SAND2017-3108C

# DATA-DRIVEN ADAPTIVE PHYSICS MODELING FOR TURBULENCE SIMULATIONS

Julia Ling and Andrew Kurzawski

June 2017

Sandia National Laboratories

THE UNIVERSITY OF TEXAS AT AUSTIN

Funding for this work was provided by the Sandia LDRD program, and its support is gratefully acknowledged. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

# Motivation

- Can't run LES of all the flows we care about


- RANS:
  - Linear eddy viscosity models often give wrong results
  - Non-linear eddy viscosity models are often hard to converge
  - Can we use machine learning to enable adaptive physics modeling: turn on correction terms only where they're needed?

# Background: Eddy Viscosity Models

- Linear Eddy Viscosity Models (LEVM)
  - Simple, stable, cannot capture Reynolds stress anisotropy

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

- Non-linear Eddy Viscosity Models
  - Up to 5th order have been proposed
  - Less numerically stable, but can better capture Reynolds stress anisotropy
  - Quadratic Eddy Viscosity Model (QEVM) implemented into in-house incompressible flow solver

$$\begin{aligned}\overline{u_i'u_j'} = \;& \frac{2}{3}k\delta_{ij} - 2\nu_t S_{ij} + C_1\frac{\nu_t k}{\tilde{\epsilon}}(4S_{ik}S_{kj} - \frac{4}{3}S_{kl}S_{kl}\delta_{ij}) \\ & + C_2\frac{\nu_t k}{\tilde{\epsilon}}(4R_{ik}S_{kj} + 4R_{jk}S_{ki}) + C_3\frac{\nu_t k}{\tilde{\epsilon}}(4R_{ik}R_{jk} - \frac{4}{3}R_{kl}R_{kl}\delta_{ij})\end{aligned}$$

# Background: Scalar Flux Models

- Gradient Diffusion Hypothesis (GDH)
  - Simple, stable, unable to capture scalar flux anisotropy

$$\overline{u_i'\Theta'} = -\frac{\nu_t}{Sc_t}\frac{d\Theta}{dx_i}$$

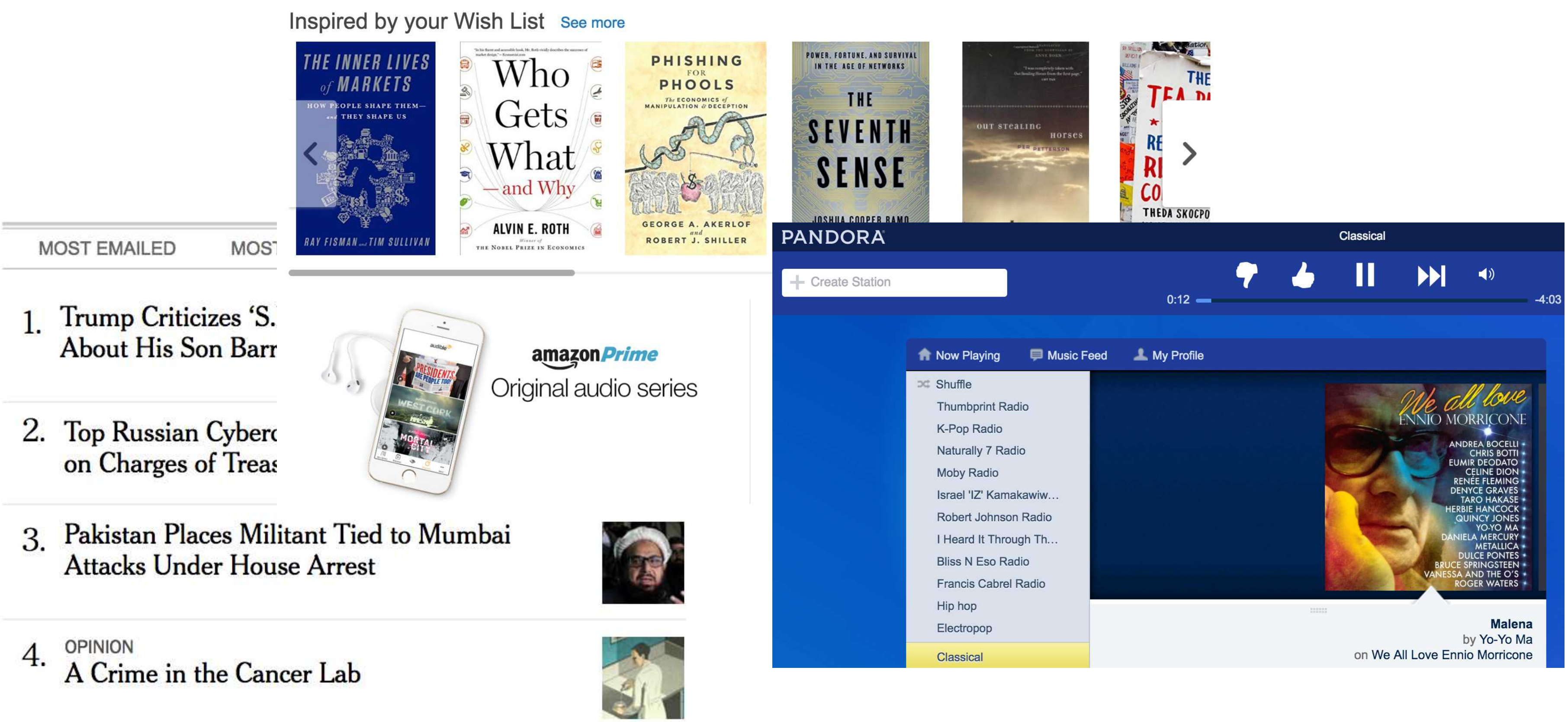
- Generalized Gradient Diffusion Hypothesis (GGDH)
  - Less stable, better able to capture scalar flux anisotropy

$$\overline{u_i'\Theta'} = -C_\theta \frac{k}{\epsilon}\overline{u_i'u_j'}\frac{d\Theta}{dx_j}$$

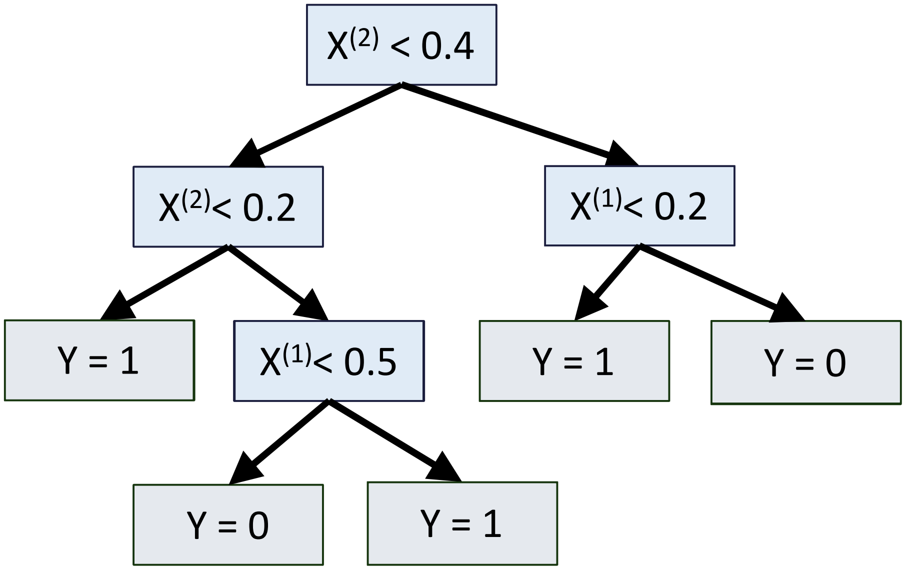
- We want to turn use LEVM/GDH in most regions of the flow, only turn on QEVM/GGDH where they're needed

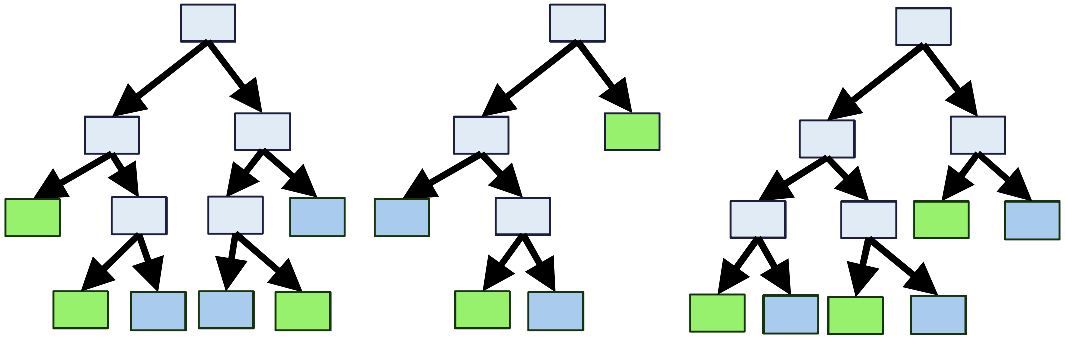
# What is Machine Learning?

- Data-driven algorithms to discern patterns and make predictions on big, high-dimensional data
- Linear regression, support vector machines, neural networks



# Random Forest Algorithm



# Using Machine Learning to Predict when the LEVM assumptions are wrong:

- Ling and Templeton (2015) developed a machine learning classifier to predict when the Reynolds stress anisotropy is high

$$f_{ML} = \begin{cases} 1, & \text{if } -2\mathrm{II}_a > \dfrac{1}{6} \\ 0, & \text{otherwise} \end{cases}$$

- Makes a prediction at each point in the flow
- Cross-validated over a data base of flows
  - Accuracy of 89% in detecting regions of high Reynolds stress anisotropy

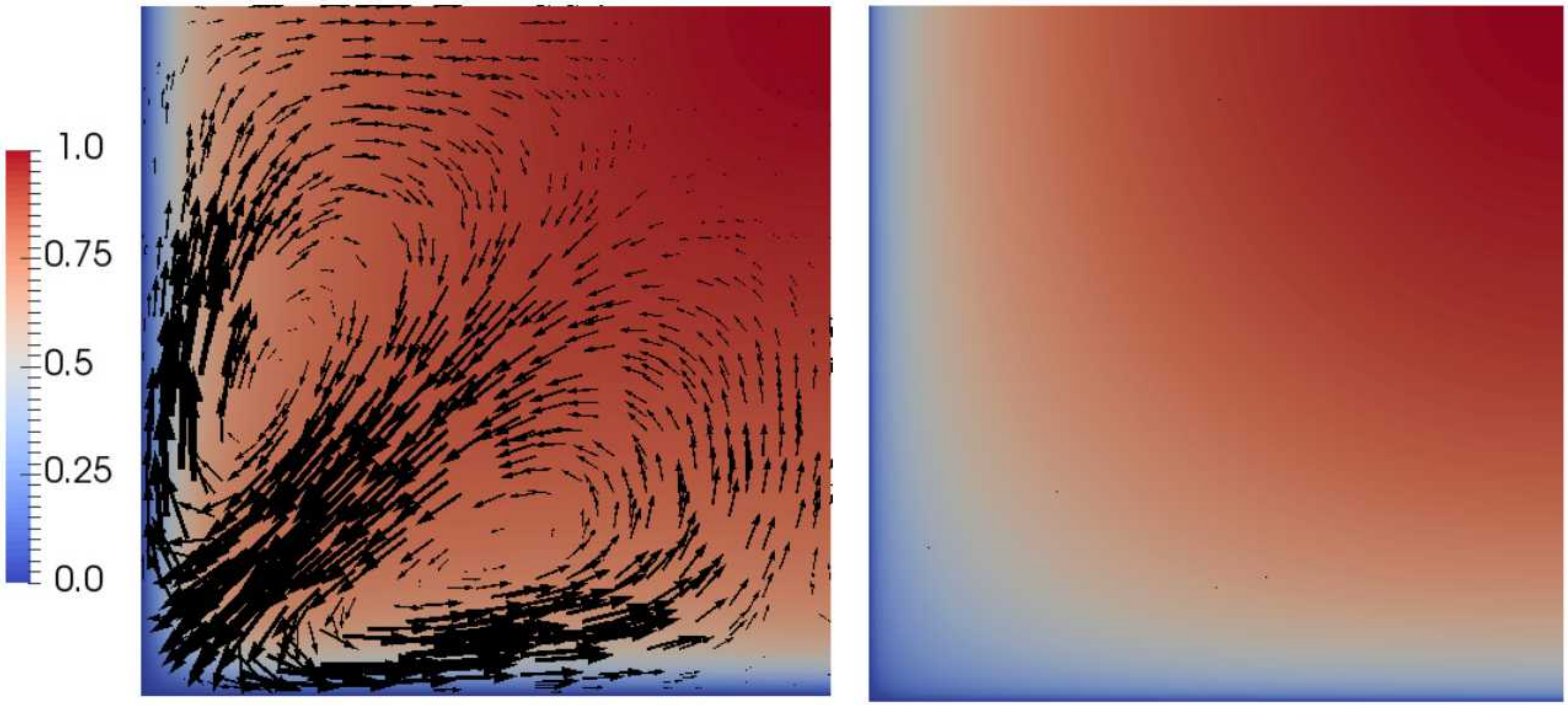
# Zonal Implementation

- Use Machine Learning (ML) classifier to trigger RANS model corrections
- Used Gaussian filter to smooth $f_{ML}$ to give smooth transitions

$$(\overline{u_i'u_j'})_{\mathrm{ZONAL}} = (1 - f_{\mathrm{ML}})(\overline{u_i'u_j'})_{\mathrm{LEVM}} + f_{\mathrm{ML}}(\overline{u_i'u_j'})_{\mathrm{QEVM}}$$

# Case Study: Turbulent Duct Flow

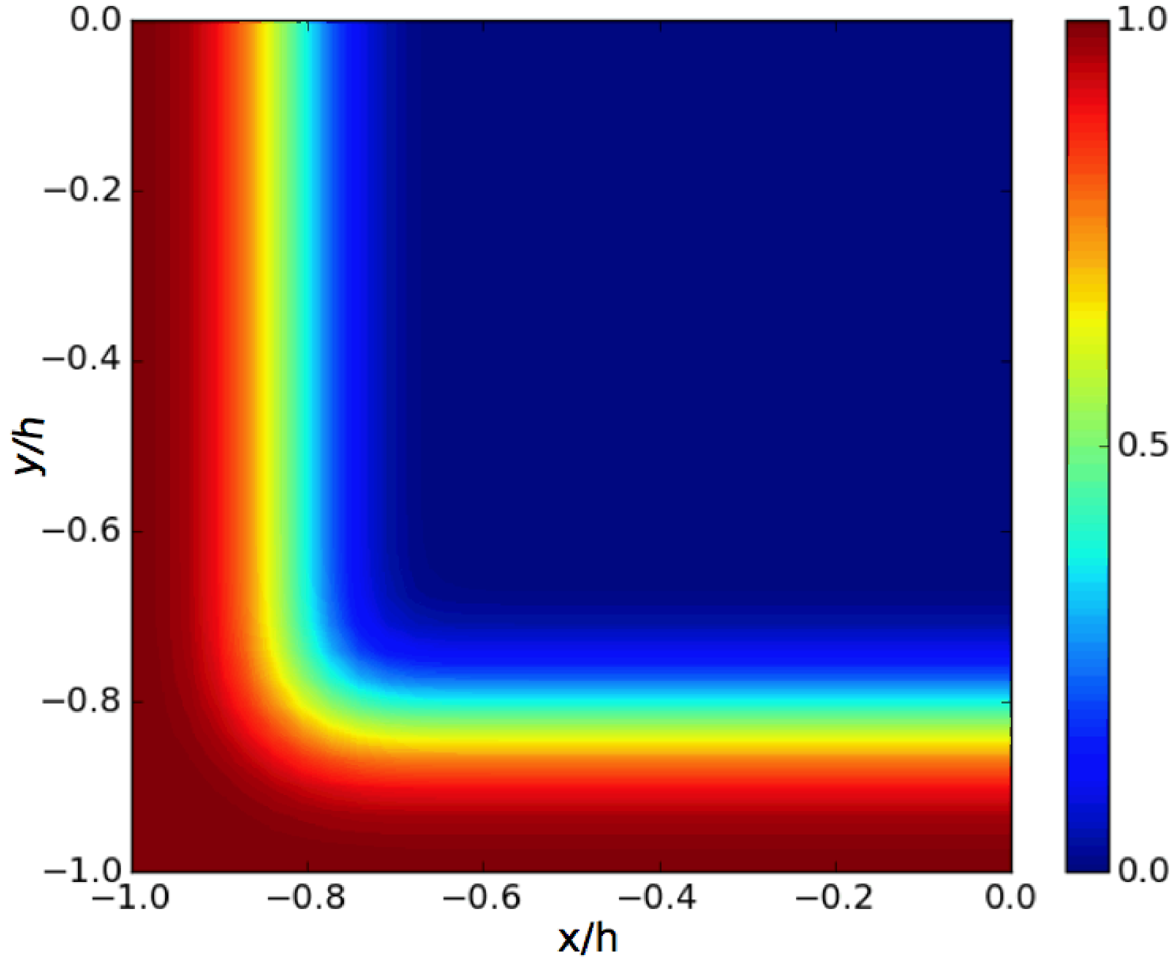
- Re = 3500 from Pinelli et al.

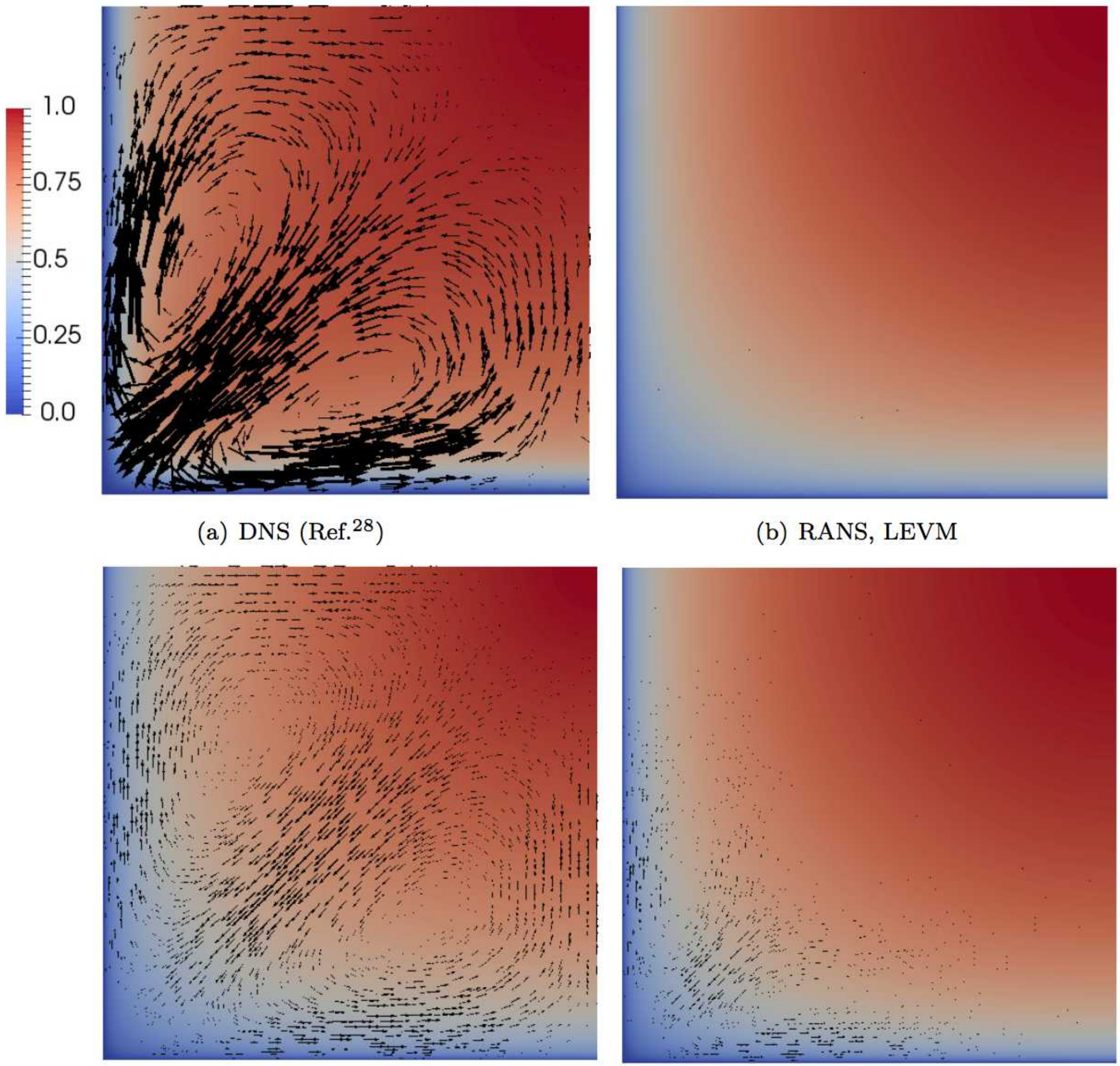



(a) DNS (Ref.[28])

(b) RANS, LEVM

# Zonal Mask: $f_{ML}$





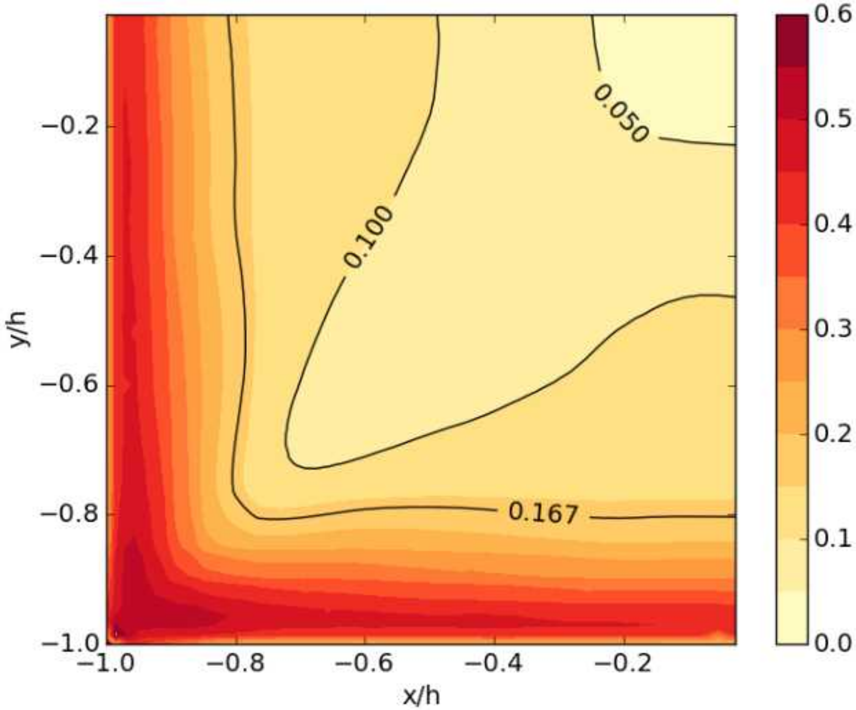

(a) DNS (Ref.[28])

(b) RANS, LEVM

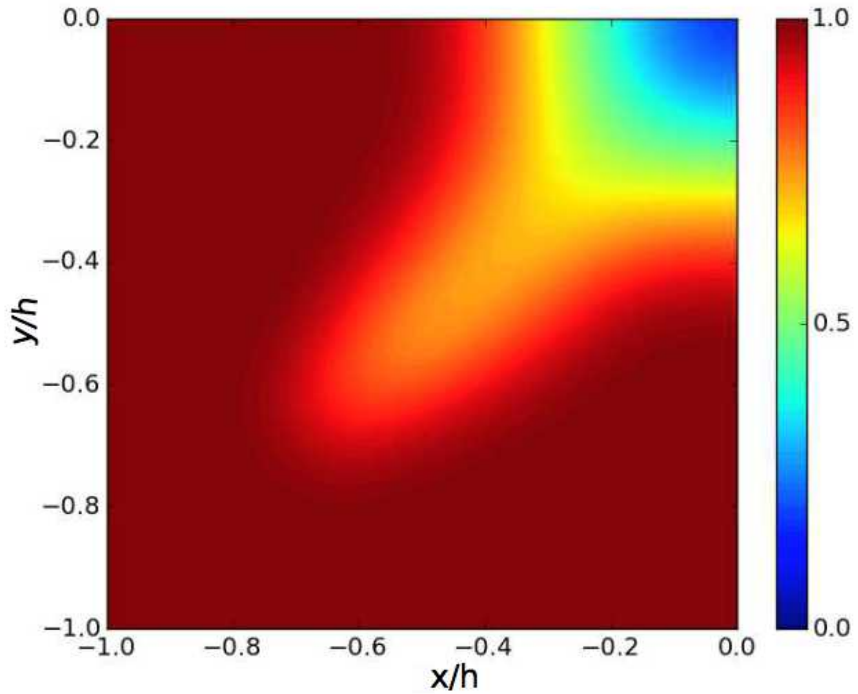
(c) RANS, QEVM

(d) RANS, Zonal QEVM

# Updating Zonal Mask

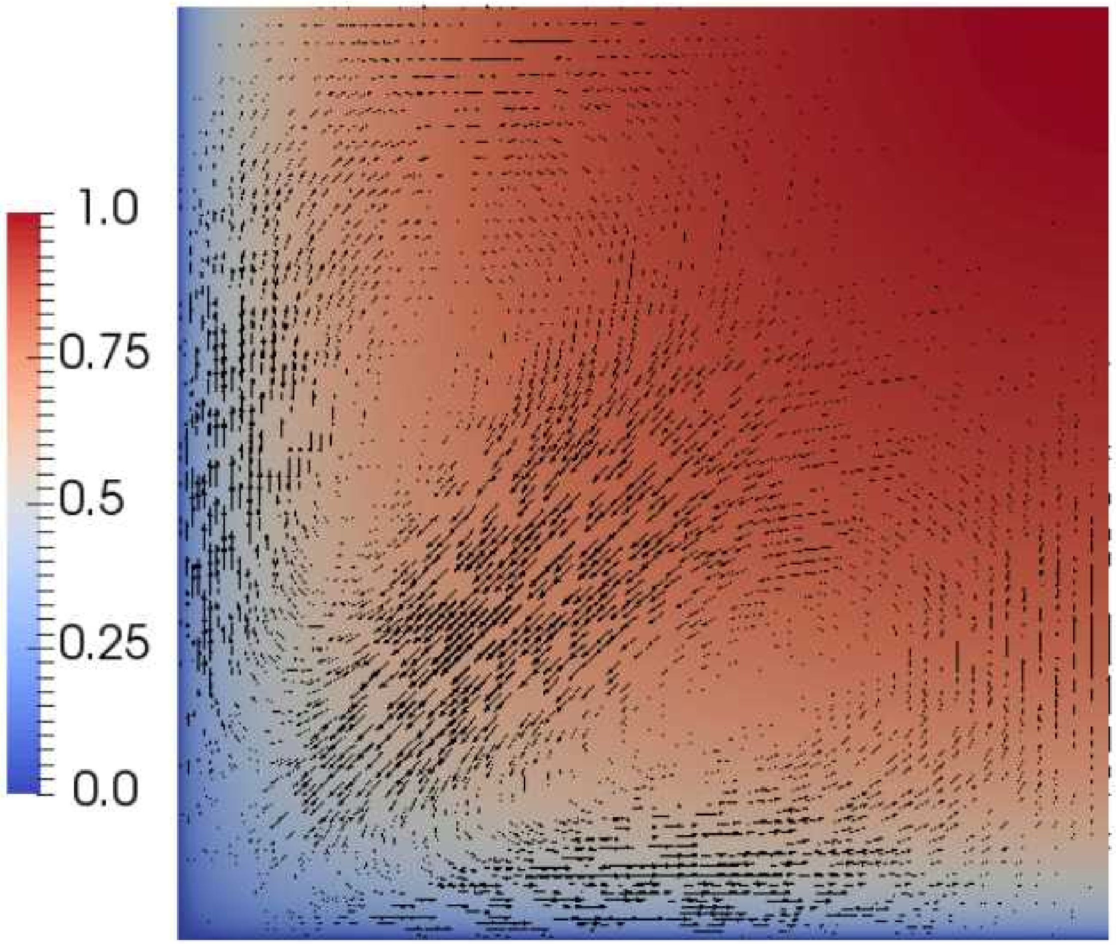



(a) Contours of $II_b$



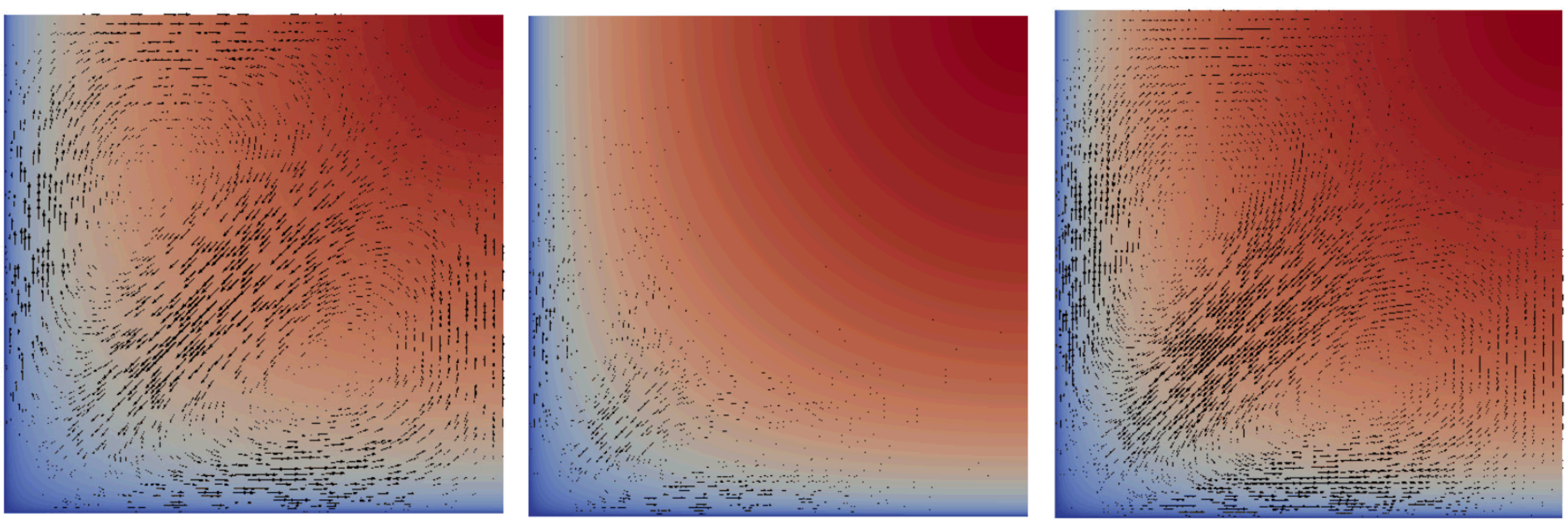

(b) Zonal mask based on $II_b$

# Results with Updated Zonal Mask



# Conclusions from Duct Flow Case Study

- The zonal approach with the original ML mask was not able to reproduce the proper strength or extent of the secondary flows
- With a modified mask that encompassed regions of lower anisotropy, the zonal approach resulted in stronger, bigger secondary flows

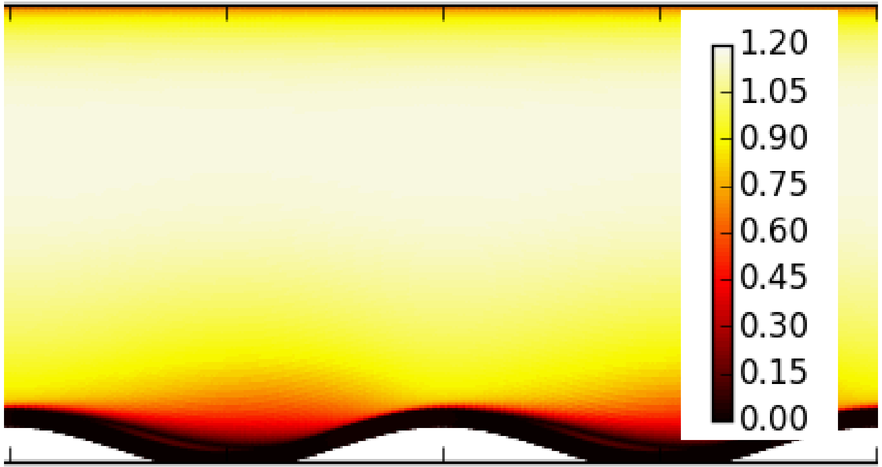


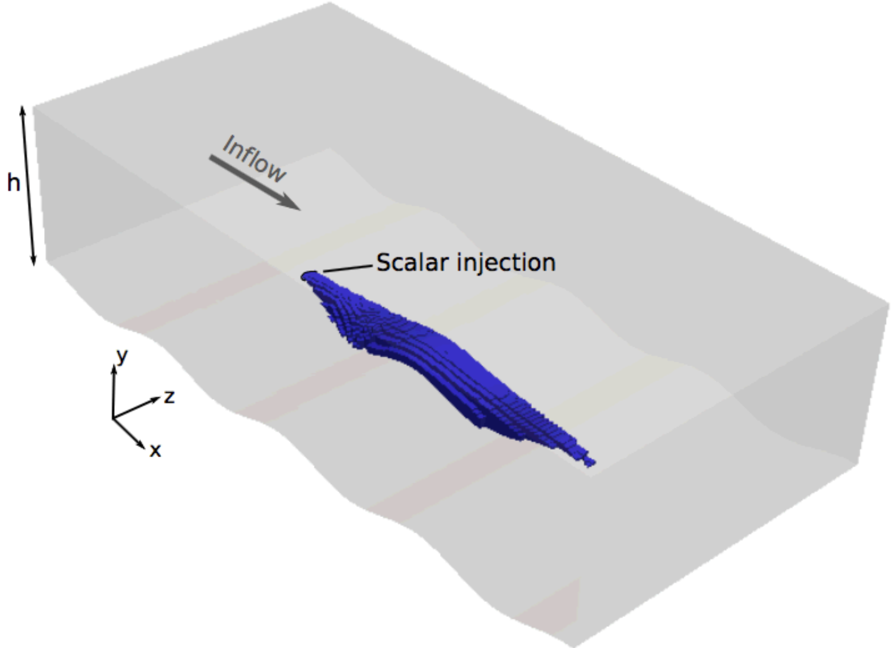
QEVM Zonal, ML mask Zonal, updated mask

# Case Study: Flow over a Wavy Wall

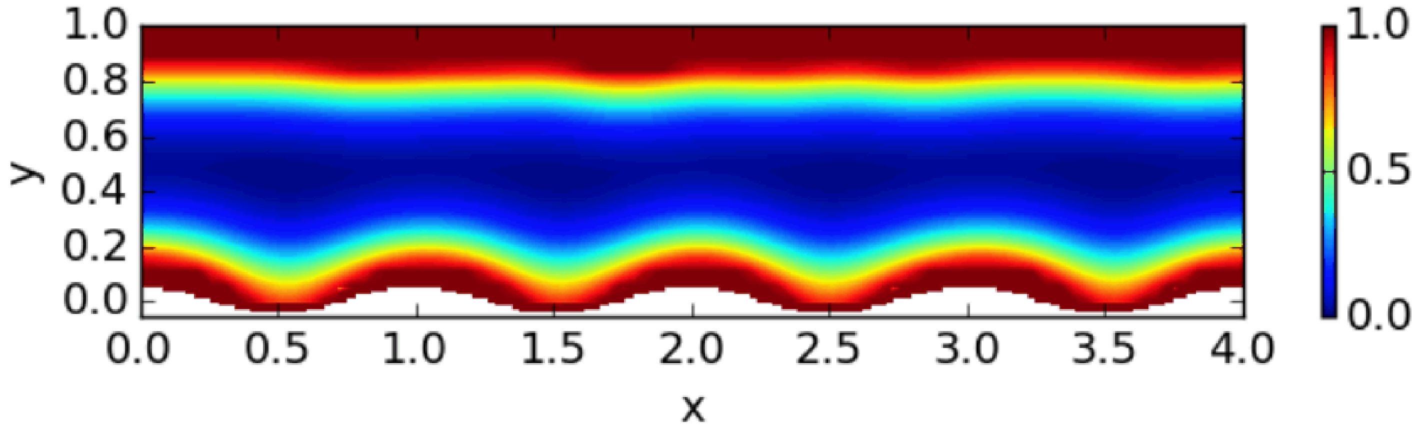
- Re = 7400, DNS from Rossi et al.

Contours of velocity magnitude

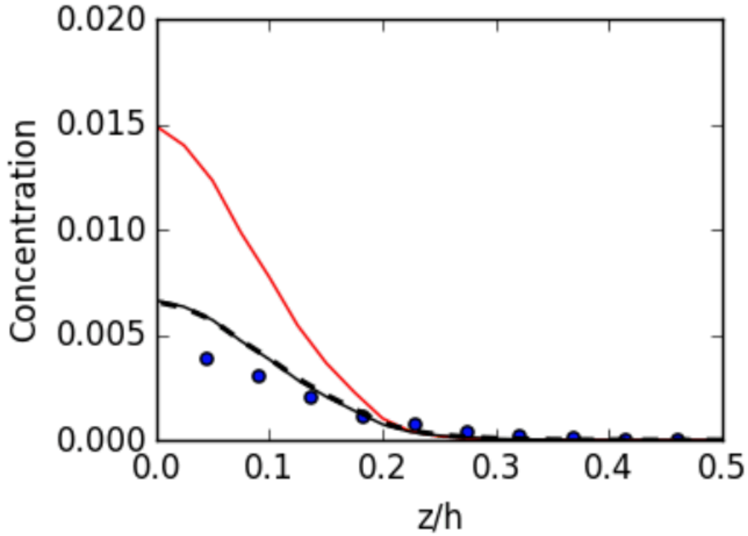


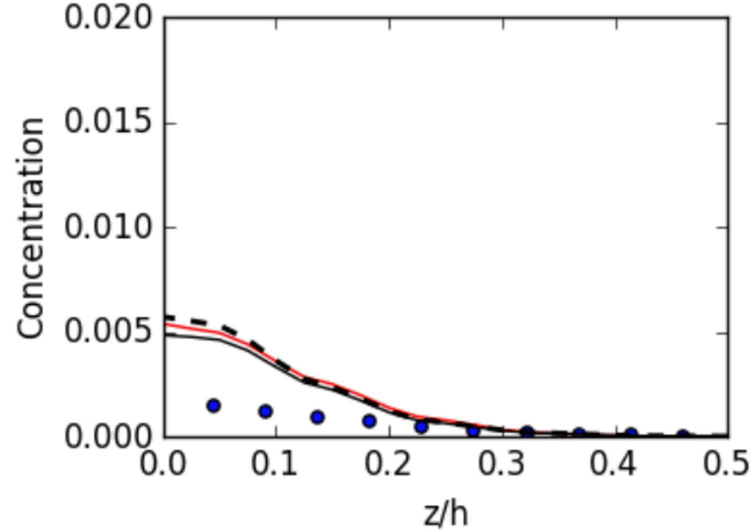
# Zonal Mask: $f_{ML}$



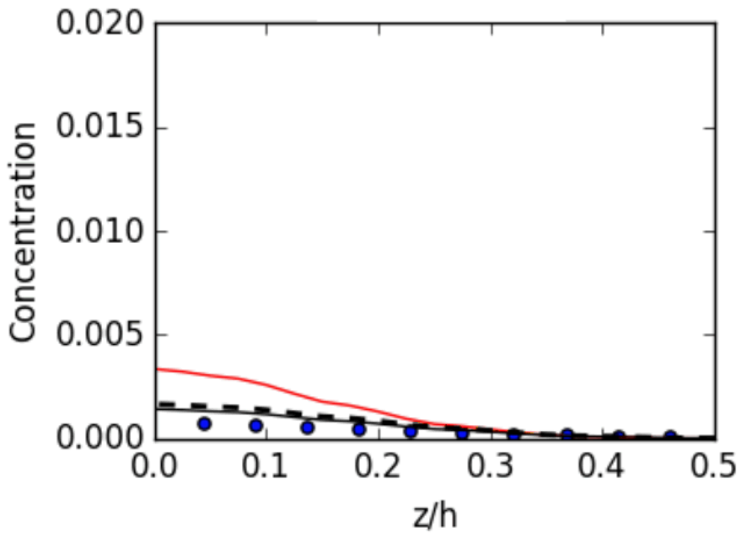

**Mask of $f_{\mathrm{ML}}$ used for zonal implementation of QEVM and GGDH.**



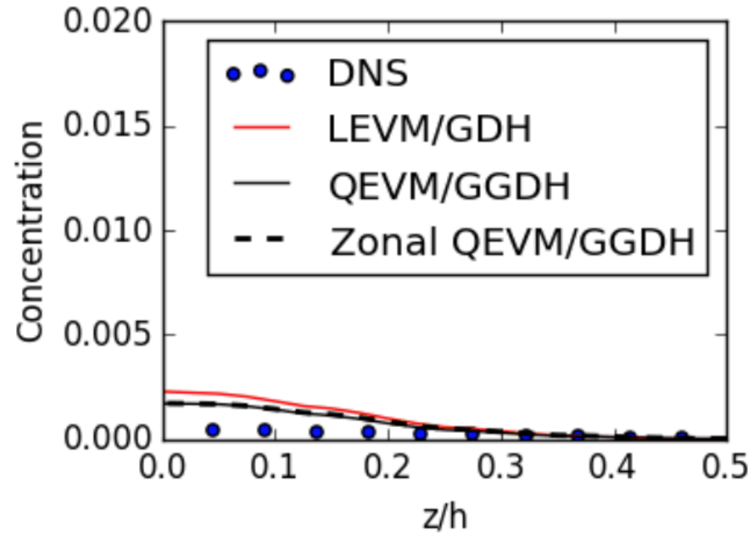

(a) $x/h = 1.5$



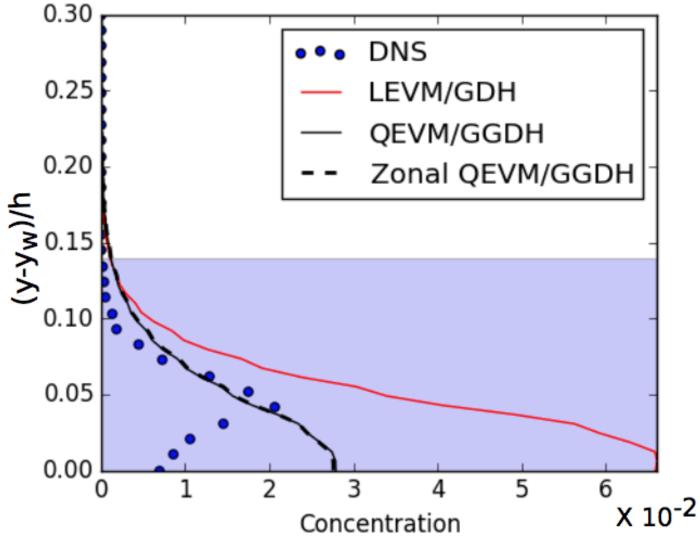

(b) $x/h = 2.0$



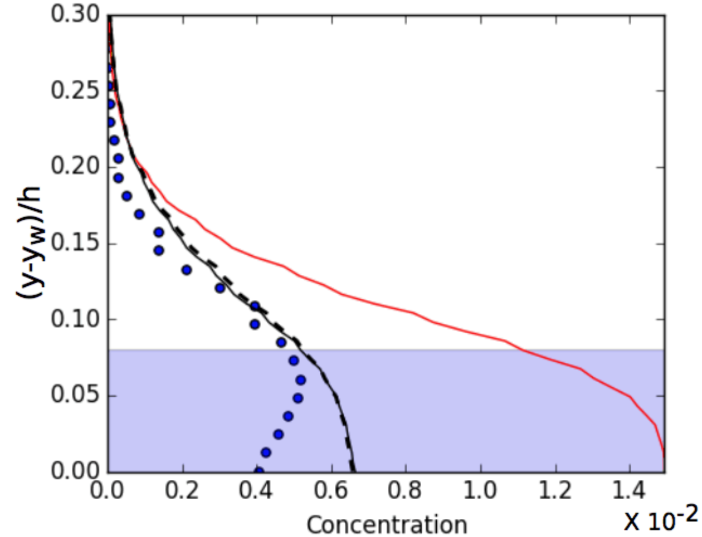

(c) $x/h = 2.5$



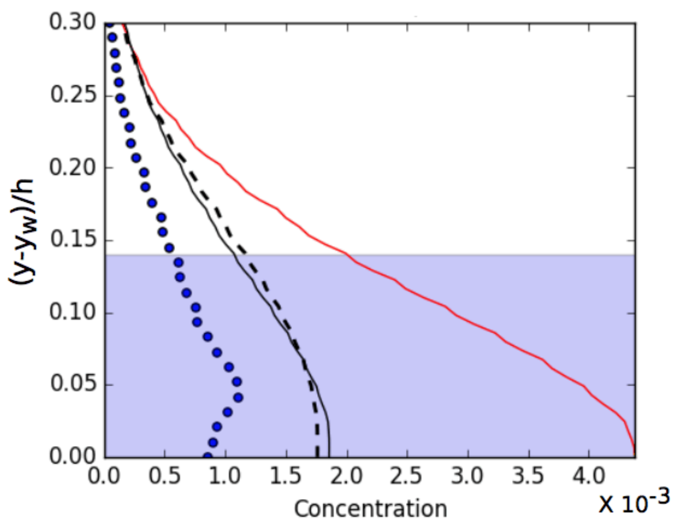

(d) $x/h = 3.0$



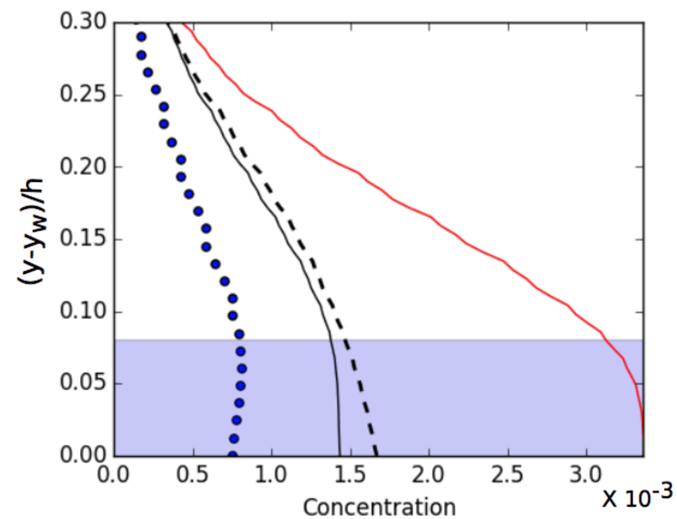

(a) $x/h = 1.25$




(b) $x/h = 1.5$

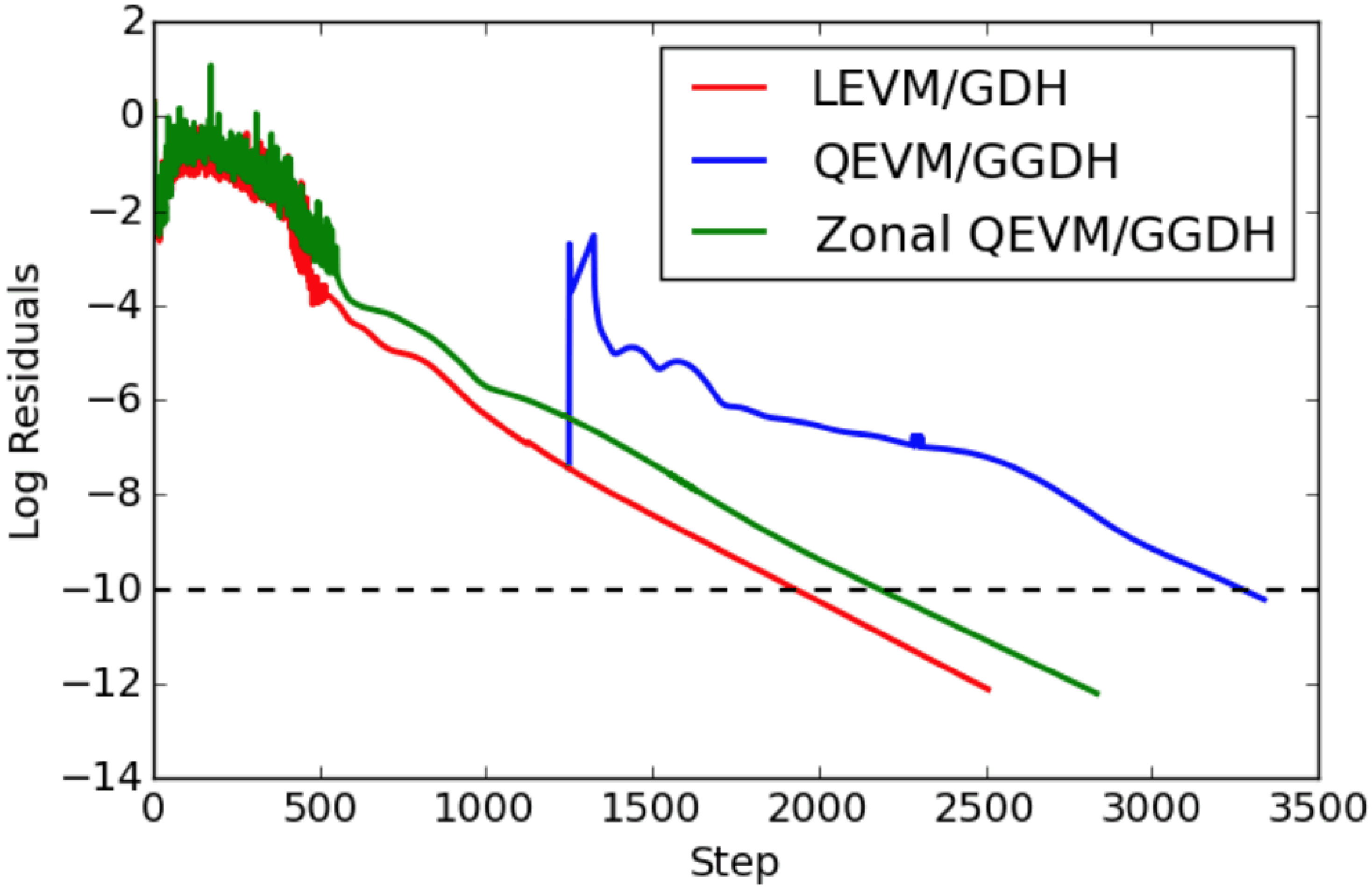



(c) $x/h = 2.25$




(d) $x/h = 2.5$

# Convergence



# Conclusions from Wavy Wall Case Study

- Zonal approach successfully reproduced accuracy of full QEVM/GGDH approach, with improved numerical stability
- Zonal approach provided improved predictions, even outside the corrected zone

# Overall Conclusions

- Presented general framework for adaptive physics modeling
  - Can use data-driven classifiers to trigger model corrections where they're needed
  - Specific correction is open-ended
  - We presented results for QEVM correction, but could use a machine learning correction, or LES, or any other higher fidelity model in these regions