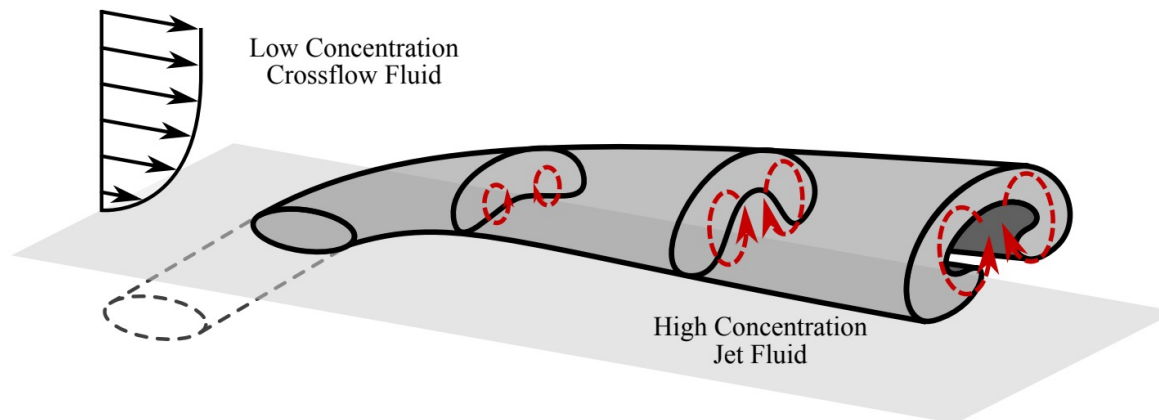
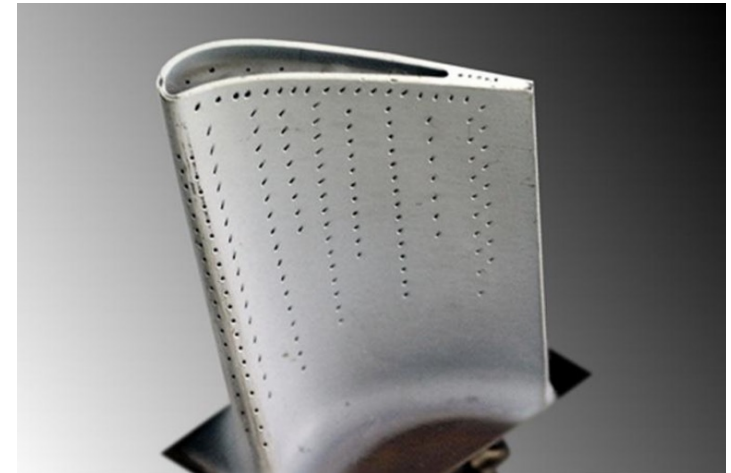
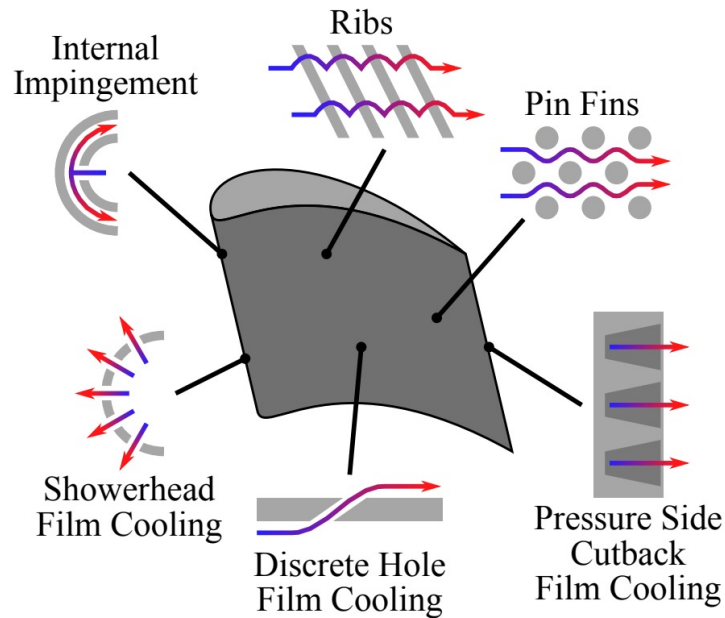


Key Questions

- Relative importance of anisotropy and auxiliary equations
- Performance bounds of model forms
- Data requirements and dealing with extrapolation

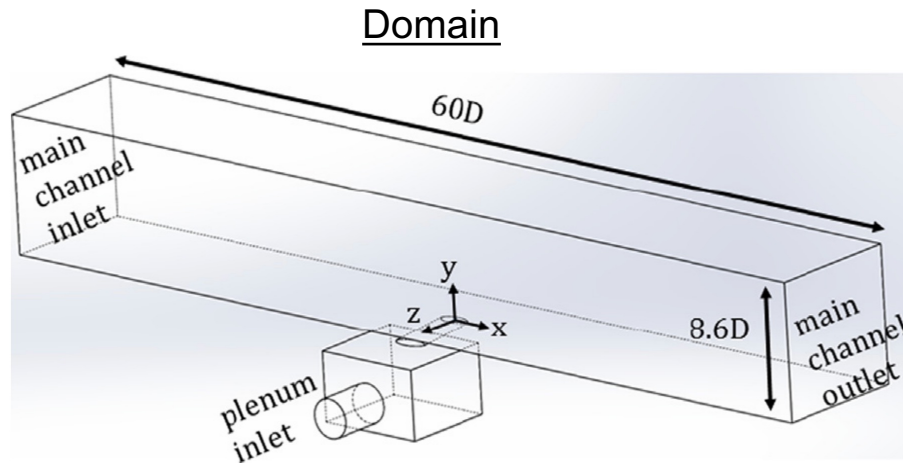


Blade surfaces are actively cooled using arrays of round and shaped holes





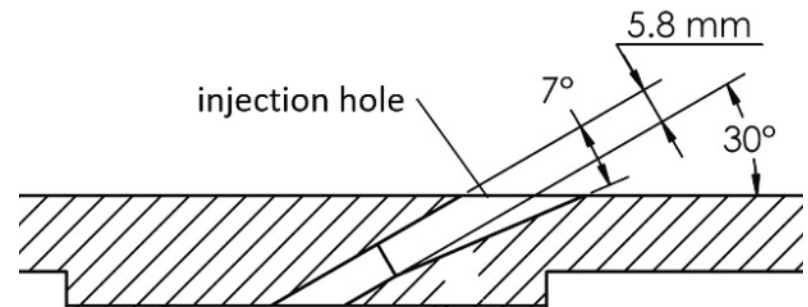
- Family of jet in crossflows



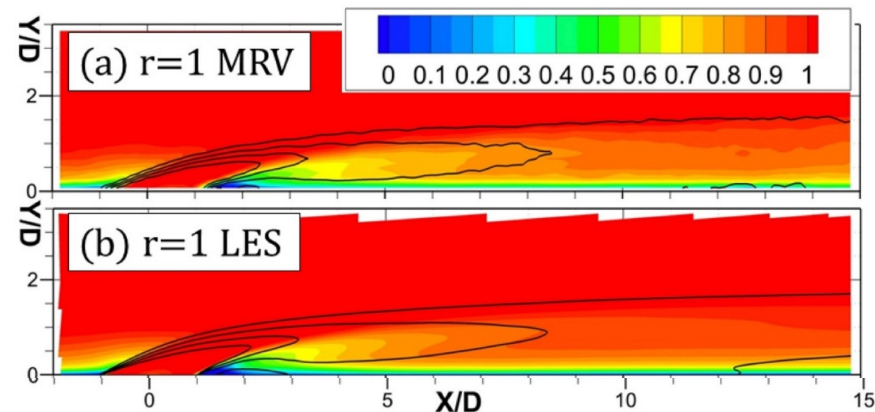
- Conditions

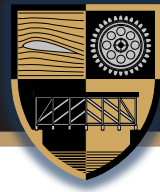
- Grid: 40M cells, wall-resolved on bottom/hole
- SGS Model: Vreman, $\nu_{SGS}/\nu < 1$
- Main flow: $Re_H = 25,000$
 $Re_\theta = 2,500$
 $\delta_{99}/D = 1.5$
- Jet: BR = 1 (based on metering hole)
 $Re_D = 2,900$

777 Diffuser Hole



- Validation against 3D MRI data

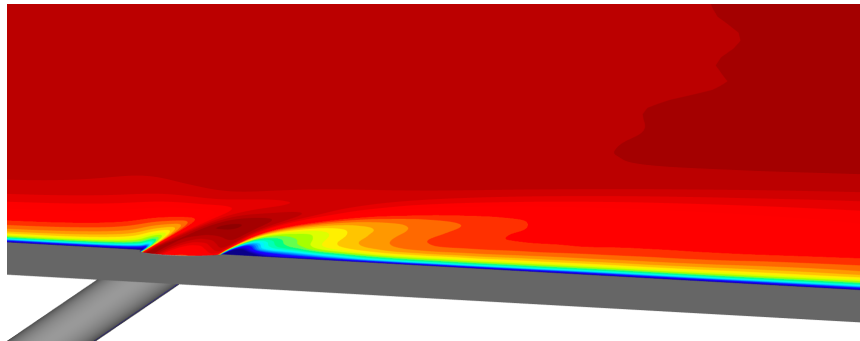




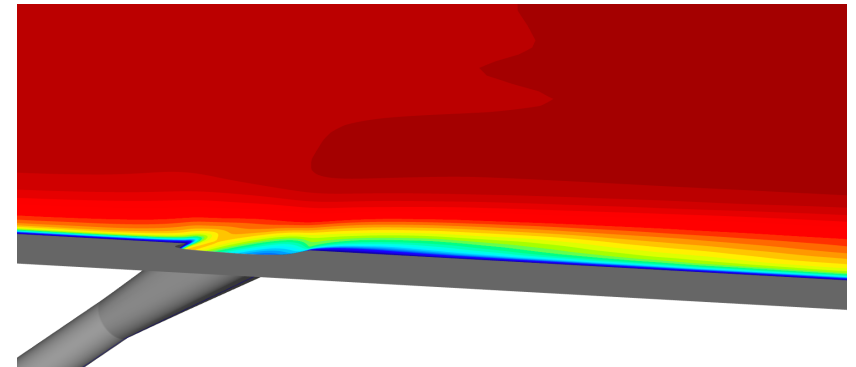
- Round hole has a strong counter-rotating vortex pair
- Diffuser hole bleeds low momentum fluid adjacent to the surface

Streamwise Velocity

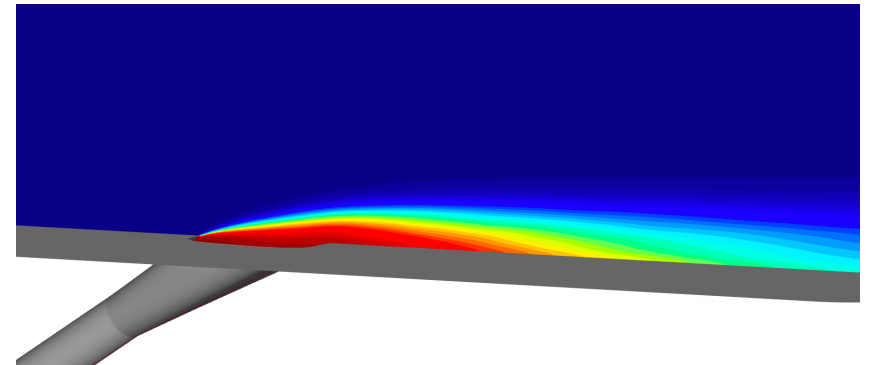
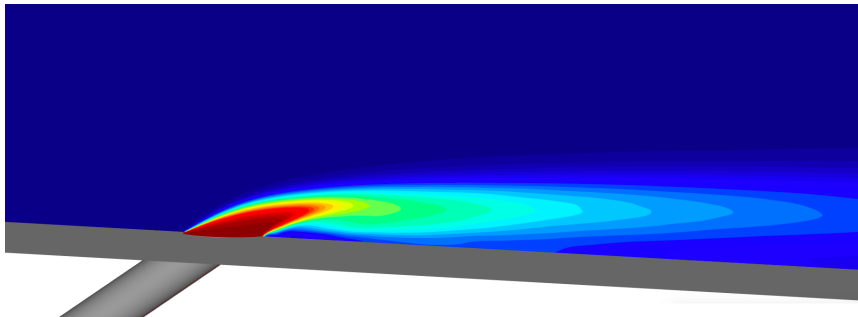
Round Hole

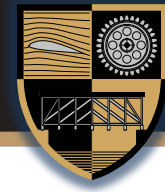


Diffuser Hole



Concentration



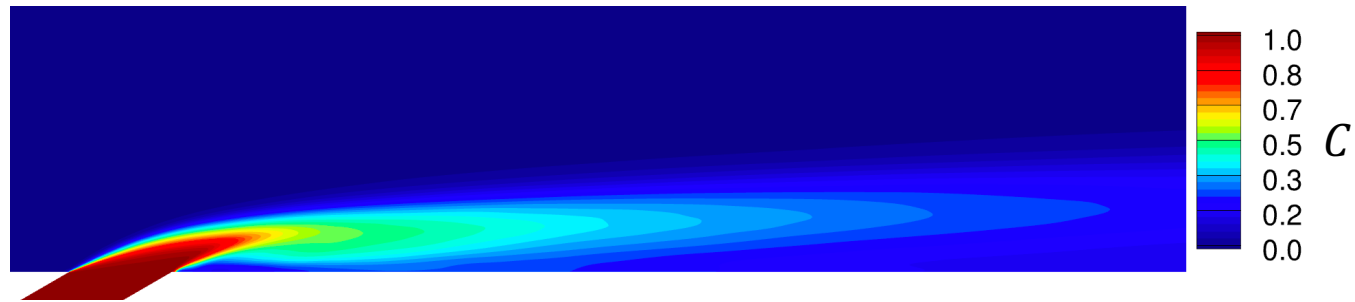


- Focus on scalar transport equation with $k - \epsilon$ as a baseline

$$\mathbf{U} \cdot \nabla C = \alpha \nabla^2 C - \nabla \cdot \langle c' \mathbf{u}' \rangle \quad \text{where} \quad \langle c' \mathbf{u}' \rangle = -\frac{\nu_T}{Pr_t} \nabla C \quad \text{and} \quad Pr_t \approx 0.85$$

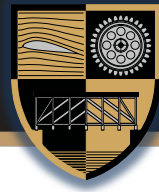
- Isolate turbulent scalar flux model
 - Same grid as LES
 - Use LES mean velocity
 - Determine k and ϵ by solving their transport equations using the LES velocity field

LES



Baseline RANS





- Turbulent scalar flux: $\langle c' u' \rangle = -\nu_T \mathbf{D}^* \nabla C$ $\mathbf{D}^* = \mathbf{F}(\mathbf{S}, \mathbf{R})$ \mathbf{S}, \mathbf{R} normalized by k/ϵ

¹Milani et al., JFM, 2021

²Banko et al., In prep.

³Zheng, 1994



- Turbulent scalar flux: $\langle c' u' \rangle = -\nu_T \mathbf{D}^* \nabla C$ $\mathbf{D}^* = f(\mathbf{S}, \mathbf{R})$ \mathbf{S}, \mathbf{R} normalized by k/ϵ
- Tensor basis neural network (TBNN-s)^{1,2}

– Input invariants

$$\begin{aligned} \lambda_1 &= \text{tr}(\mathbf{S}^2) & \lambda_3 &= \text{tr}(\mathbf{S}^3) & \lambda_5 &= \text{tr}(\mathbf{S}^2 \mathbf{R}^2) & \lambda_7 &= \sqrt{k}d/\nu \\ \lambda_2 &= \text{tr}(\mathbf{R}^2) & \lambda_4 &= \text{tr}(\mathbf{S} \mathbf{R}^2) & \lambda_6 &= \text{tr}(\mathbf{S}^2 \mathbf{R}^2 \mathbf{S} \mathbf{R}) & \lambda_8 &= \nu_T/\nu \end{aligned}$$

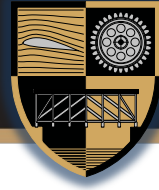
– Tensor basis (derived from vector basis³)

$$\begin{aligned} \mathbf{T}^{(1)} &= \mathbf{I} & \mathbf{T}^{(3)} &= \mathbf{R} & \mathbf{T}^{(5)} &= \mathbf{R}^2 \\ \mathbf{T}^{(2)} &= \mathbf{S} & \mathbf{T}^{(4)} &= \mathbf{S}^2 & \mathbf{T}^{(6)} &= \mathbf{S} \mathbf{R} + \mathbf{R} \mathbf{S} \end{aligned}$$

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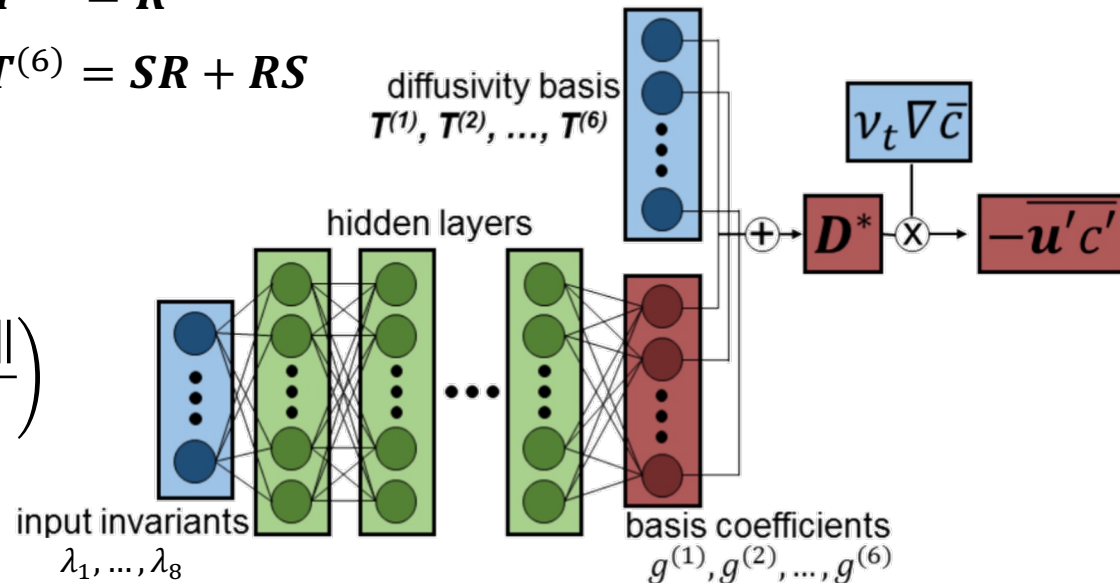
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- 8 layers, 20 nodes/layer
- Loss function

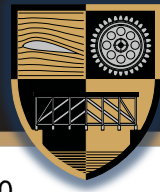
$$L = \log \left(\frac{\|\langle \mathbf{u}' c' \rangle_{ML} - \langle \mathbf{u}' c' \rangle_{LES}\|}{\|\langle \mathbf{u}' c' \rangle_{LES}\|} \right)$$



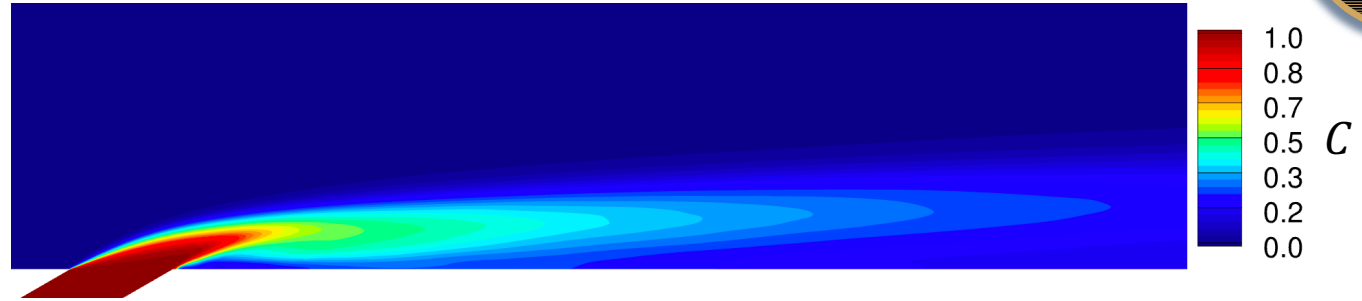
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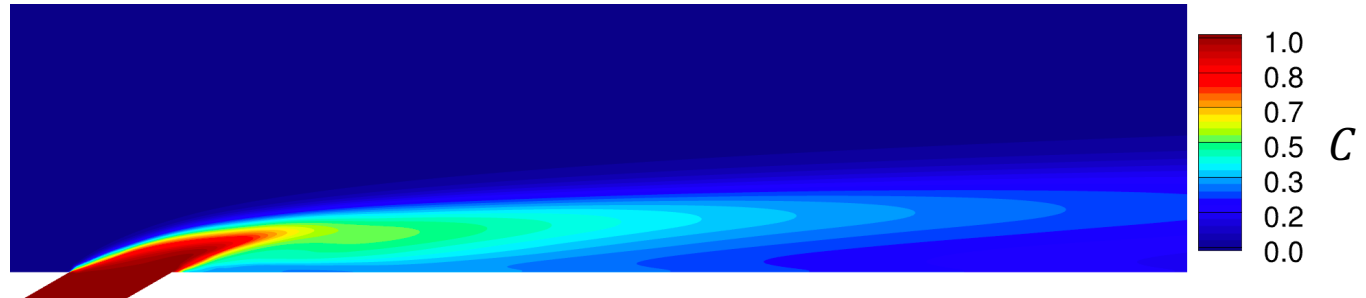
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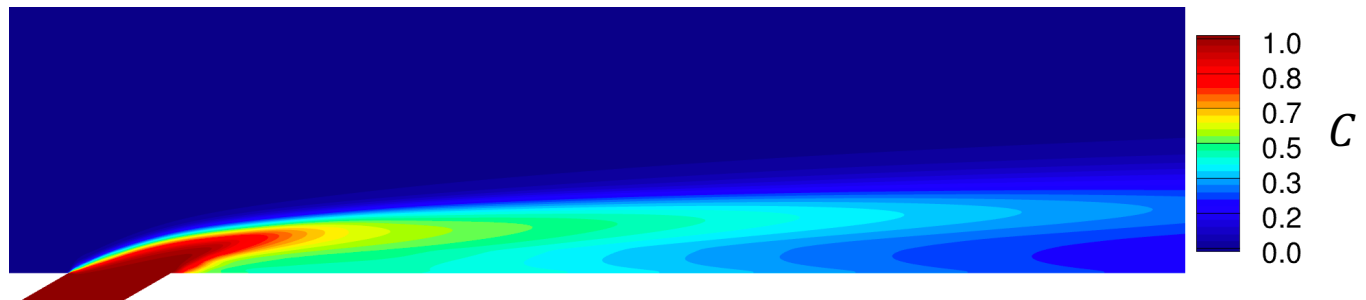
LES



Trained on
Round Hole



Trained on
Diffuser Hole

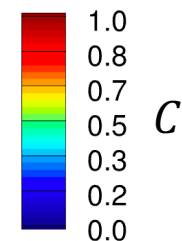
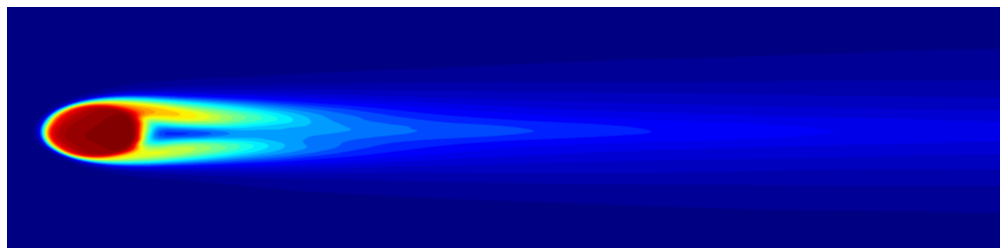


Baseline RANS

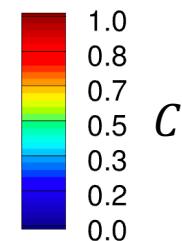
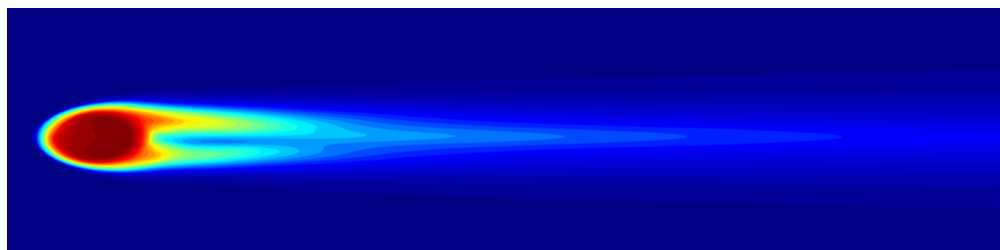




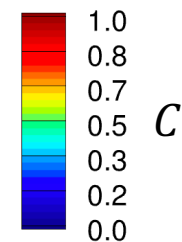
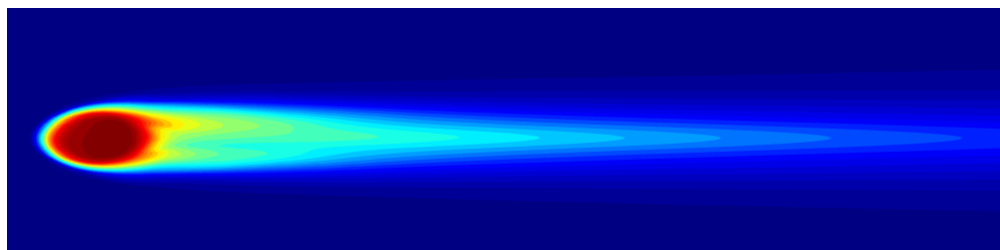
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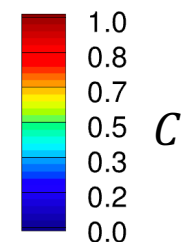
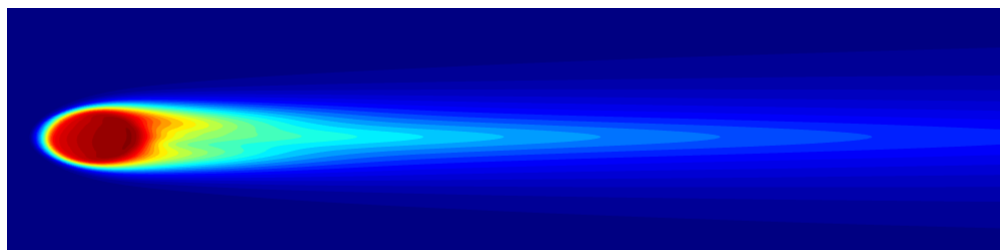
Trained on
Round Hole

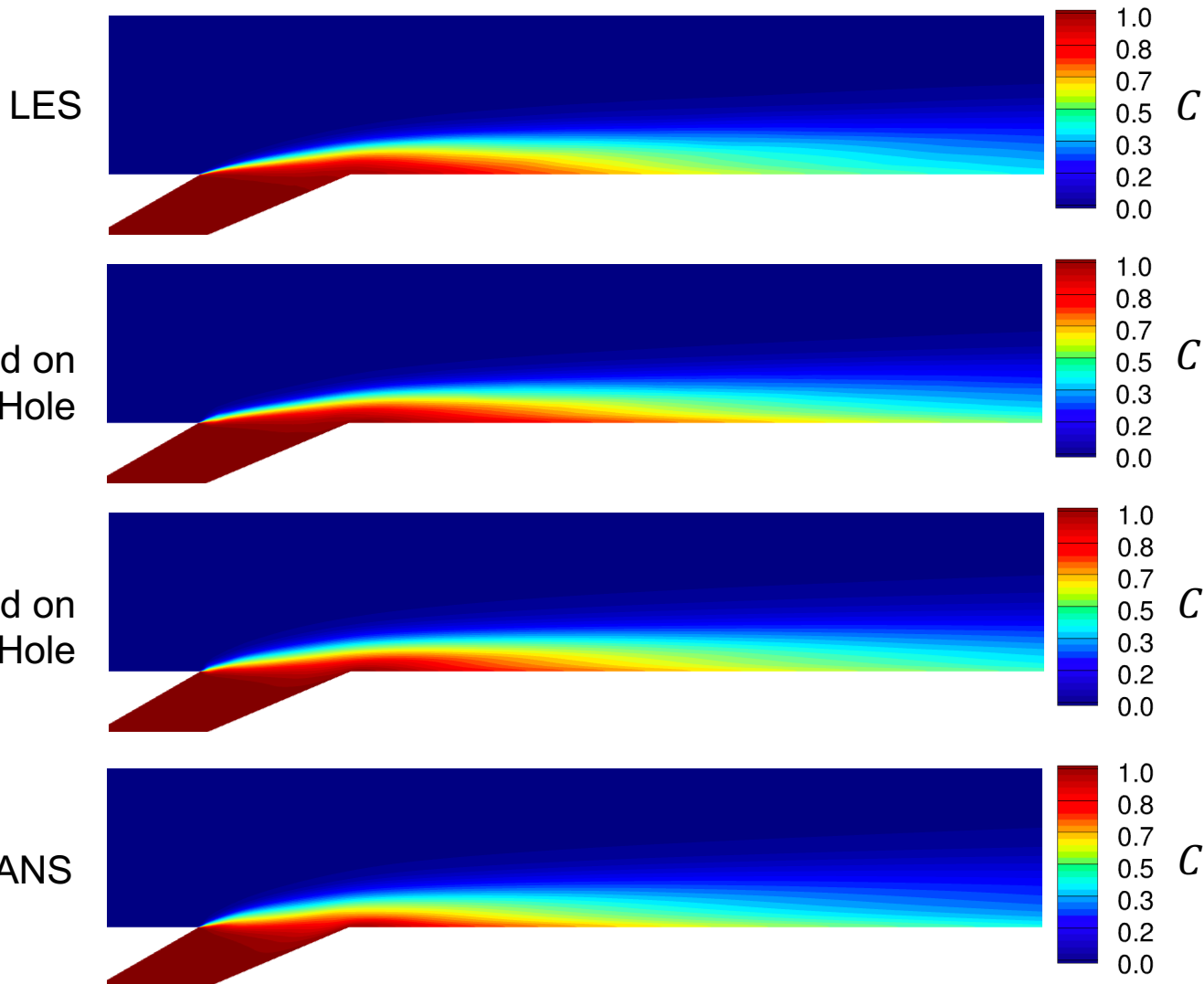


Trained on
Diffuser Hole



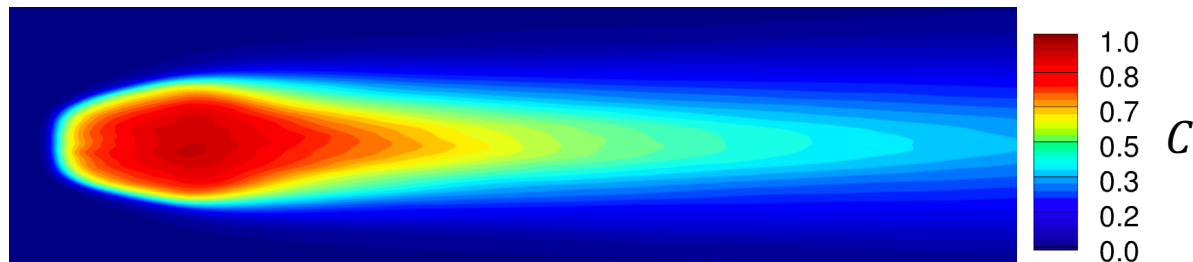
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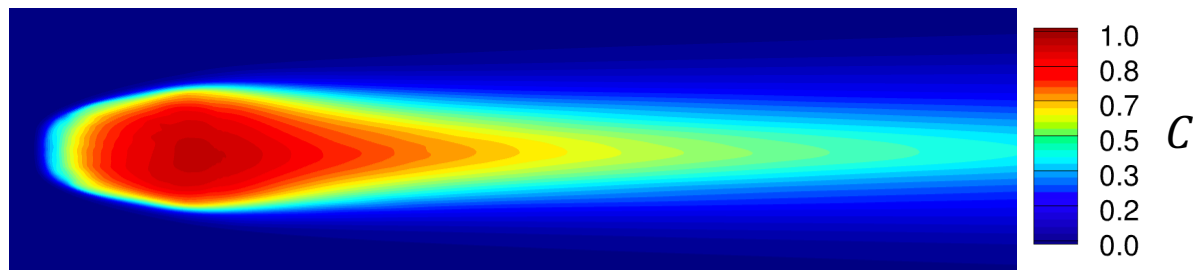




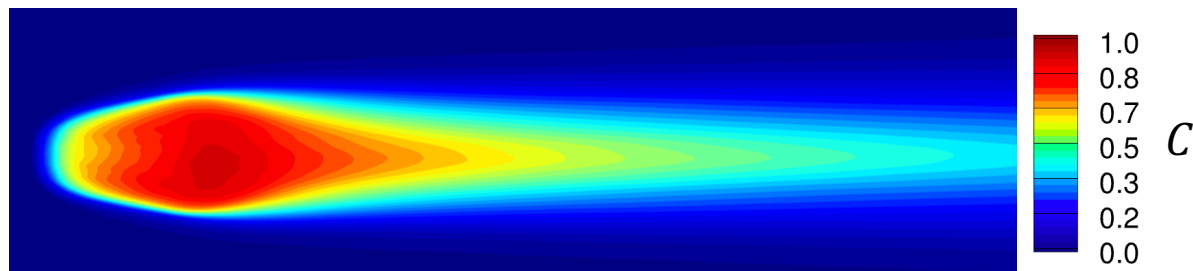
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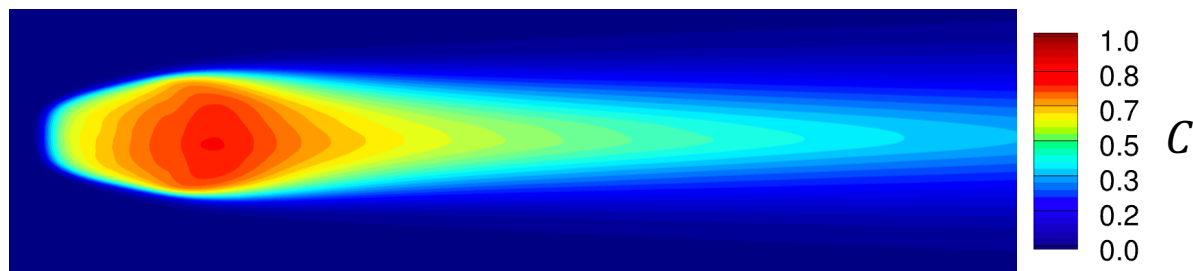
Trained on
Diffuser Hole



Trained on
Round Hole

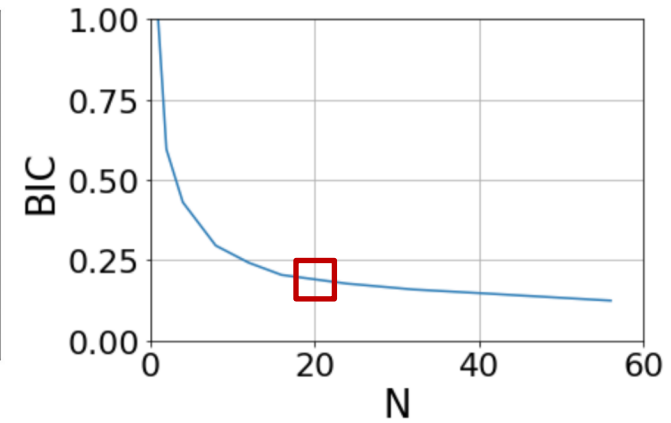
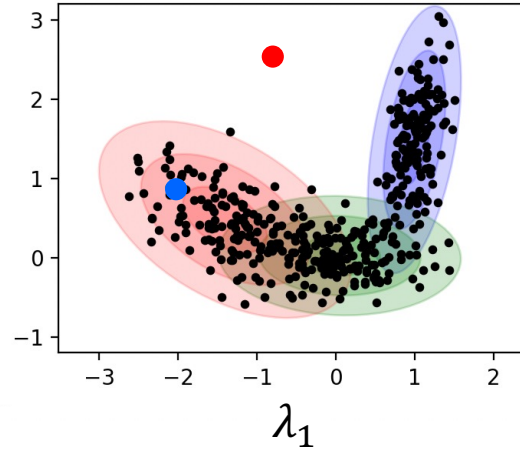
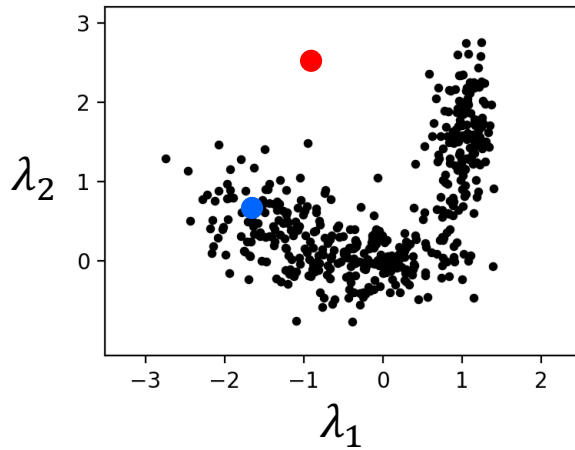


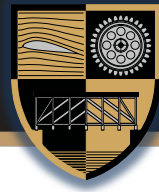
Baseline RANS



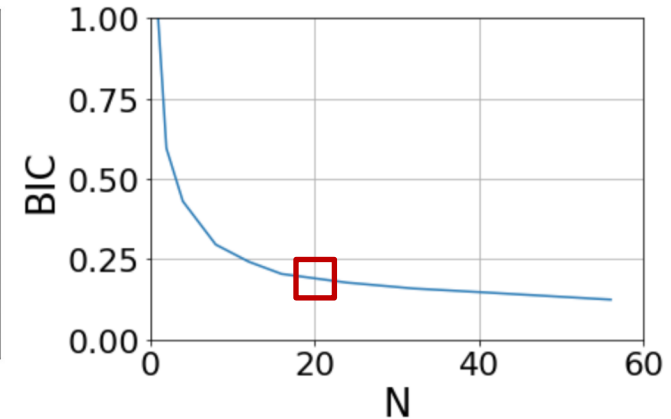
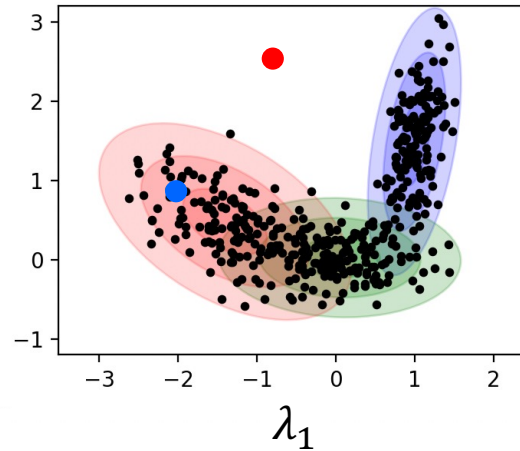
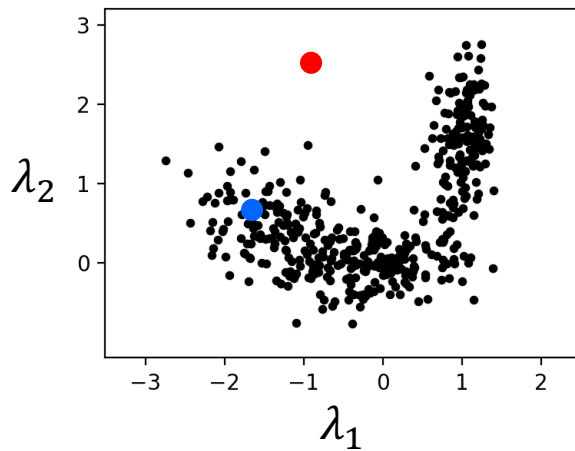


- Gaussian mixture model



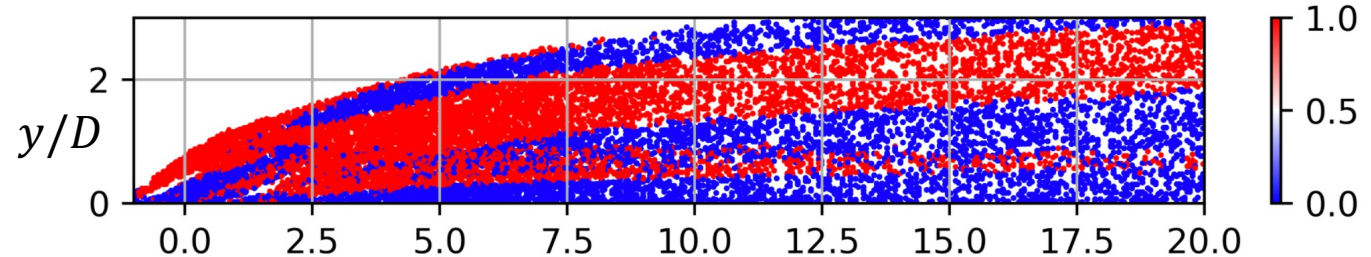


- Gaussian mixture model

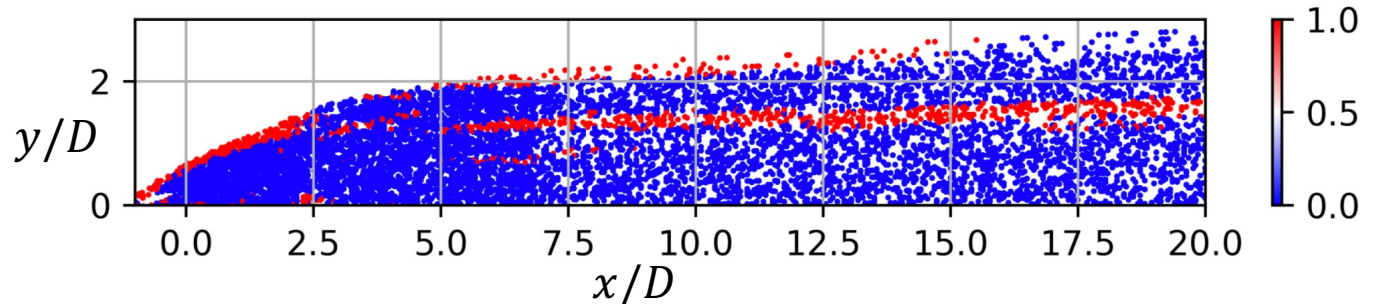


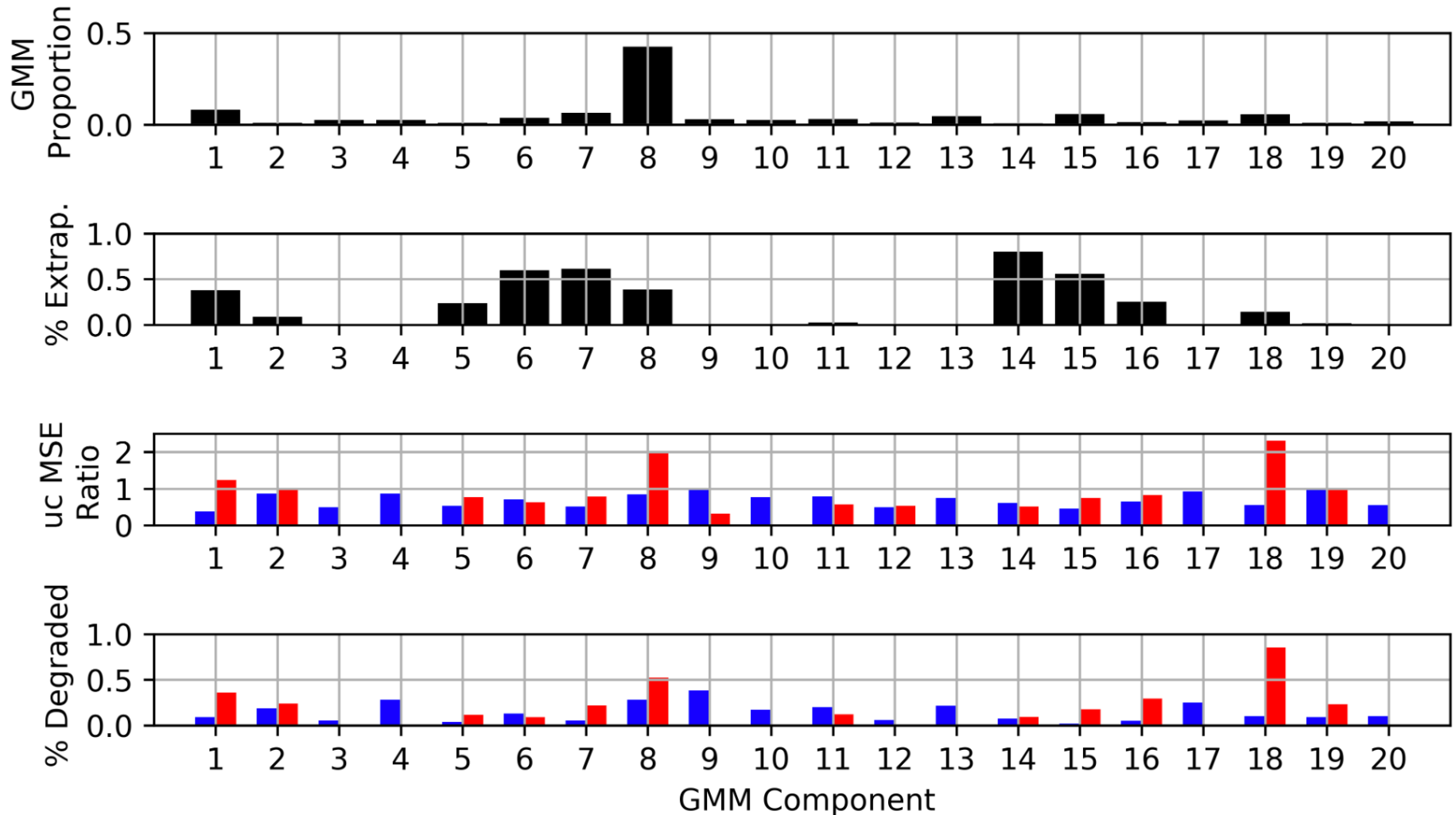
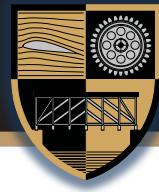
- Extrapolatory points: Blue = interpolating Red = extrapolating

Round Hole
(Train on Diffuser)



Diffuser
(Train on Round)



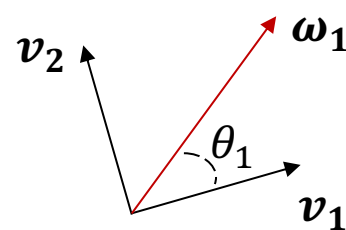


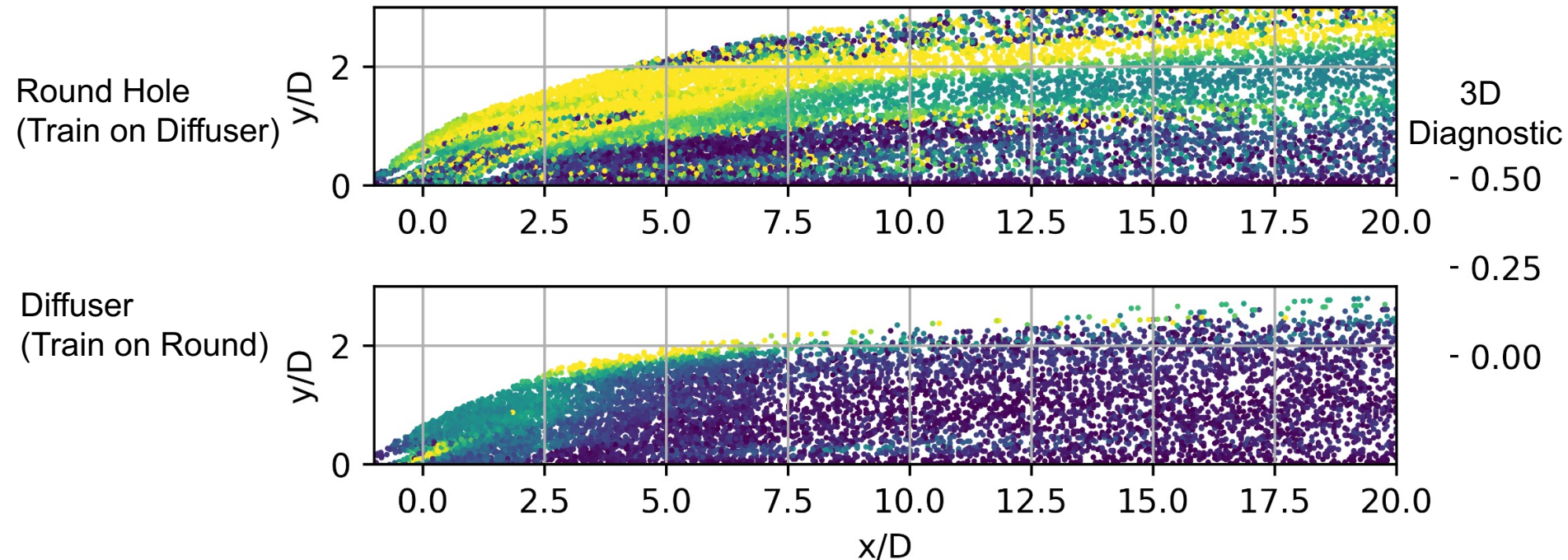
Blue = interpolating Red = extrapolating



- Detecting statistically 2D vs. 3D flow

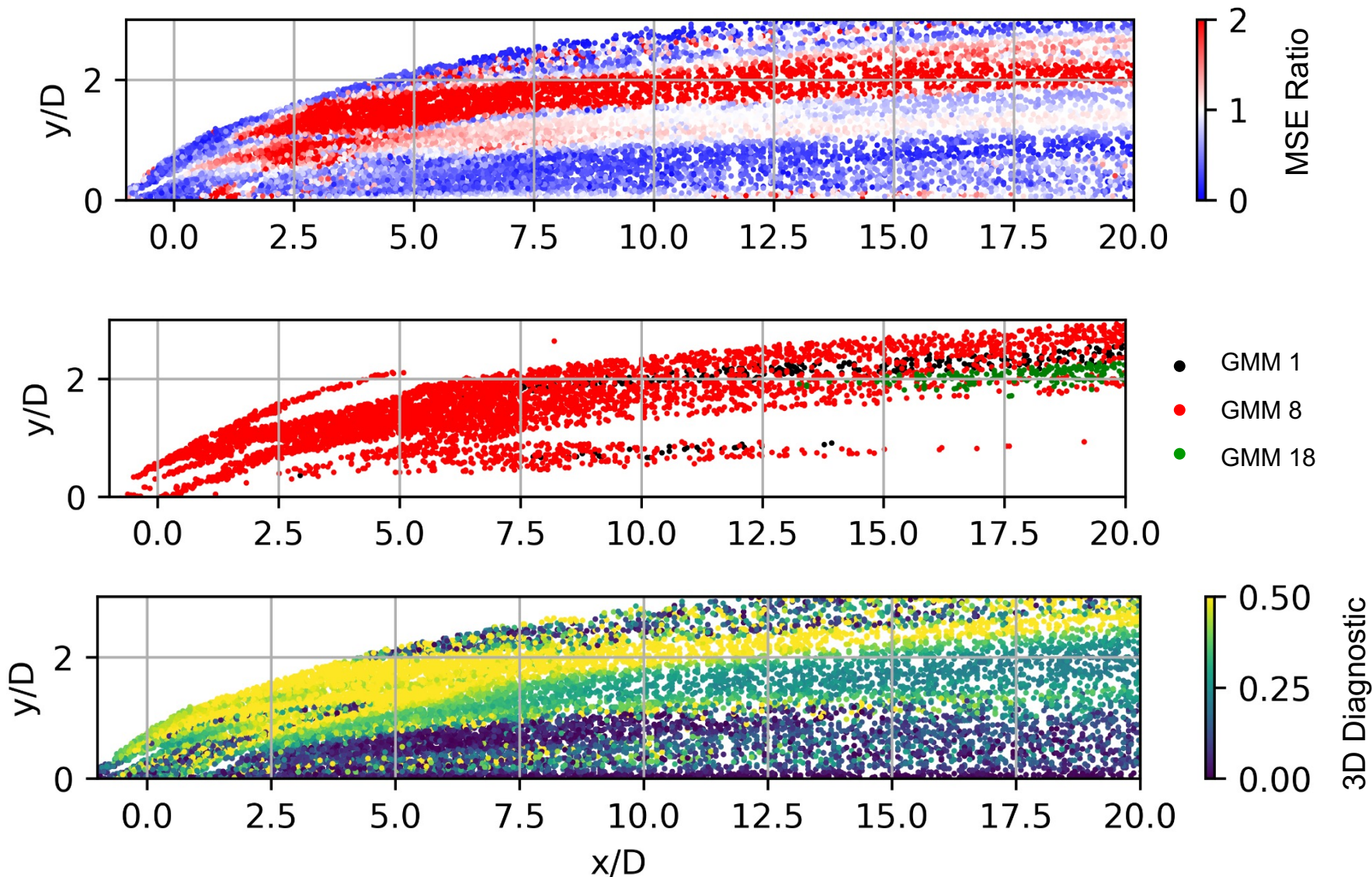
$$\lambda_5 = \text{tr}(\mathbf{S}^2 \mathbf{R}^2) = \frac{1}{4} \omega^2 \sum_{i=1}^3 \cos^2 \theta_i s_i = \begin{cases} \neq 0 & \text{if 3D} \\ = 0 & \text{if 2D} \end{cases}$$

$$\mathbf{S} = \mathbf{V} \begin{bmatrix} s_1 & & \\ & s_2 & \\ & & s_3 \end{bmatrix} \mathbf{V}^T$$






“2D”-Trained Network Extrapolates in “3D”



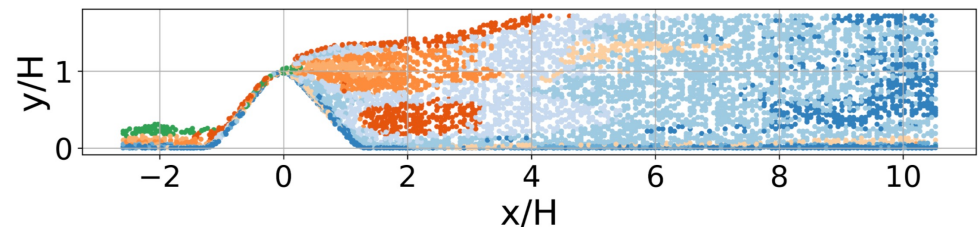
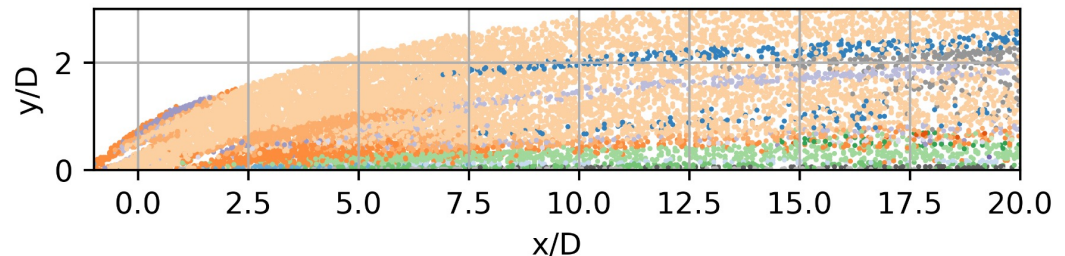


- GMM efficiently characterizes interpolation and extrapolation points
- Predictions were improved on average for interpolation cases
Caution: High error for interpolating points is possible
- Extrapolation and error were significant when moving from quasi-2D flow to 3D flow
3D: 5 independent invariants → 2D: 1 indep. inv. → 1D: 1 indep. inv.
- Big picture: an irony of data limitation

40 million CVs

≠

40 millions useful training
points





- Collaborators
 - Jad Nasrallah (Mainspring Energy)
 - Pedro Milani (Google X)
 - David Ching (Sandia National Labs)
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 - National Science Foundation
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