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A Data-Driven, Physics-Informed Approach Towards *Predictive Turbulence Modeling*

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Acknowledgment of Collaborators

- My graduate students:

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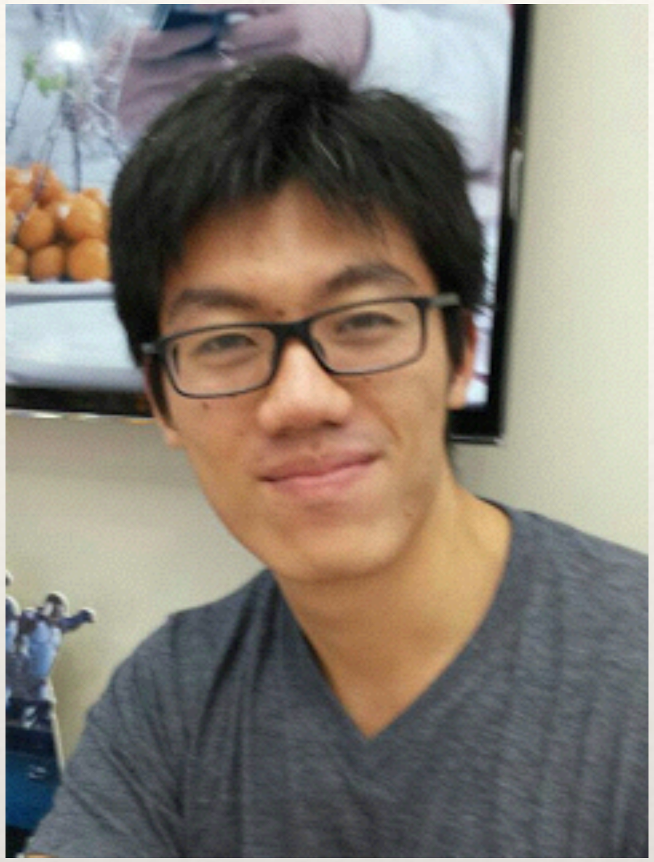

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- Colleague & collaborator: Chris J. Roy (Virginia Tech)

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Publications Related to This Talk

[1]. H. Xiao, J.-L. Wu, J.-X. Wang, R. Sun, and C. J. Roy. Quantifying and reducing model-form uncertainties in Reynolds averaged Navier-Stokes equations: An open-box, physics-based, Bayesian approach. Submitted to JCP, 2015. Also available at arxiv:1508.06315

[2]. J.-X. Wang, J.-L. Wu, and H. Xiao. Incorporating prior knowledge for quantifying and reducing model-form uncertainty in RANS simulations. Submitted to IJUQ, 2015. Also available at arxiv:1512.01750

[3]. J.-L. Wu, J.-X. Wang, and H. Xiao. A Bayesian calibration-prediction method for reducing model-form uncertainties with application in RANS simulations. Flow, Turbulence and Combustion, 2016. In press. DOI: 10.1007/s10494-016-9725-6 Also available at arxiv: 1510.06040

[4]. H. Xiao, J. X. Wang and R. G. Gahnem. A Random Matrix Approach for Quantifying Model-Form Uncertainties in Turbulence Modeling. Submitted to CMAME, 2016. Available at arxiv:1603.09656

[5]. J. X. Wang, R. Sun, H. Xiao. Quantification of Uncertainty in RANS Models: A Comparison of Physics-Based and Random Matrix Theoretic Approaches. Submitted, 2016. Available at arxiv:1603.05549

[6]. J.-L. Wu, J.-X. Wang, and H. Xiao. Quantifying Model Form Uncertainty in RANS Simulation of Wing–Body Junction Flow. Submitted to FTC.

Google my Google Site: Heng Xiao, VT

RANS as Work-Horse Tool in CFD

- Turbulence are everywhere in natural and industrial flows (see examples below).
- RANS (Reynolds Averaged Navier-Stokes) models are still the work-horse tool in practical applications, because high-fidelity methods (LES and DNS) are still too expensive for practical flows.

Landscape of Turbulence Modeling

- Standard (one/two eqn) RANS models: k-e, k-w, SA
- Advanced turbulence model: RSTM, EARSM
- Hybrid LES/RANS: DES and its variants, PANS, among others
- Wall-modeled LES (WALES)
- Fully resolved LES or DNS

The drawback of RANS: poor performance in flows with *separation, mean pressure gradient, mean flow curvature.* Need to quantify the uncertainties in the RANS predictions for high-consequence applications (e.g., nuclear power plants or airplanes).

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- Standard (one/two eqn) RANS models: k-e, k-w, SA
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- Fully resolved LES or

The drawback of RA
with *separation, mec*
curvature. Need to q
RANS predictions for
(e.g., nuclear power plants or airplanes).

Landscape of RANS Model Uncertainty

- Parametric and Bayesian model averaging approaches [Oliver & Moser et al.; Edling, Cinnella & Dwight]

Nonparametric Approaches.
with uncertainties injected in:

- RANS predicted turbulent viscosity [Dow and Wang]
- Source terms discrepancy in turbulent transport equations, e.g., v_t in SA model, ω in k-ω model [Duraisamy et al.]
- RANS predicted Reynolds stresses [Oliver & Moser]
- Decomposed RANS-predicted Reynolds stresses: TKE, anisotropy, orientation. [Emory, Gorle, Iaccarino et al.]
- Dynamics (time derivatives) of Reynolds stresses (Mishra & Girimaji): preliminary studies.

RANS Model Uncertainty: Black-Box vs. Openbox

- Kennedy & O'Hagan approach: introduce a discrepancy term to the QoI (e.g., drag and lift), and then calibrate the discrepancy with data => band-aid approach.
- Drawback: **black-box, physics-neutral**, not an efficient use of data; difficult to incorporate prior knowledge.
- Most of the methods discussed in this talk (except for the parametric approaches) are open-box, physics informed.

Parametric/Model Averaging Approaches

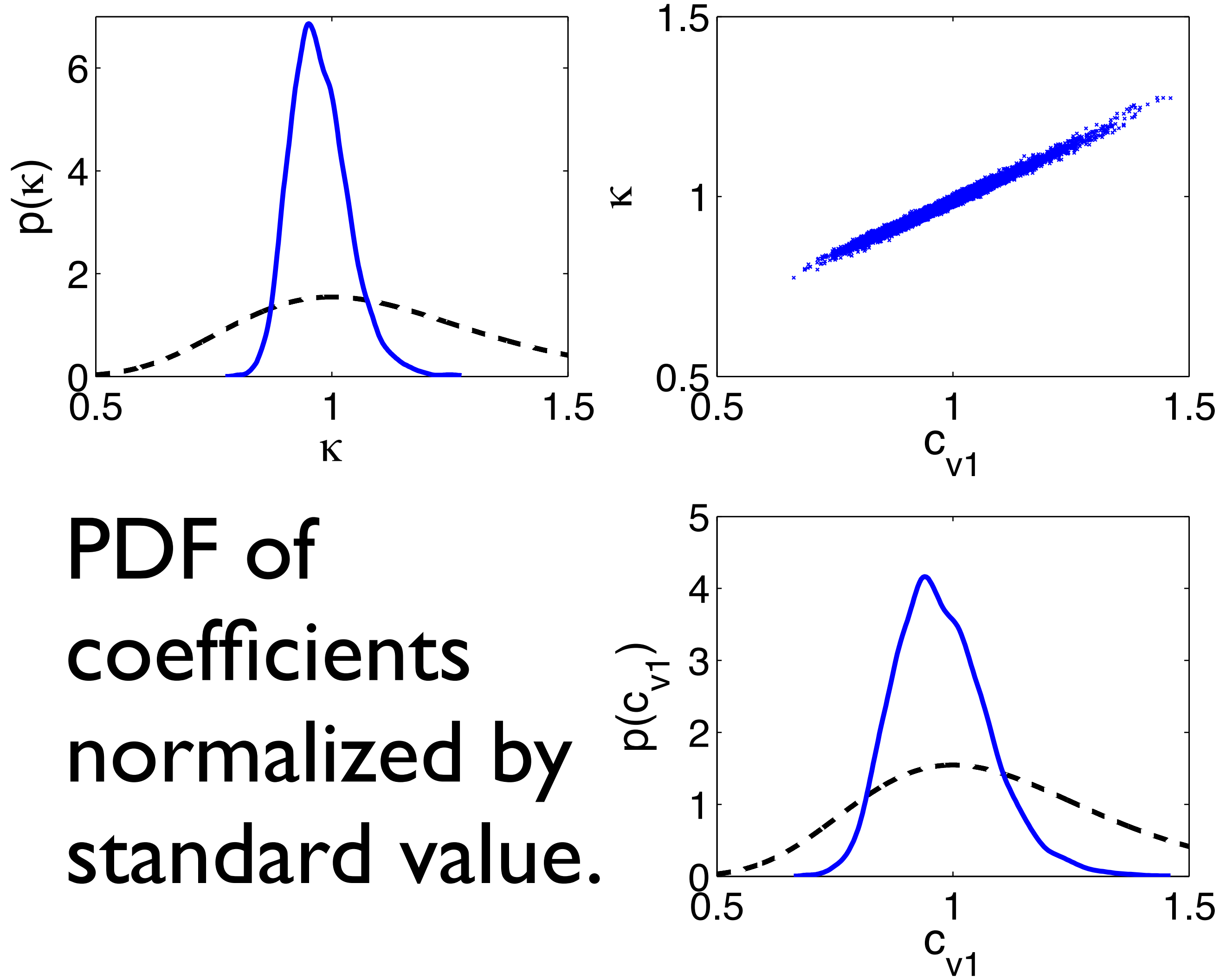
Simply stated: given experimental data, Bayesian inference methods are used to infer:

- How likely is each model (e.g., SA, Chien, v2f) correct?
- For a given model, what are the possible values/likelihood of the coefficients?

Bayesian Inference with Data

Table 2. $\log(E)$ value for each model.

	BL	SA	Chien	v^2-f
IND	44.19	8.862	21.78	20.23
SE	41.71	8.045	19.94	40.45
VLSE	159.5	164.0	175.5	169.8
ARSM	135.0	169.0	157.5	158.9



PDF of coefficients normalized by standard value.

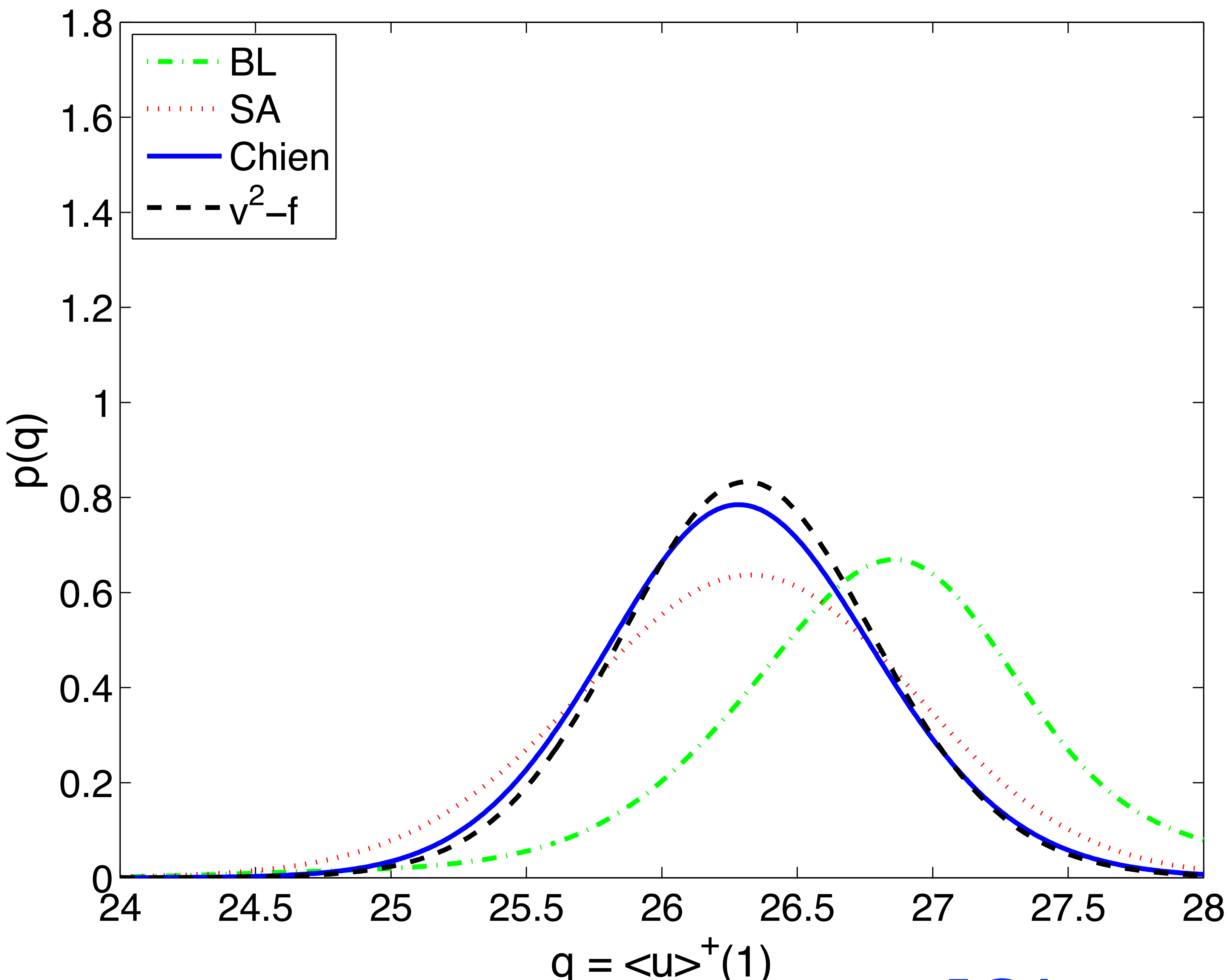
(a) SA: κ and c_{v1}

[Oliver & Moser]

Oliver, T. A., & Moser, R. D. (2011). Bayesian uncertainty quantification applied to RANS turbulence models. In *Journal of Physics: Conference Series* 318 (4), p. 042032. IOP Publishing.

Prediction with Posterior of Models/Coefficients

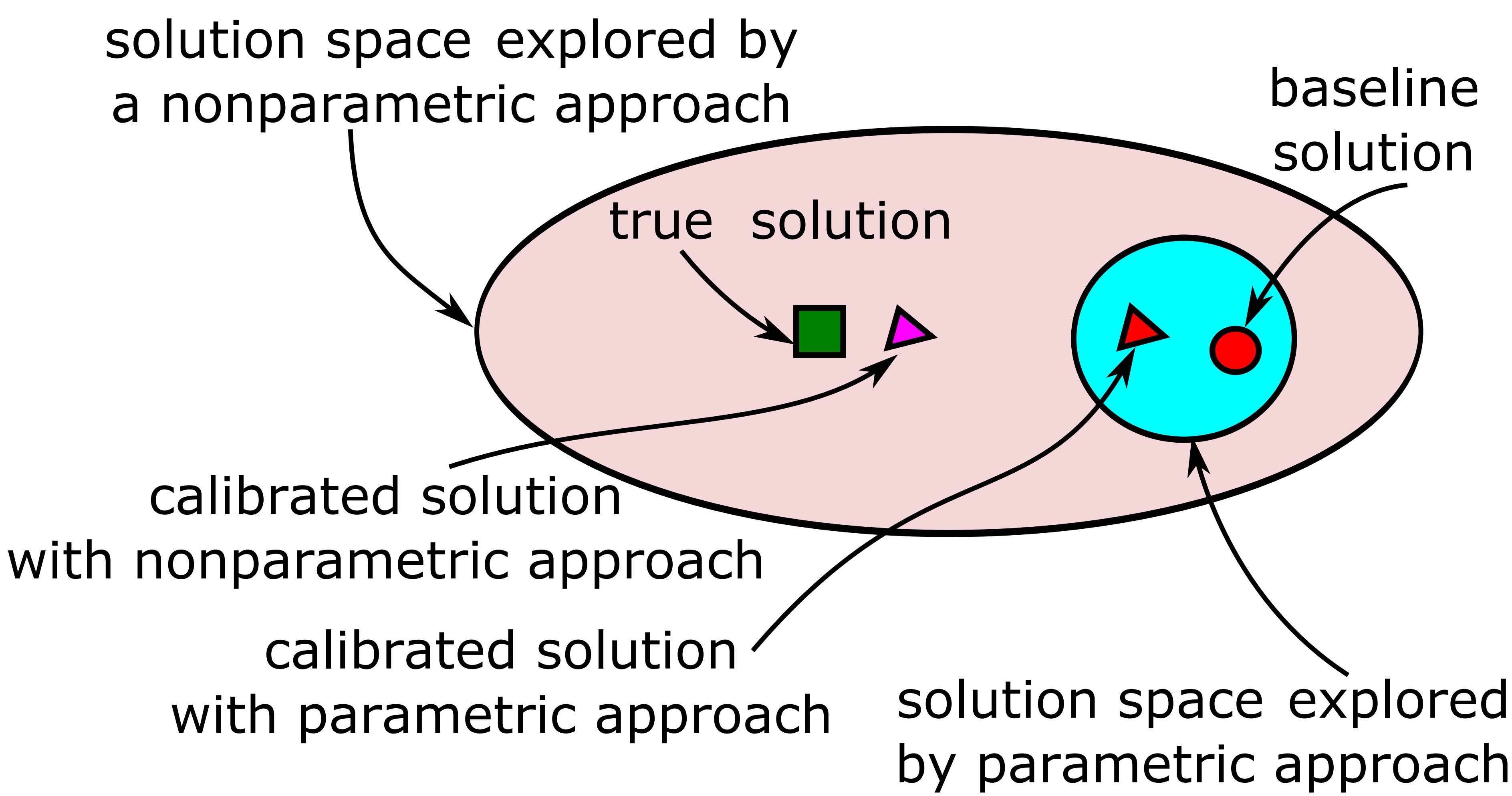
- Probability of predicted Quantity of Interest (mean velocity at a given location)



[Oliver & Moser]

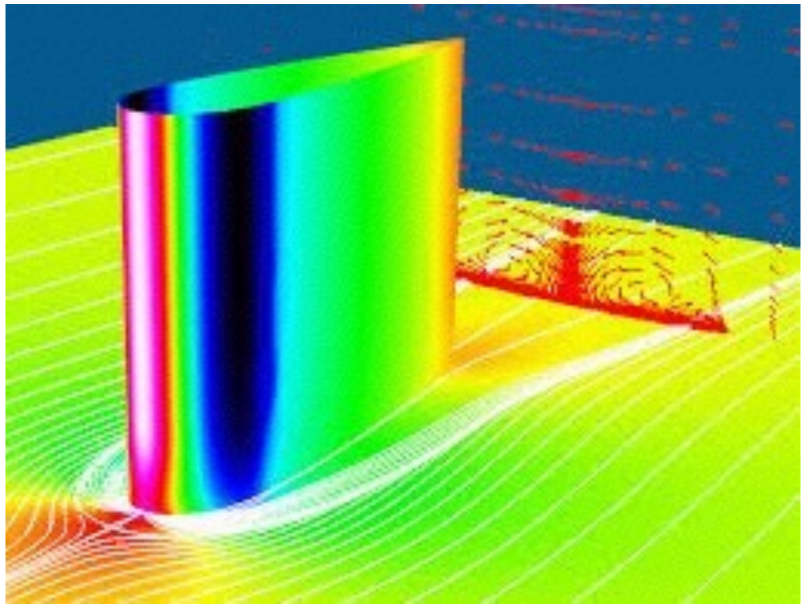
Parametric vs. Non-parametric Approaches

- + Parametric approaches are easy to implement.
- – Restricted by the model(s): e.g., Bousinessq assumption if all candidate models are EVM. Cannot explore the solution manifold outside the assumption!

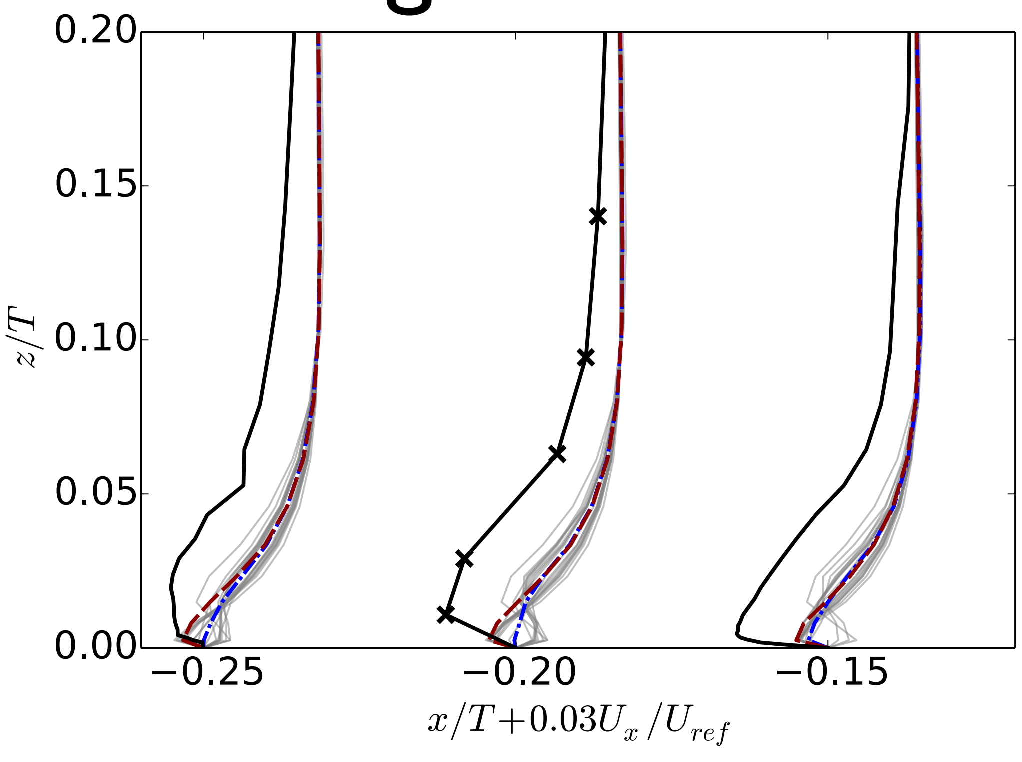


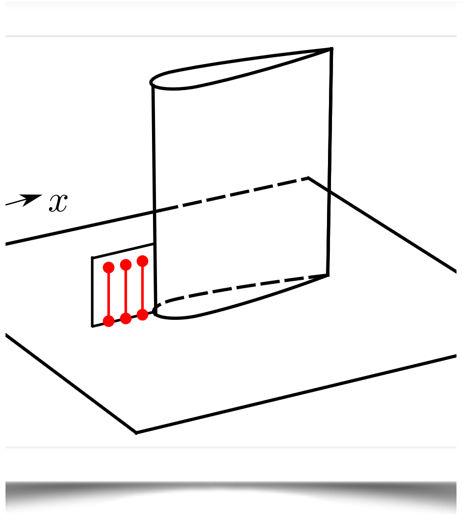
Example: Wing-Body Junction Flow

- In the leading edge region, scatter in velocity is very limited as long as the Reynolds stress is aligned with the mean rate of strain tensor **S**.

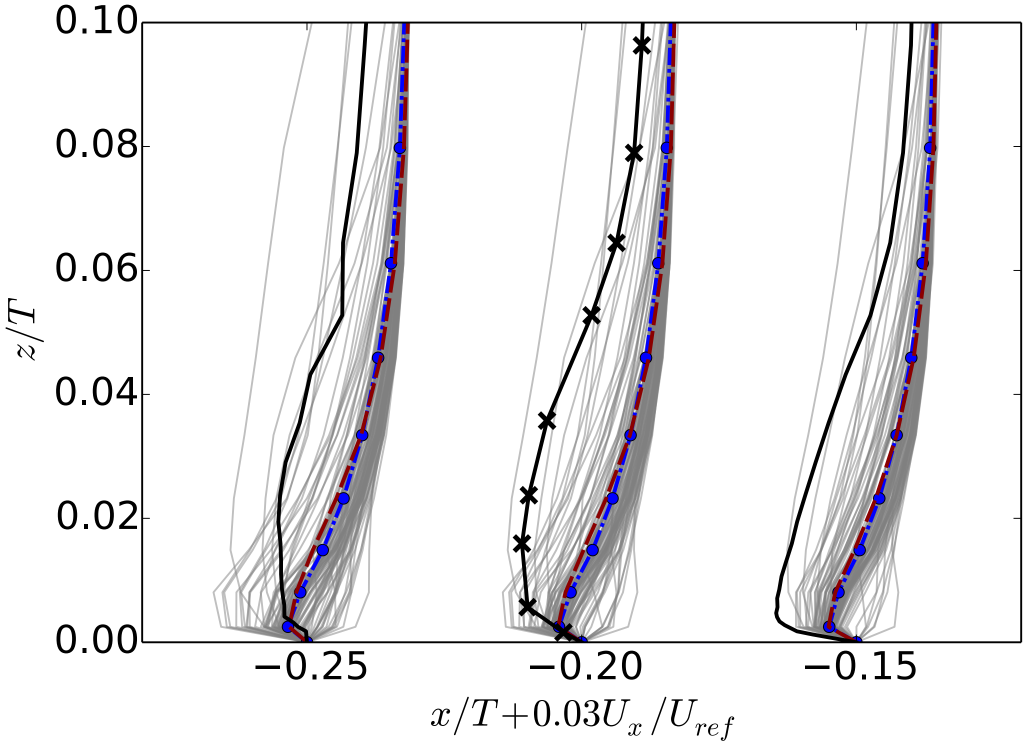


Aligned w/ S





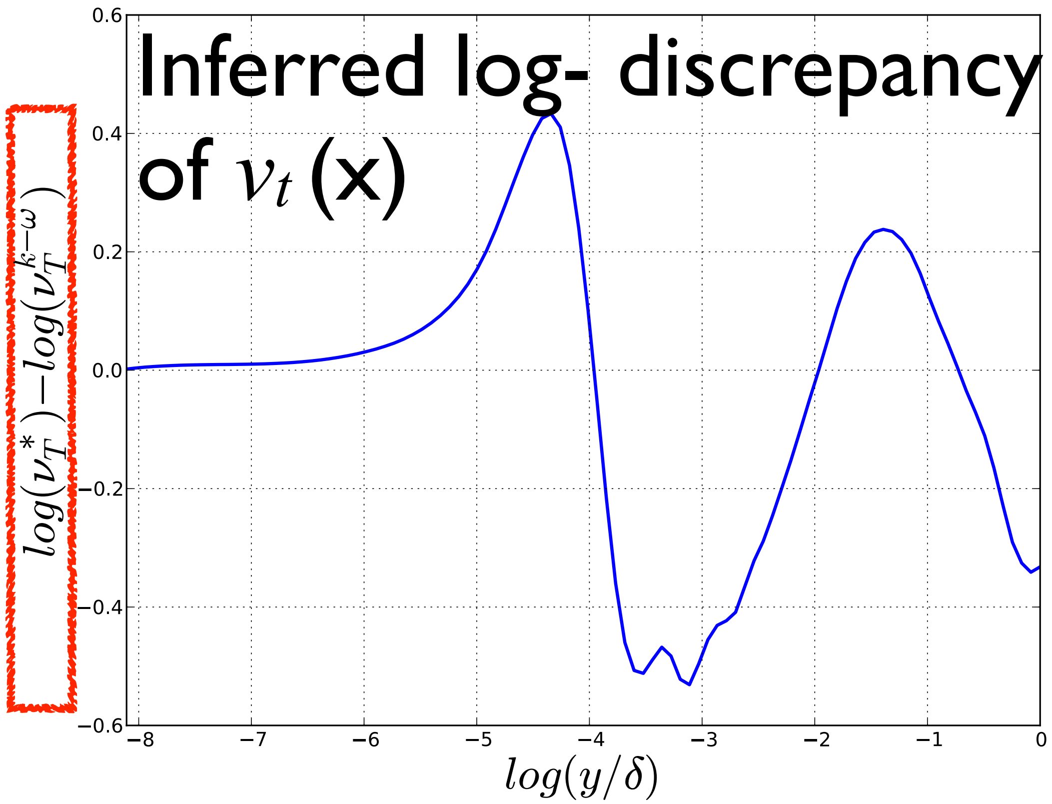
Not aligned w/ S



[6]. J.-L. Wu, J.-X. Wang, and H. Xiao. Quantifying Model Form Uncertainty in RANS Simulation of Wing–Body Junction Flow. Submitted to FTC, 2016.

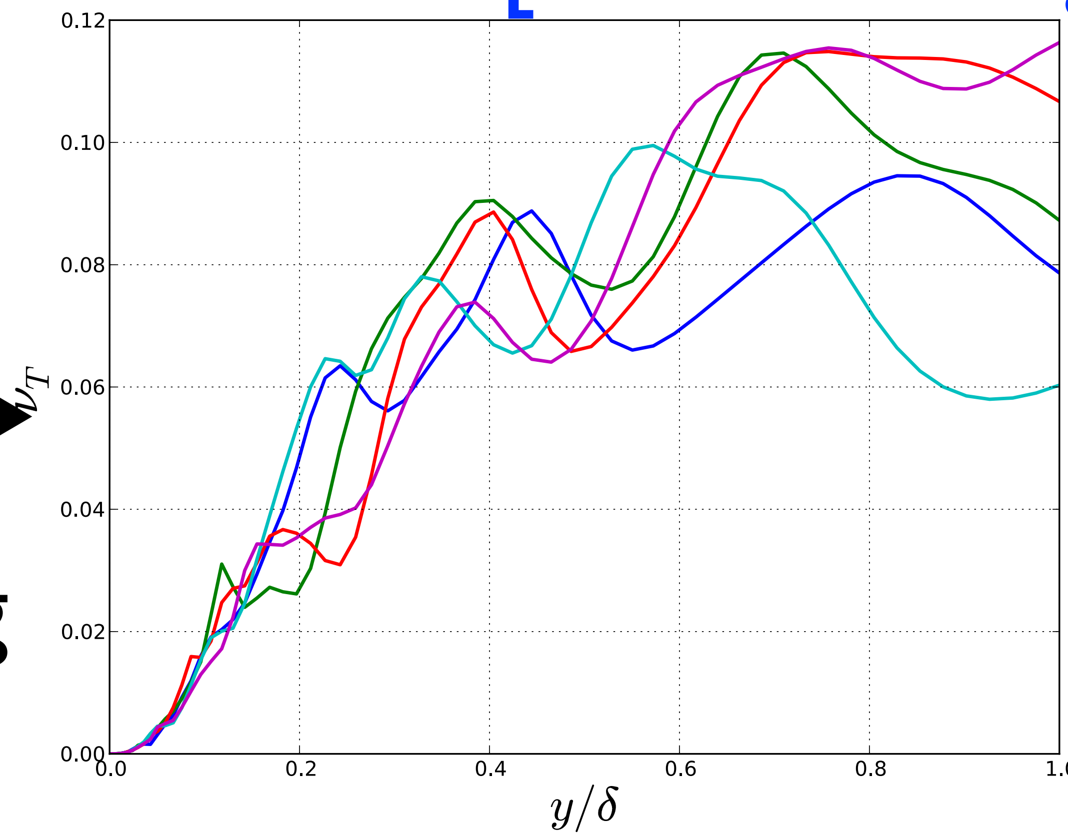
Inferring Turbulent Viscosity Field

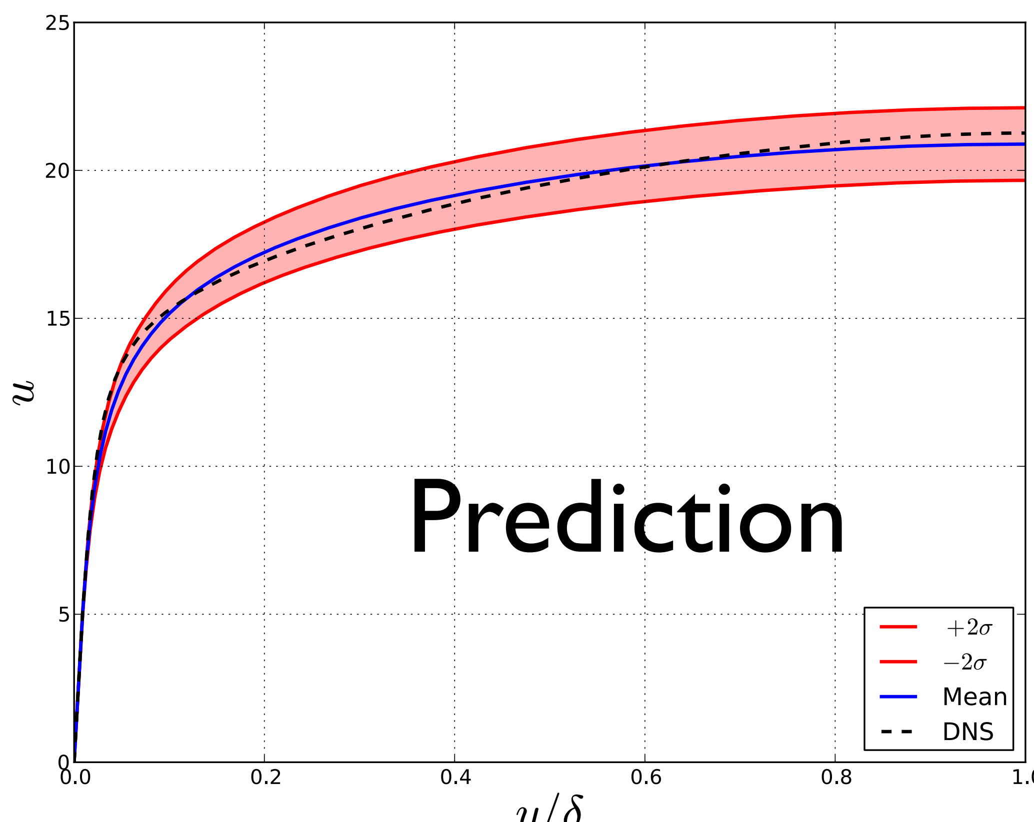
[Dow & Wang]



Gaussian Process

Sampling





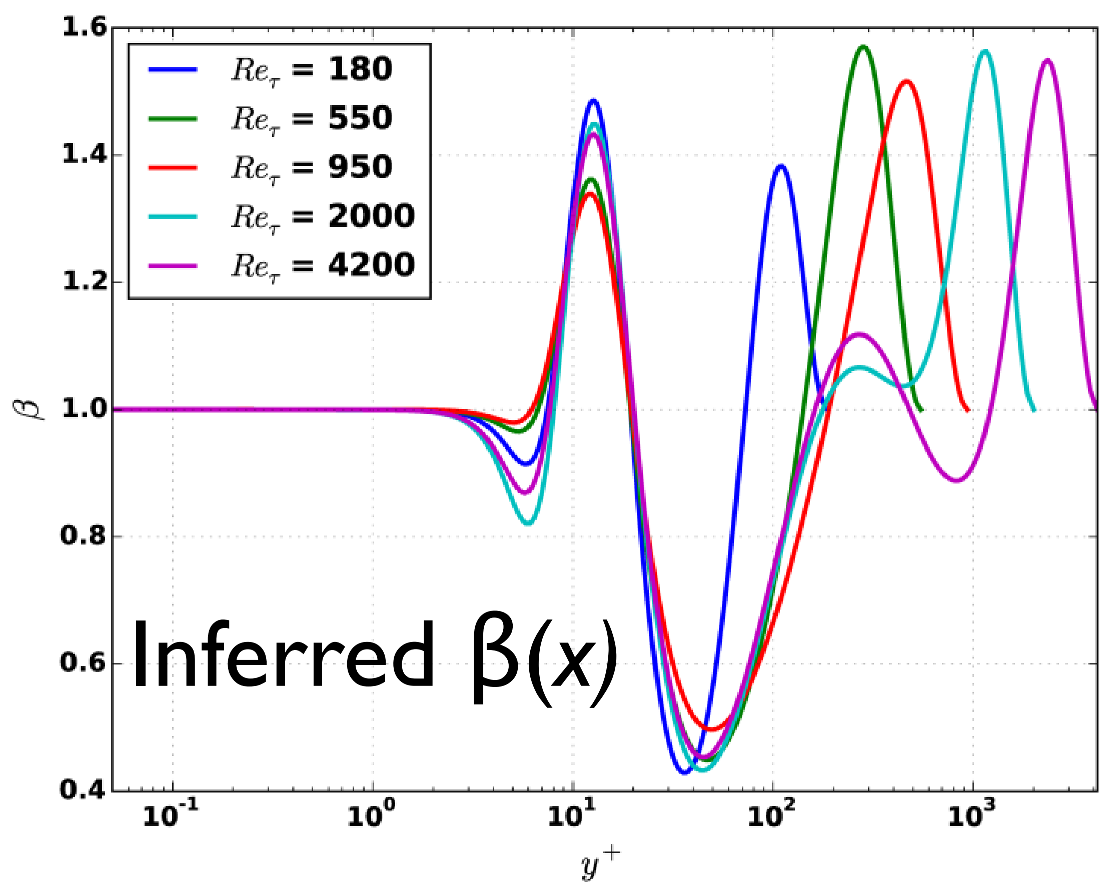
- +++ Full field inversion with adjoint model!!
- Constrained by Boussinesq assumption.
- * Uncertainty estimation (vs. reduction.)

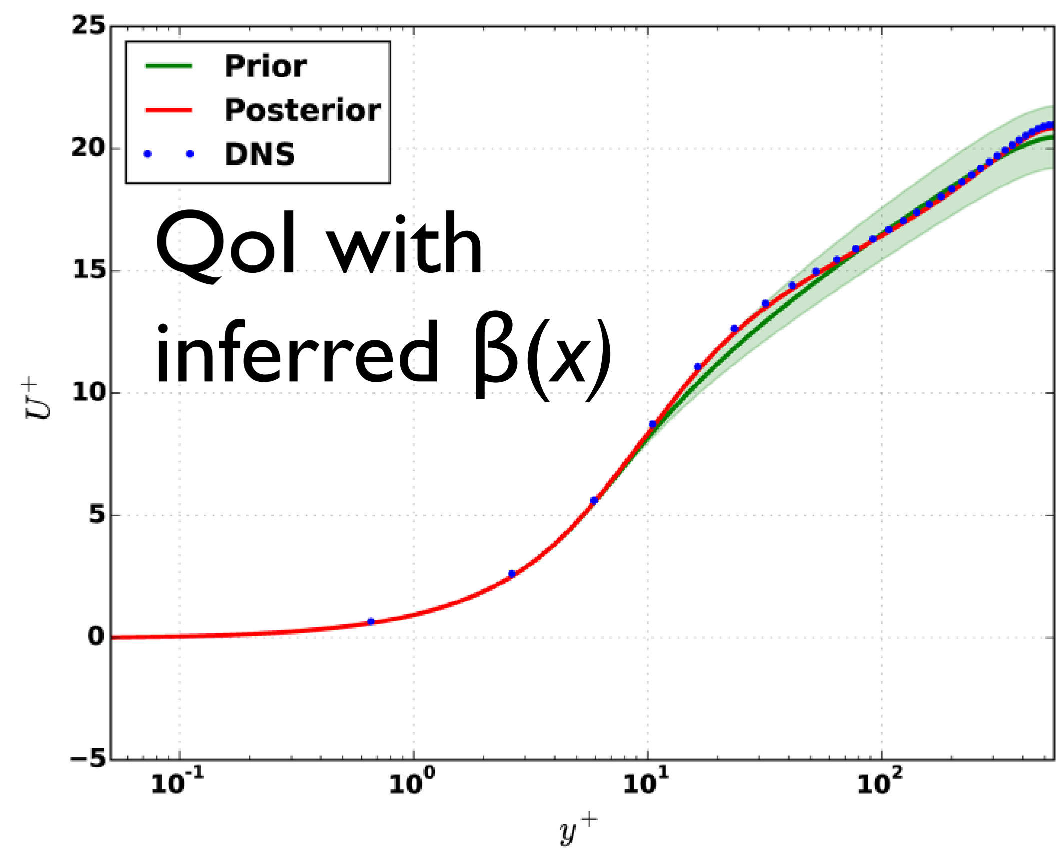
Dow & Wang, Quantification of Structural Uncertainties in the k-w Turbulence Model, AIAA 2011-1762

Inferring Discrepancy in Turb. Quantity Equations
[Duraisamy et al.]

$$\frac{D\tilde{\nu}_t}{Dt} = \boxed{\beta(x)} P(\tilde{\nu}_t, \mathbf{U}) - D(\tilde{\nu}_t, \mathbf{U}) + T(\tilde{\nu}_t, \mathbf{U})$$

$$\frac{D\omega}{Dt} = \boxed{\beta(x)} P(\omega, \mathbf{U}) - D(\omega, \mathbf{U}) + T(\omega, \mathbf{U})$$





Singh & Duraisamy. Using field inversion to quantify functional errors in turbulence closures. POF, 28, 045110, 2016.

Assessment: Novelties

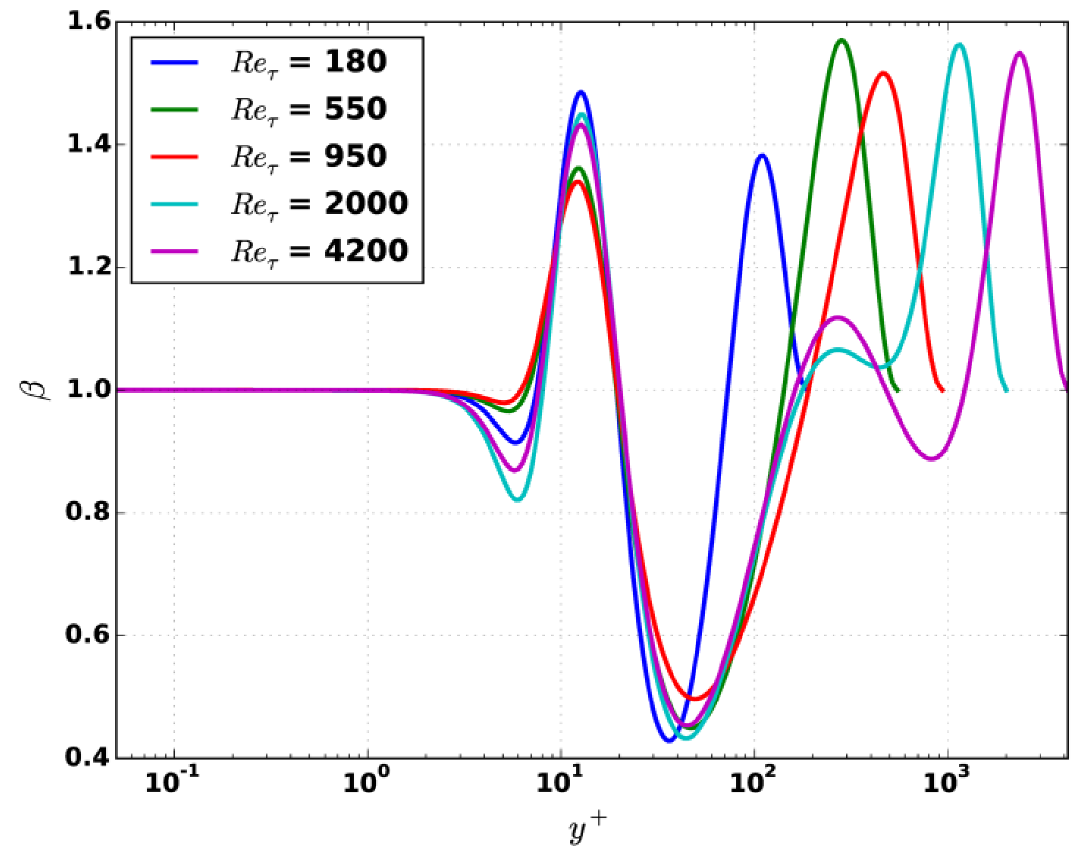
$$\frac{D\tilde{\nu}_t}{Dt} = \boxed{\beta(x)} P(\tilde{\nu}_t, \mathbf{U}) - D(\tilde{\nu}_t, \mathbf{U}) + T(\tilde{\nu}_t, \mathbf{U})$$ [Duraisamy et al.]

- +++ Bayesian: Can use integral data (e.g., surface pressure) or sparse data to infer the multiplicative correction term β(x). Then, use posterior of β(*x*) to obtain QoI (e.g., velocity).
- +++ Full field inversion! Better than parametric approaches.
- +? Model specific: different inference formulation for each model (e.g., SA, k-ω). Can be + or –. Why plus? Intimate connection with model: increases inference effectiveness!
- +? Universality of β(*x*) and extrapolation to similar flows suggested but yet to be demonstrated.
- +? Constrained by assumption of the baseline model (e.g., Boussinesq assumption) but the flexibility may be sufficient!

Assessment: Limitations

$$\frac{D\tilde{\nu}_t}{Dt} = \boxed{\beta(x)} P(\tilde{\nu}_t, \mathbf{U}) - D(\tilde{\nu}_t, \mathbf{U}) + T(\tilde{\nu}_t, \mathbf{U})$$ Duraisamy et al.

- * No physical basis to **validate or invalidate** the inferred β(**x**).
- * Different data (particularly for partial/sparse data) may give different β(**x**).
- * **Physical identifiability difficulty**: when data suggest understimated production (β > 1), it could well be overestimated dissipation, or too much transport to the neighborhood.



- ++ But: Provides valuable guidance for turbulence model development.

Injecting Uncertainty in Reynolds Stresses

RANS Equations: Composite Model Theory

- The theories are reliable (based on conservation of momentum) [Oliver, Moser, et al.]

$$\nabla \cdot (\boldsymbol{\tau}_{\mathrm{rans}})$$

$$\boxed{\frac{\partial U_i}{\partial t} + \underbrace{\frac{\partial (U_i U_j)}{\partial x_j}}_{\text{convection}} + \underbrace{\frac{1}{\rho}\frac{\partial p}{\partial x_i}}_{\text{pressure grad.}} - \nu \underbrace{\frac{\partial^2 U_i}{\partial x_j \partial x_j}}_{\text{diffusion}}} = \boxed{\underbrace{-\frac{\partial \overline{u_i u_j}}{\partial x_j}}_{\text{div. of Reynolds stress}}}$$

Mathematically rigorous/correct

Reynolds stresses need closure model

- Uncertainties are mostly caused by the closure model for the Reynolds stress.

$$\boxed{\mathcal{N}(U)} = \boxed{\nabla \cdot (\boldsymbol{\tau}_{\mathrm{rans}})}$$

with

$$\boldsymbol{\tau}_{\mathrm{rans}} = \boxed{\frac{\nu_t}{2}}(\nabla U + \nabla^t U)$$

Injecting Uncertainty in Reynolds Stresses

[Oliver, Moser et al.]

- +++ Introduce Reynolds stress discrepancy tensor to RANS equation and model with stochastic differential equation.
- The SDE is similar but simpler than RSTM equations. Driven by Wiener process (white noise).

$$\frac{d\epsilon}{d\eta} = \sigma \left(\frac{1}{Re_\tau} + \nu_t(\bar{u}^+) \right)^{3/4} \left(\frac{d\bar{u}^+}{d\eta} \right)^{5/4} \frac{dW}{d\eta}$$

channel flow

- Proof of concept in Burger's eqn. and channel flow.
- *Yet to be applied to more realistic flows.

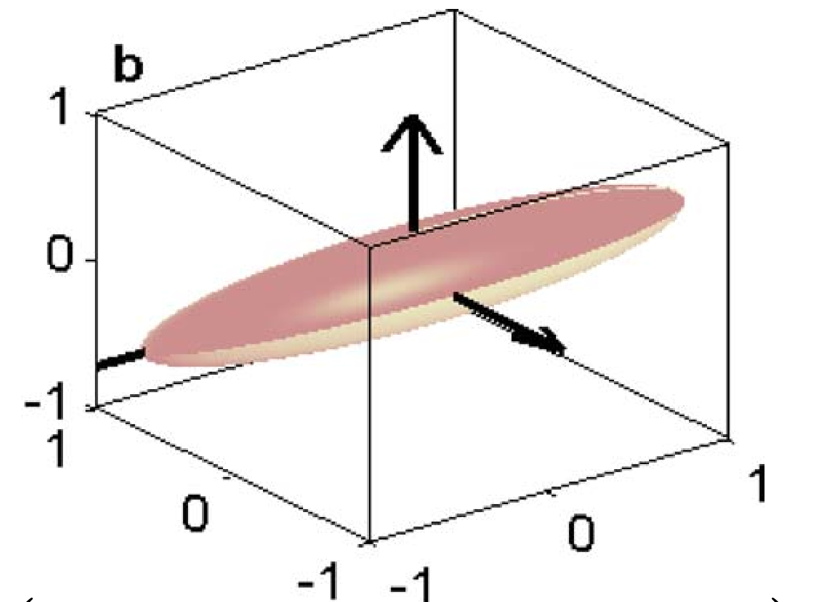
Injecting Uncertainty in Reynolds Stresses

Emory, Gorle, Iaccarino, et al.

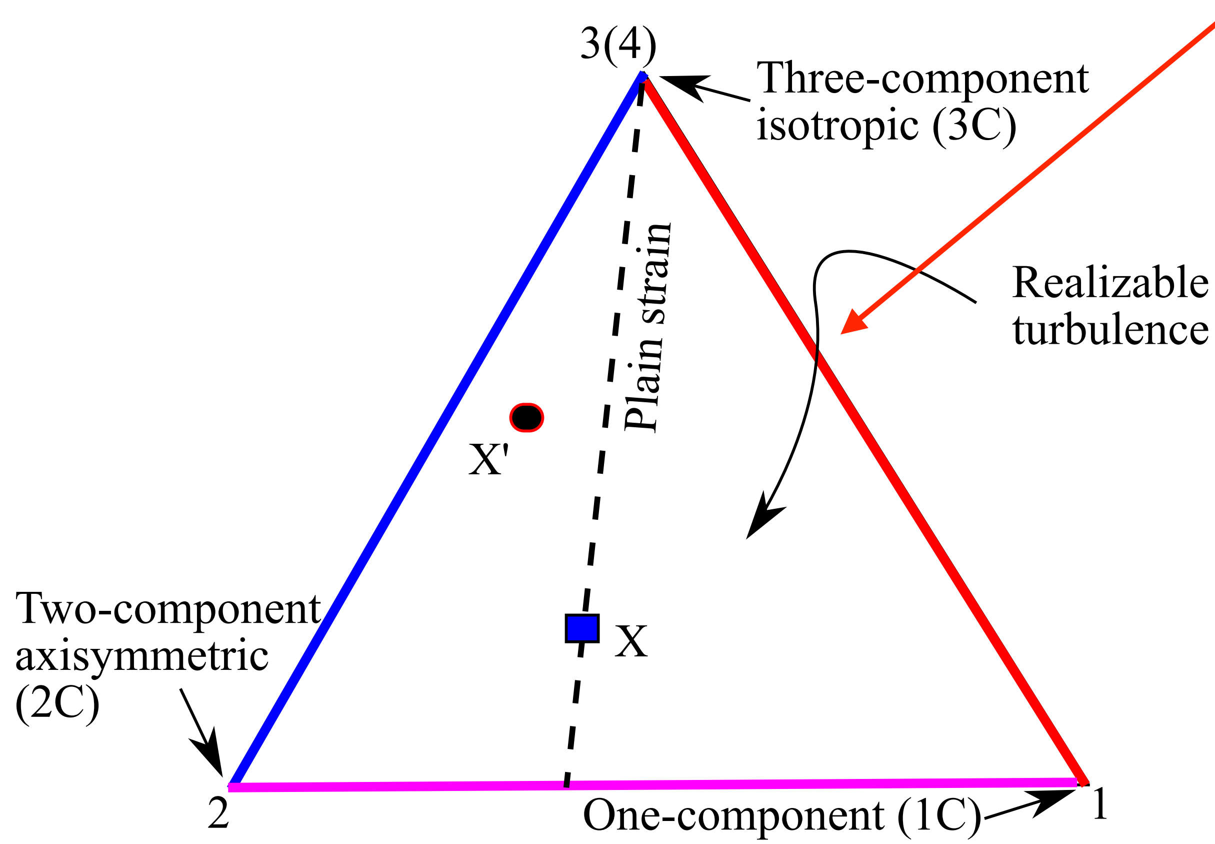
Fig. from Simonsen & Krogstad, POF 2005

- Perturb towards three limiting states in Barycentric triangle (realizability map)

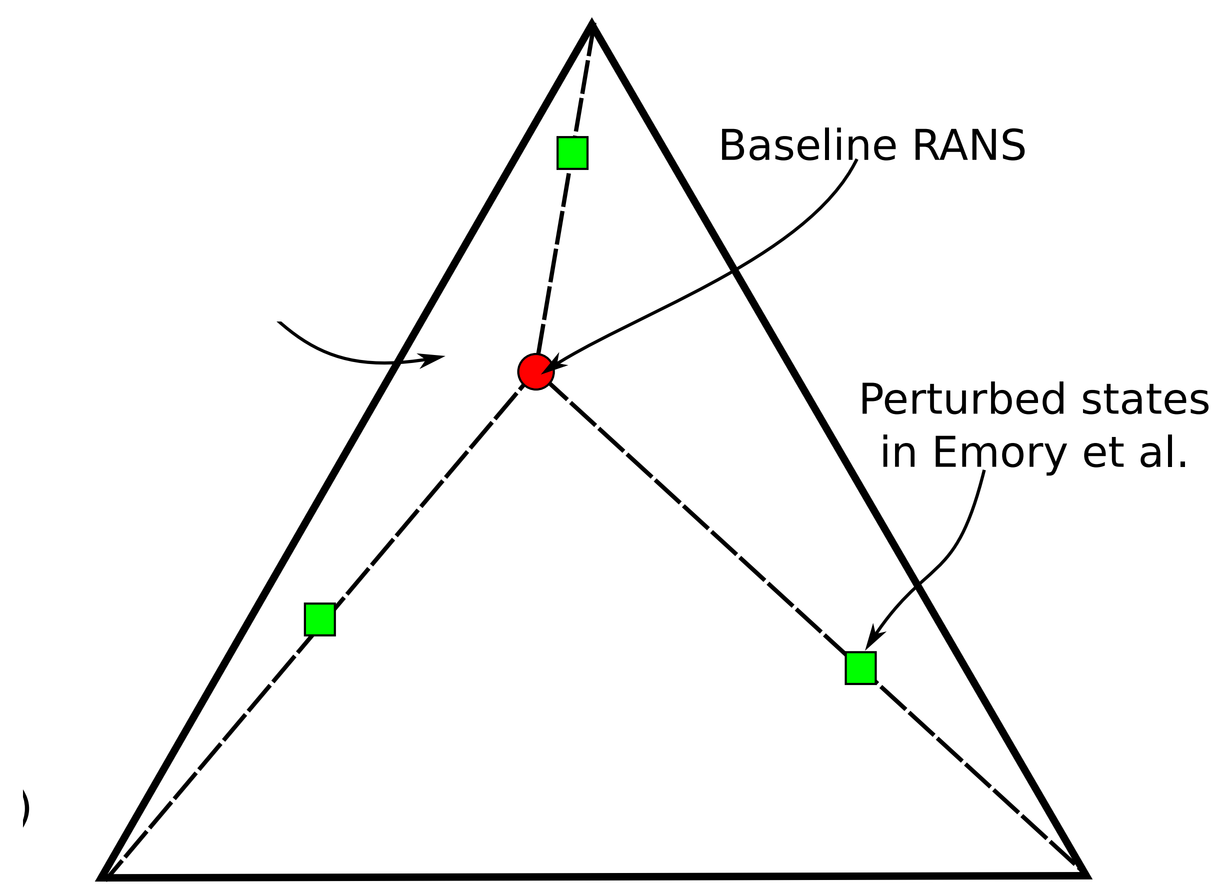
$$\boldsymbol{\tau} = 2k\left(\frac{1}{3}\mathbf{I} + \mathbf{a}\right) = 2k\left(\frac{1}{3}\mathbf{I} + \mathbf{V}\Lambda\mathbf{V}^T\right)$$



$$\boldsymbol{\tau} \longrightarrow (k, \xi, \eta, \varphi_1, \varphi_2, \varphi_3)$$



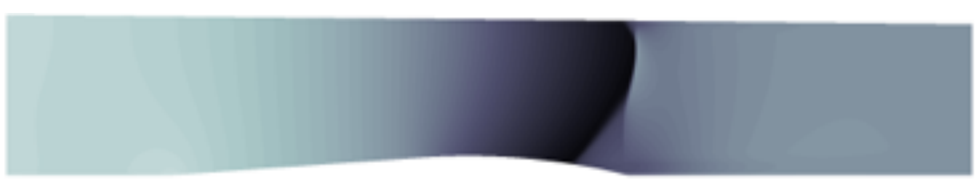
(a) Barycentric coordinate



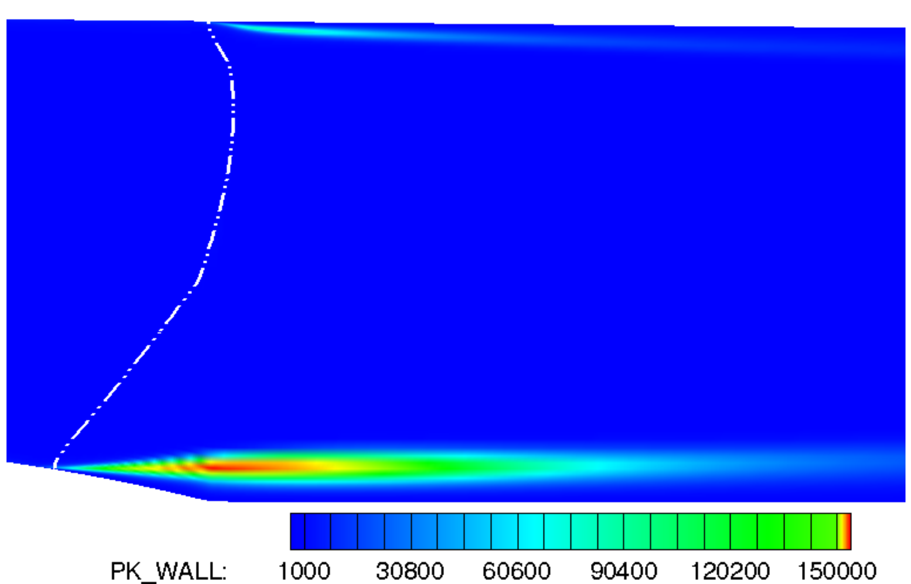
Injecting Uncertainty in Reynolds Stresses

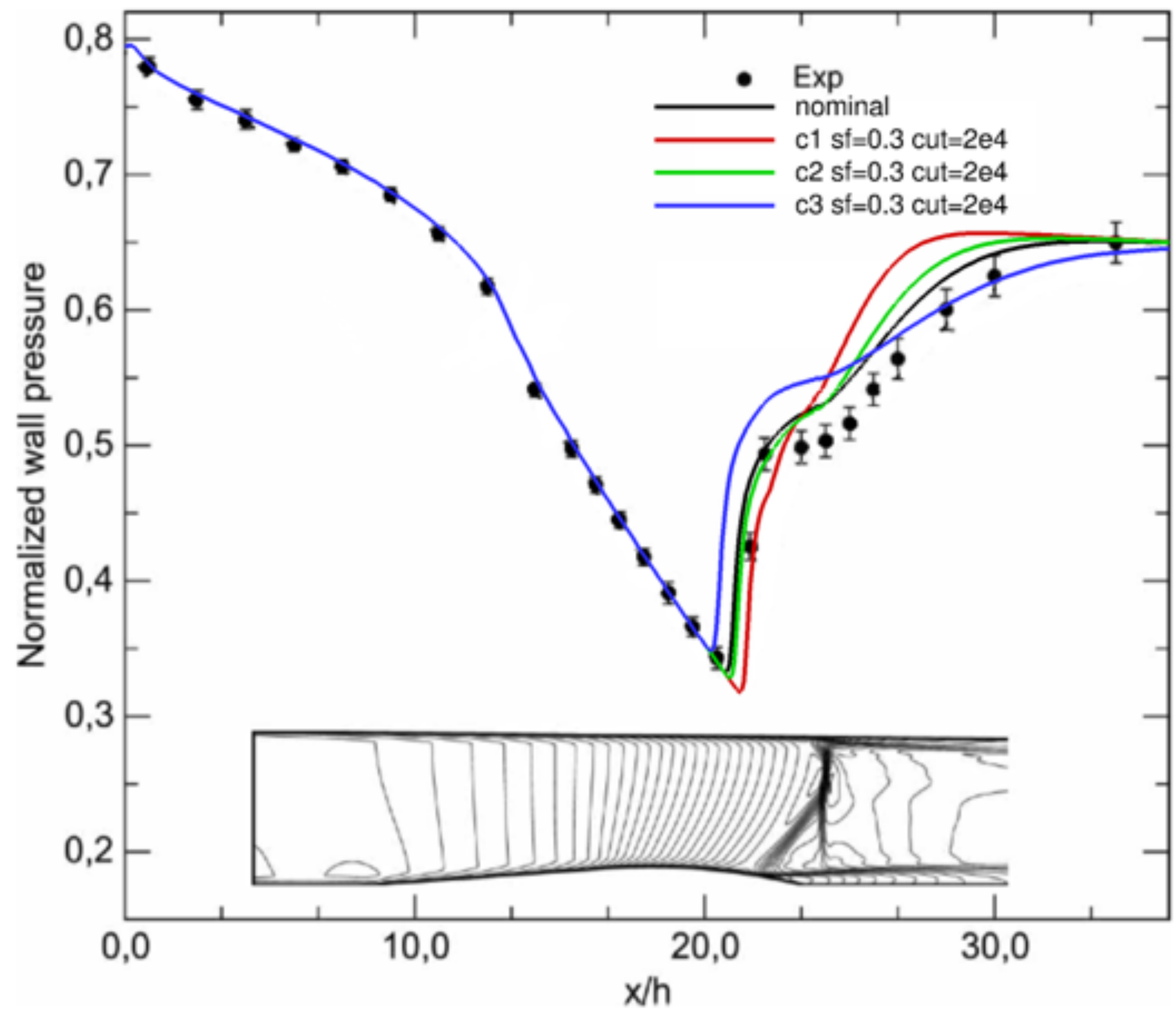
Emory, Iaccarino, et al.

- Use empirical marker function to specify the extent of perturbation towards realizable limit (vertices).
- Propagate to velocities and QoIs



Marker function





Assessment: Major Novelties

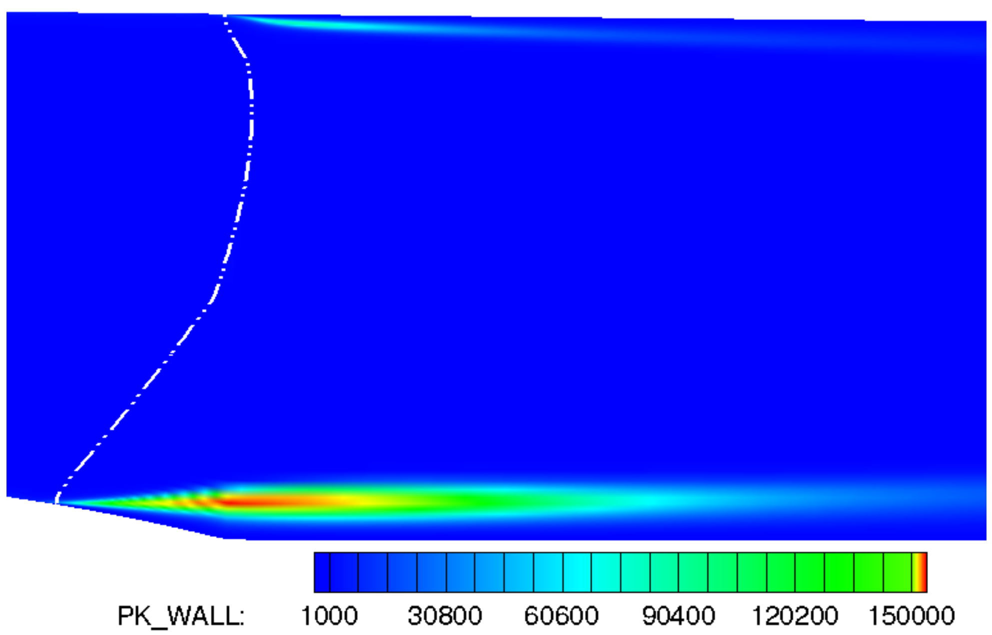
Emory, Gorle, Iaccarino, et al.

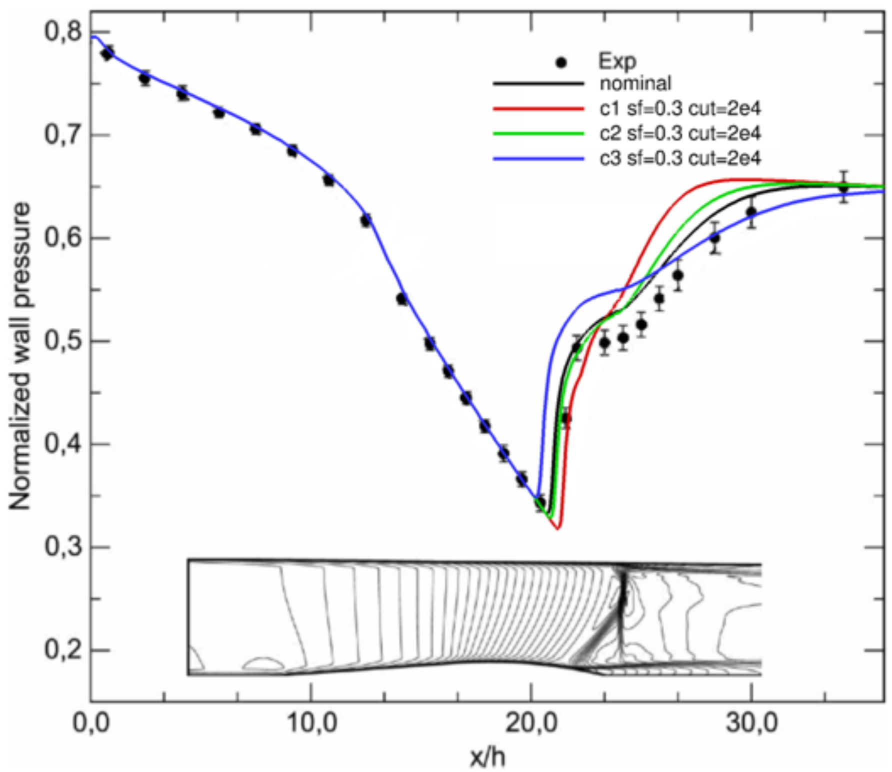
- +++ First to use realizability constraints to quantify RANS model form uncertainty (pioneering work!)
- * But: realizability only provides bound for anisotropy perturbations. Only weak constraints on TKE and orientation.
- +++ Not constrained by the Boussinesq assumption.
- +++ Directly perturb Reynolds stress: same procedure for different models.
- * Three evaluations: not a comprehensive exploration of the high dimensional uncertainty space.

Assessment: Other Minor Pros and Cons

Emory, Gorle, Iaccarino, et al.

- \+ Low computational overhead. Only three simulations needed: three perturbations; one marker function.
- – Empirical function needed for spatial distribution of the perturbations.





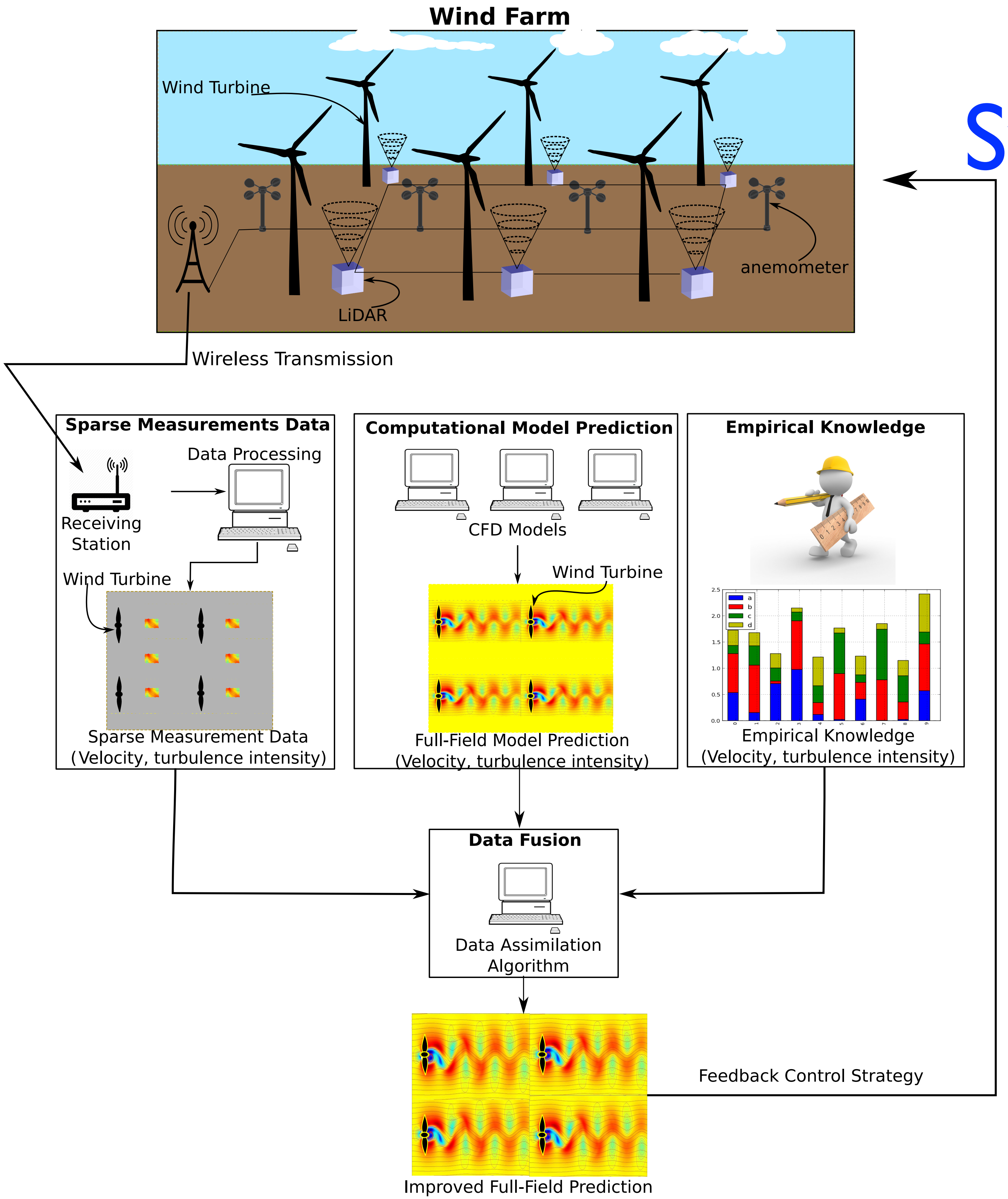
Our Approach

A Data-Driven, Physics-Informed Approach Based on Bayesian Inference

Two Scenarios of Industrial CFD Simulations

- Monitoring / Forecasting
- Support Design/Optimization

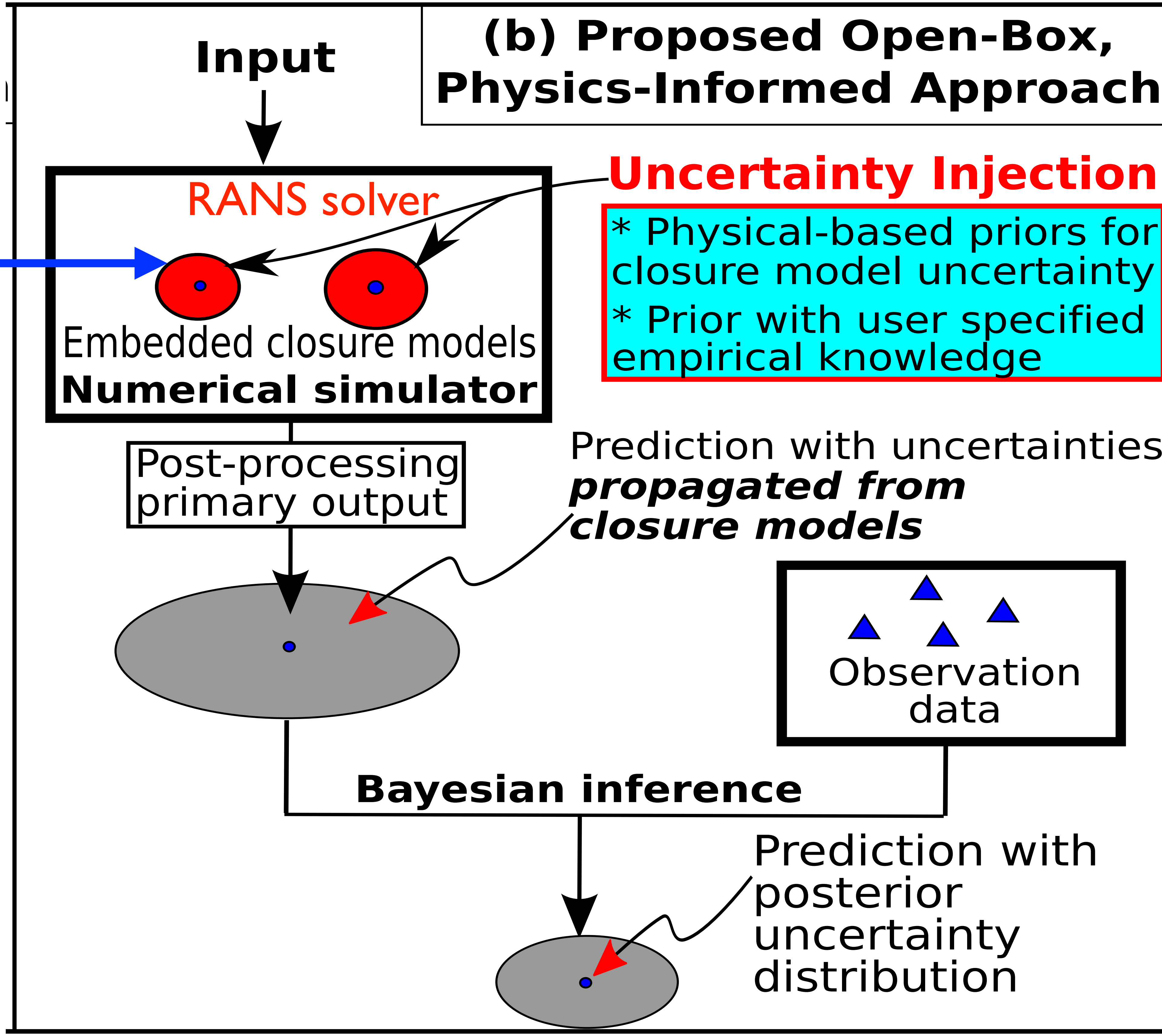
CFD to Support System Monitoring



Real-time streamed sensor data are available but are sparse

$$\mathcal{N}(U) = \nabla \cdot (\boldsymbol{\tau}_{\text{rans}} + \delta\boldsymbol{\tau})$$

Model the discrepancy as zero mean random field.

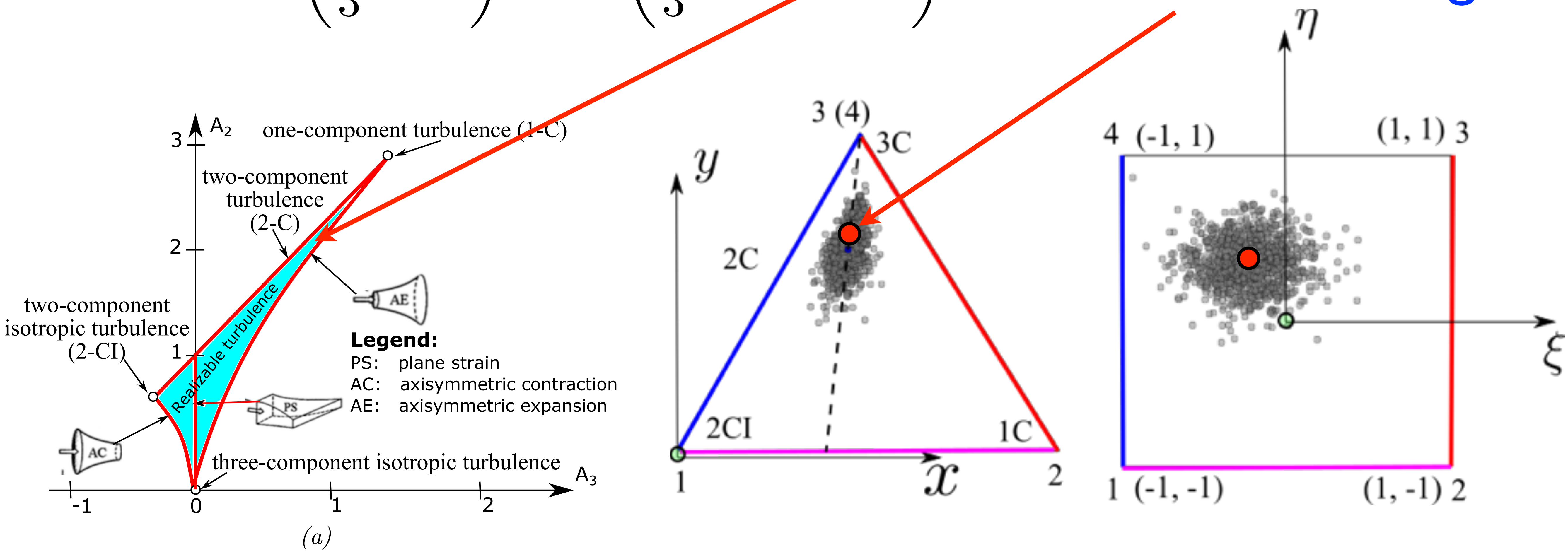


What do we know about Reynolds stresses?

- Symmetric tensor field with physical realizability **constraints**:

$$\boldsymbol{\tau} = 2k\left(\frac{1}{3}\mathbf{I} + \mathbf{a}\right) = 2k\left(\frac{1}{3}\mathbf{I} + \mathbf{V}\Lambda\mathbf{V}^T\right)$$

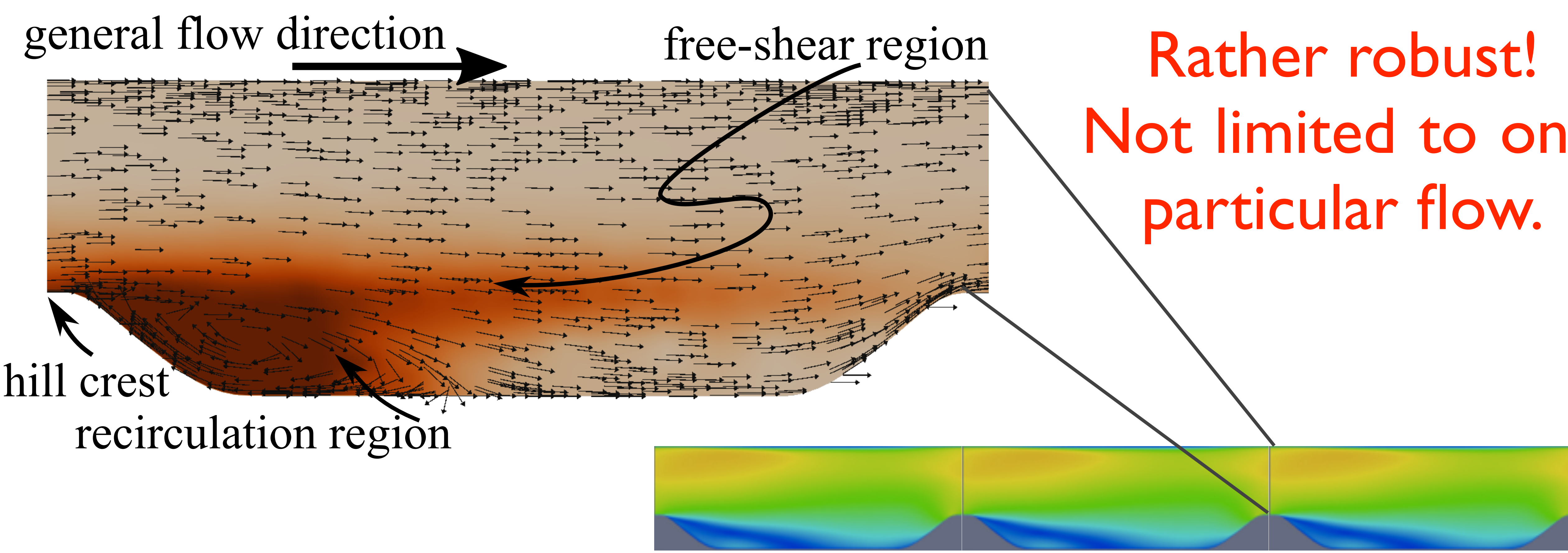
Inject uncertainty only in the realizable range



References: M. Emory, R. Pecnik, G. Iaccarino, AIAA 2011; C. Gorle, G. Iaccarino, POF 2013; M. Emory, J. Larsson, G. Iaccarino, POF 2013;

What do we know about Reynolds stresses?

- Reynolds stress field (and its discrepancies) are smooth, with length scales comparable to the length scale of the mean flow features.
- Certain regions are more problematic for RANS models: separation, mean flow curvature, adverse pressure gradient etc.



Rather robust!
Not limited to one particular flow.

Physics Based Prior: Summary

Perform RANS baseline simulation:

$$\boldsymbol{\tau} \rightarrow (k, \lambda_1, \lambda_2) \rightarrow (k, C_1, C_2) \rightarrow (k, \xi, \eta)$$

truth — RANS prediction — discrepancy

$$\boxed{\begin{aligned} k(x) \\ \xi(x) \\ \eta(x) \end{aligned}} = \boxed{\begin{aligned} \tilde{k}^{rans}(x) \\ \tilde{\xi}^{rans}(x) \\ \tilde{\eta}^{rans}(x) \end{aligned}} \begin{aligned} &\boxed{\exp[\delta^k(x)]} \\ &+\boxed{\delta^\xi(x)} \\ &+\boxed{\delta^\eta(x)} \end{aligned}$$

$$\delta^k(x, \theta^k) = \sum_{i=1}^{\infty} \omega_i^k|_{\theta^k}\ \phi_i(x)$$

$$\delta^\xi(x, \theta^\xi) = \sum_{i=1}^{\infty} \omega_i^\xi|_{\theta^\xi}\ \phi_i(x)$$

$$\delta^\eta(x, \theta^\eta) = \sum_{i=1}^{\infty} \omega_i^\eta|_{\theta^\eta}\ \phi_i(x)$$

basis functions

Reynolds stress field is parameterized with a small number of coefficients:

$$\boldsymbol{\omega} \equiv [\omega_1^k,\ \omega_1^\xi,\ \omega_1^\eta,\ \omega_2^k,\ \omega_2^\xi,\ \omega_2^\eta,\ \cdots\ ,\ \omega_m^k,\ \omega_m^\xi,\ \omega_m^\eta]$$

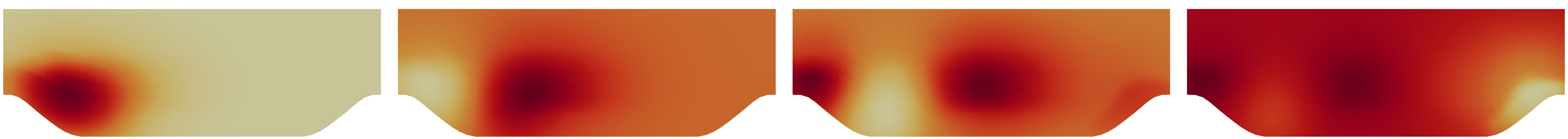
Physics Based Dimension Reduction!

Modes and Realizations of Discrepancy

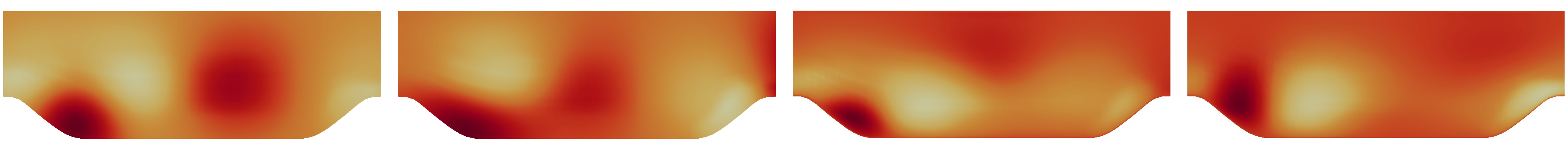
- The prior is modeled as a Gaussian process:

$$K(x, x') = \sigma(x)\sigma(x') \exp\left(-\frac{|x - x'|^2}{l^2}\right)$$

- Basis functions are obtained with Karhunen-Loeve expansion. **The prior knowledge is encoded in the basis functions.**

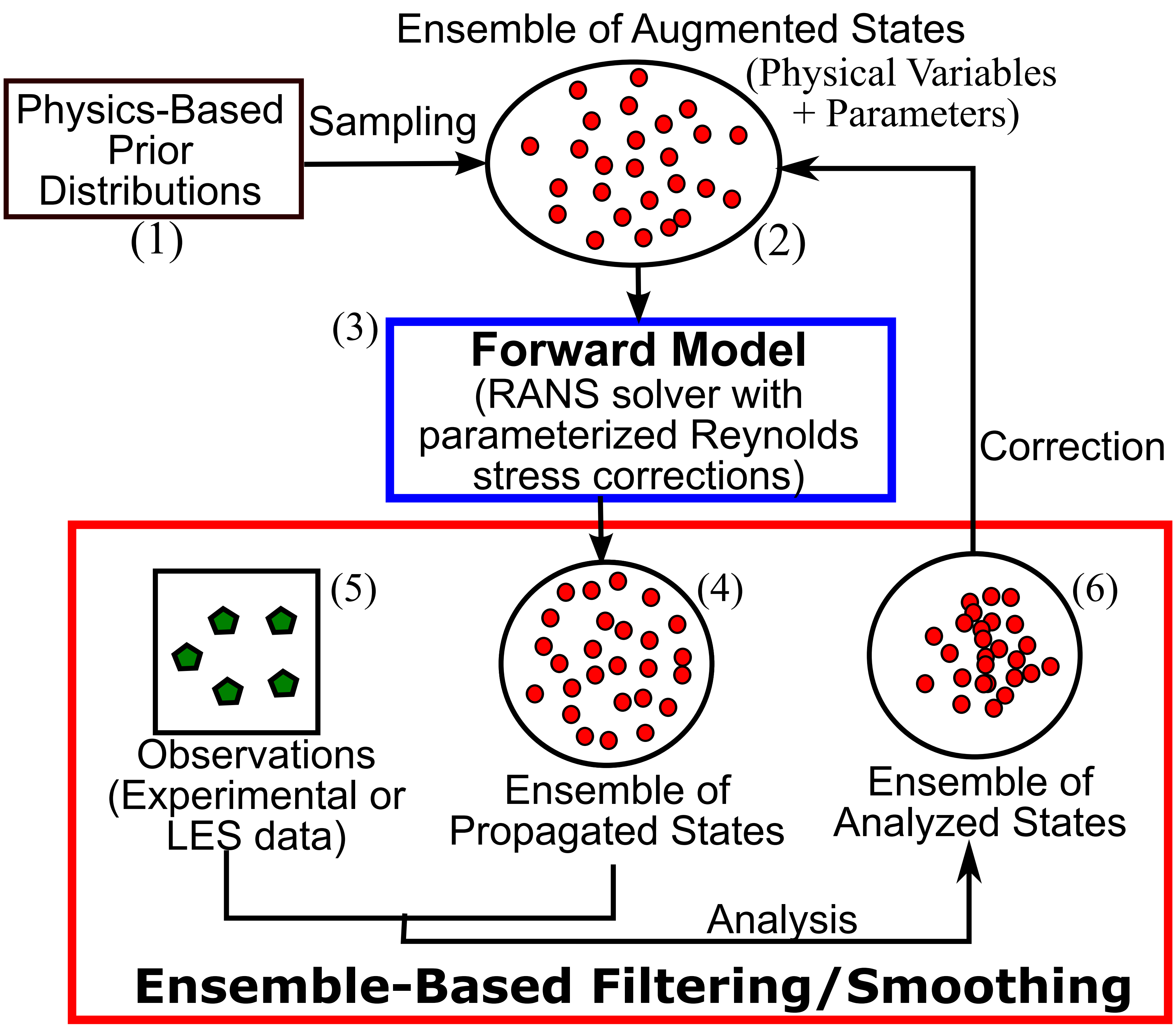


(a) mode 1 (b) mode 2 (c) mode 3 (d) mode 4



(e) mode 5 (f) mode 6 (g) realization 1 (h) realization 2

Summary of the UQ Algorithm



M. A. Iglesias, K. J. Law, A. M. Stuart, Ensemble Kalman methods for inverse problems, Inverse Problems 29 (4) (2013) 045001.

Simple Model (standard RANS models)

+

Sparse Data (velocity observations)

+

Physics-Based Prior Knowledge

=

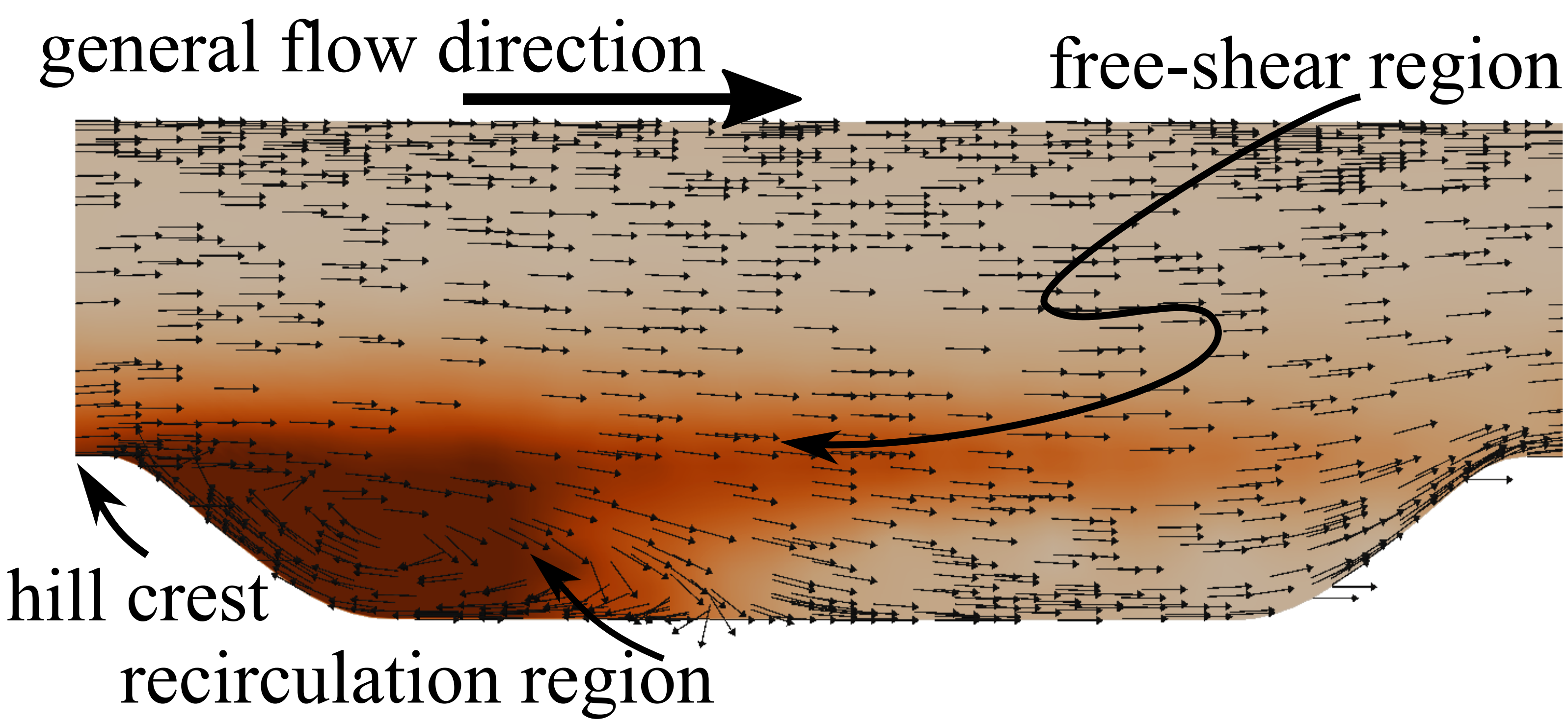
Predictions

(better than advanced models)

with quantified uncertainties

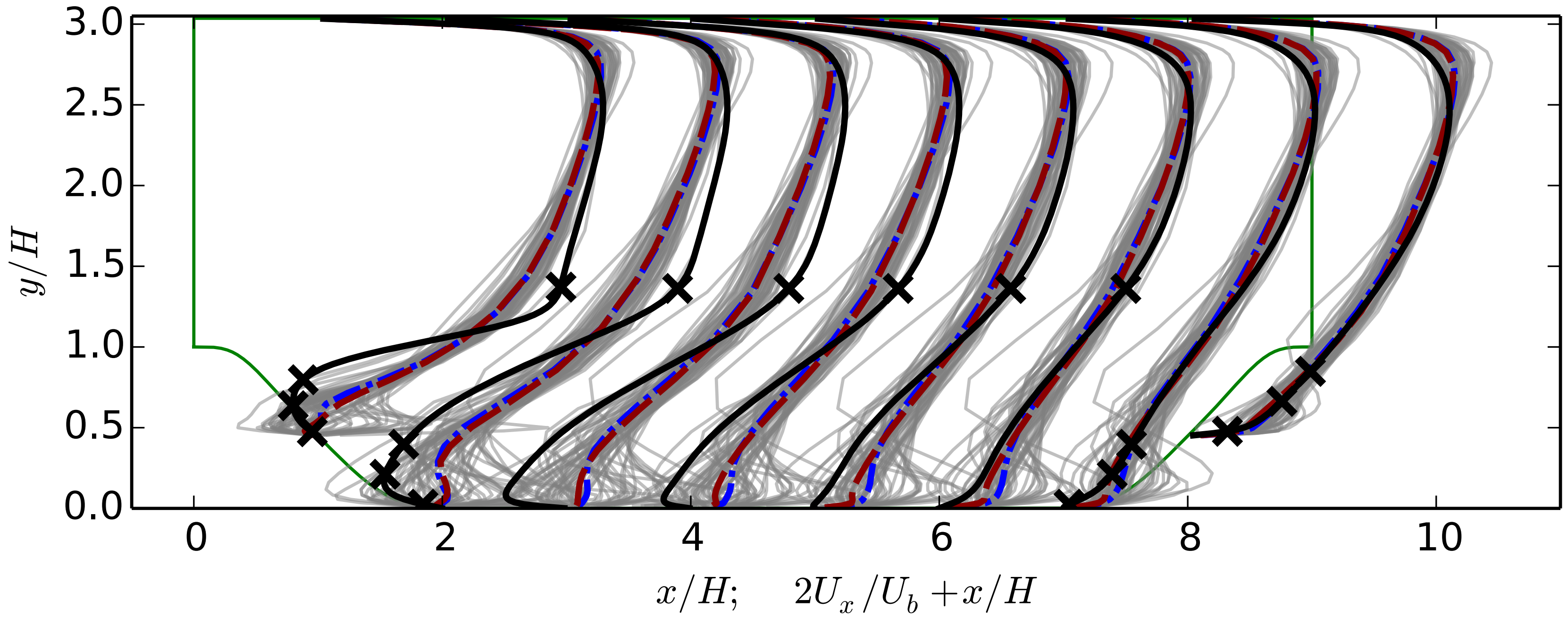
[1]. H. Xiao, J.-L. Wu, J.-X. Wang, R. Sun, and C. J. Roy. Quantifying and reducing model-form uncertainties in Reynolds averaged Navier-Stokes equations: An open-box, physics-based, Bayesian approach. Submitted to JCP, 2015.

Test Case 1:
Flow Over Periodic Hills



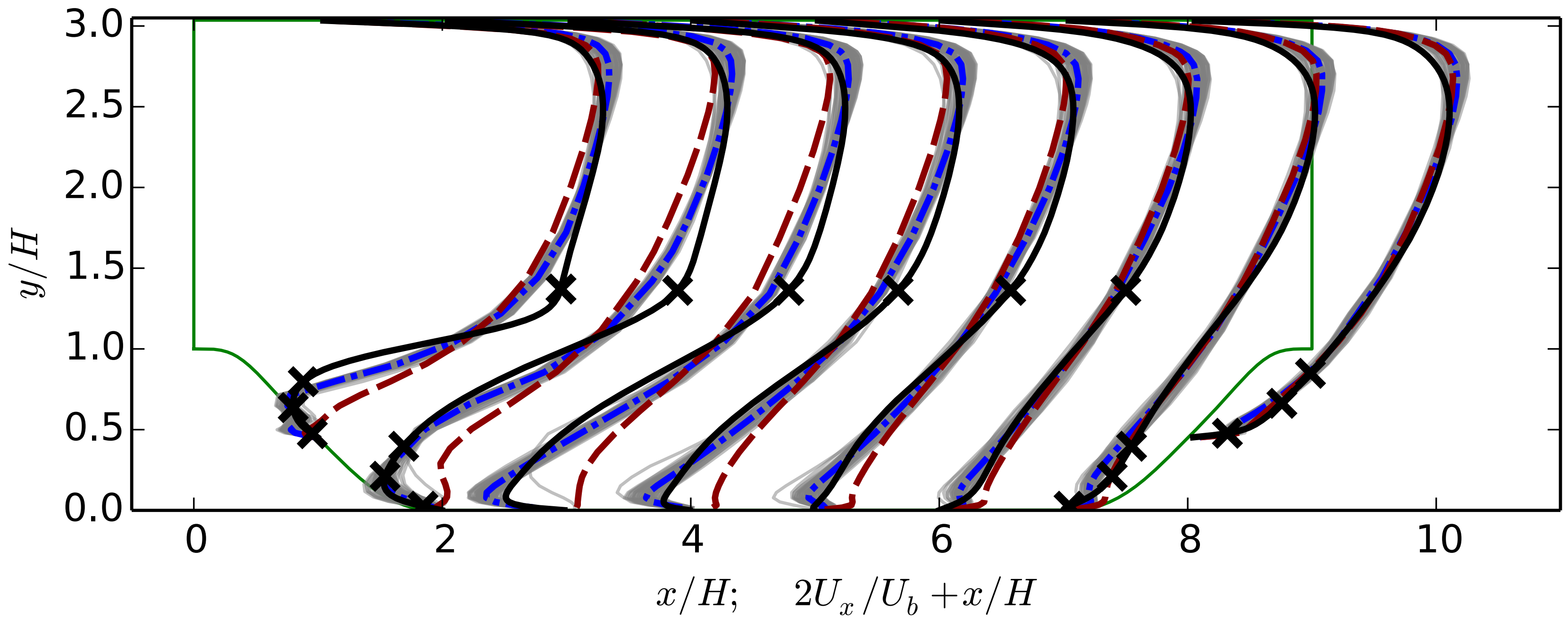
Shown previously.

Prior and Posterior Velocities



(a) Prior velocities ensemble

Prior



(b) Posterior velocities ensemble

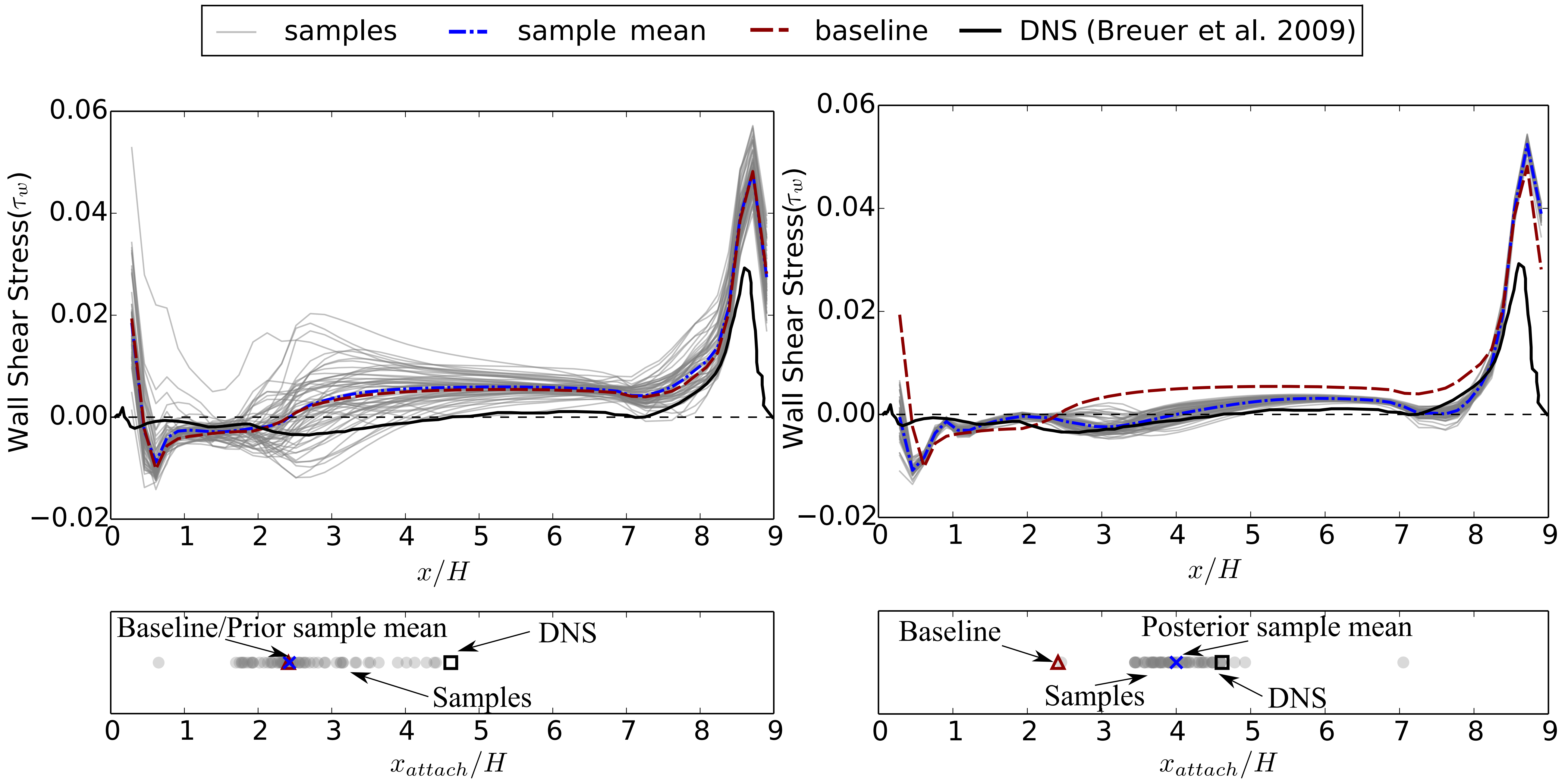
Posterior

samples sample mean baseline

DNS × × observations

Prior and Posterior of Other QoIs

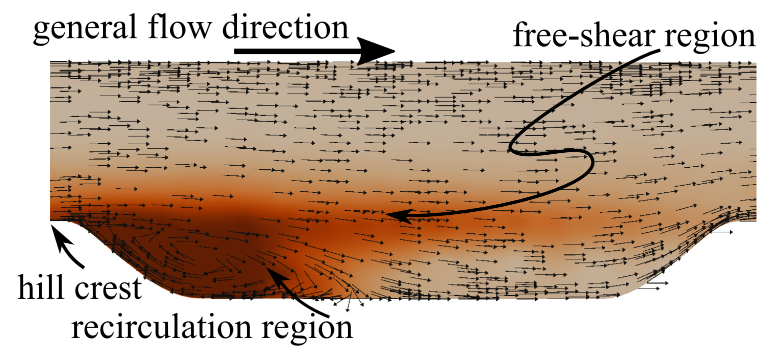
QoIs: Shear stress on bottom wall; reattachment point (obtained by post-processing of velocity field)



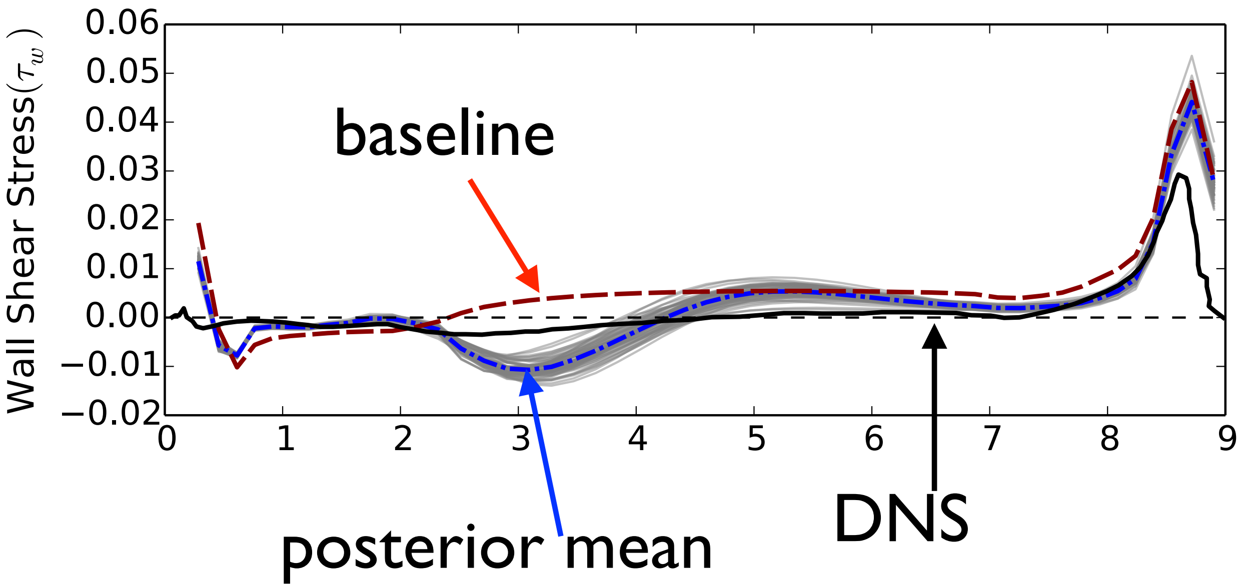
(a) Prior ensemble (b) Posterior ensemble

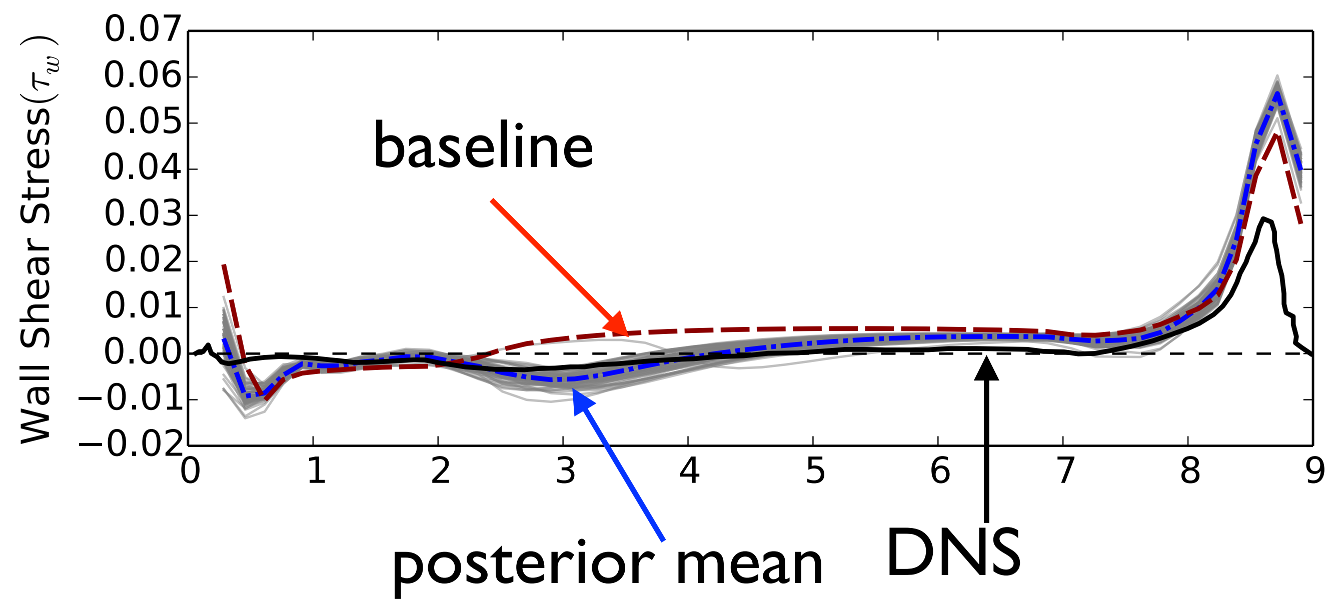
Effects of Physical Prior Knowledge

- Prior knowledge helps improving results. (Wang et al. 2015)
- It is easy to incorporate prior knowledge in the current framework, even for those empirical, imprecise experiences in engineering.

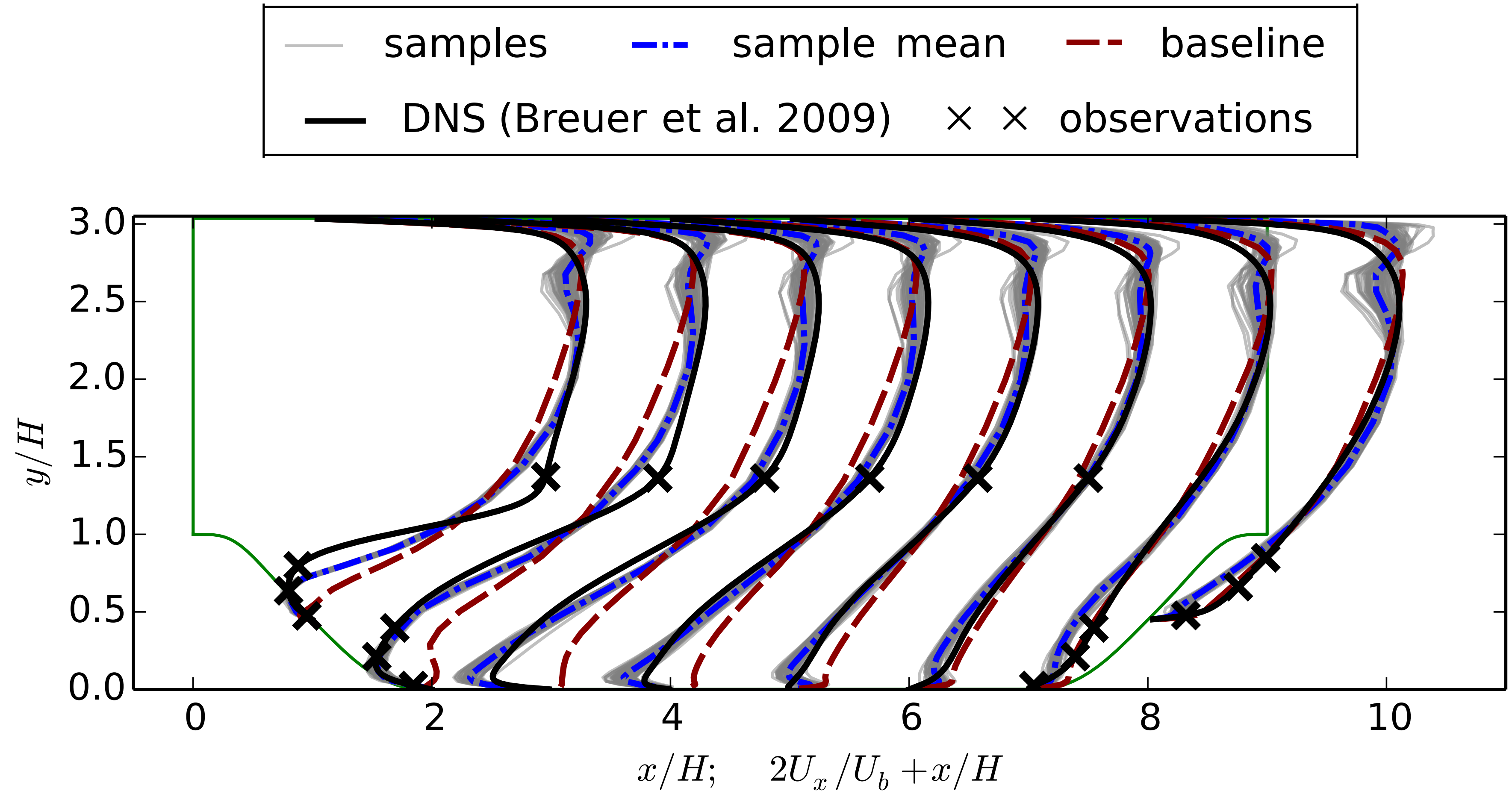


Constant variance
(no prior knowledge)

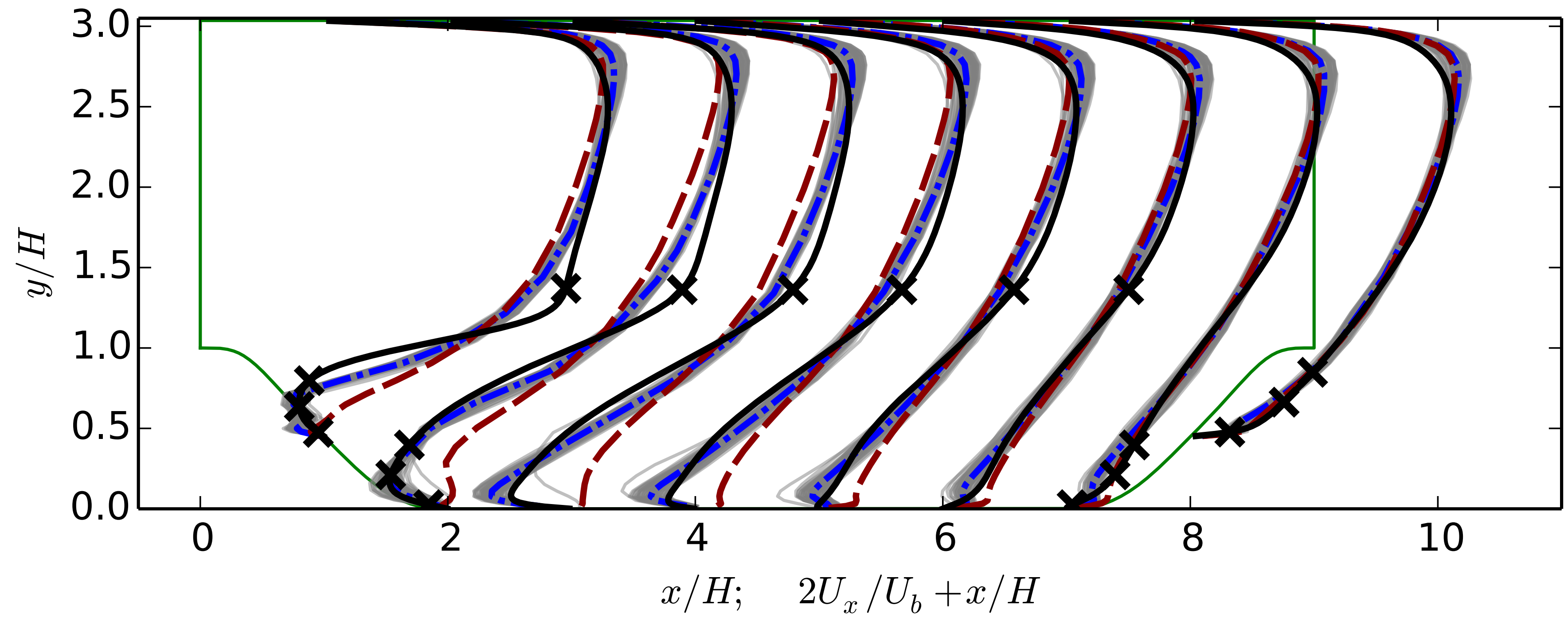




[2] J.-X. Wang, J.-L. Wu, and H. Xiao. Incorporating prior knowledge for quantifying and reducing model-form uncertainty in RANS simulations. Submitted to IJUQ, November, 2015.

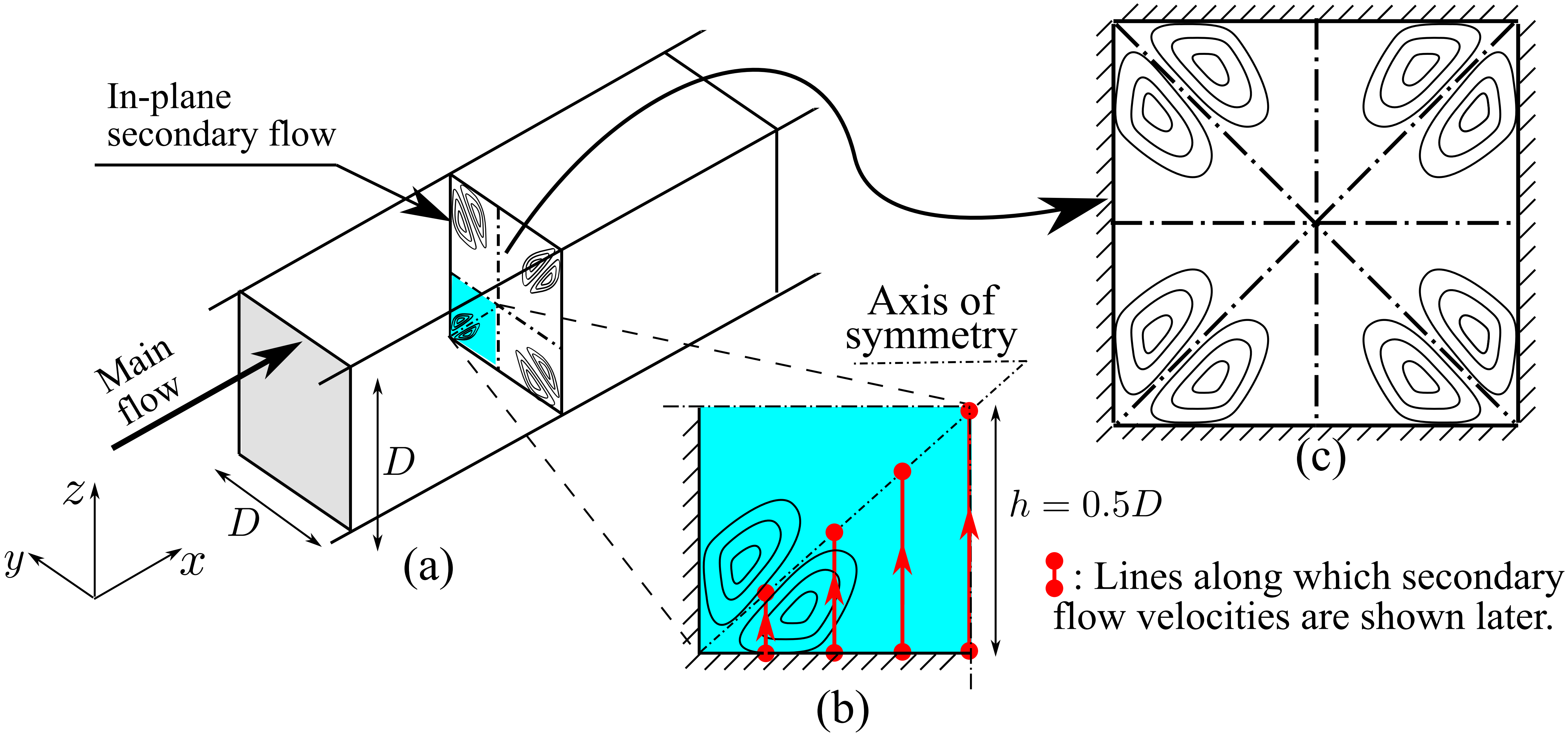


(a) U_x with non-informative $\sigma(x)$



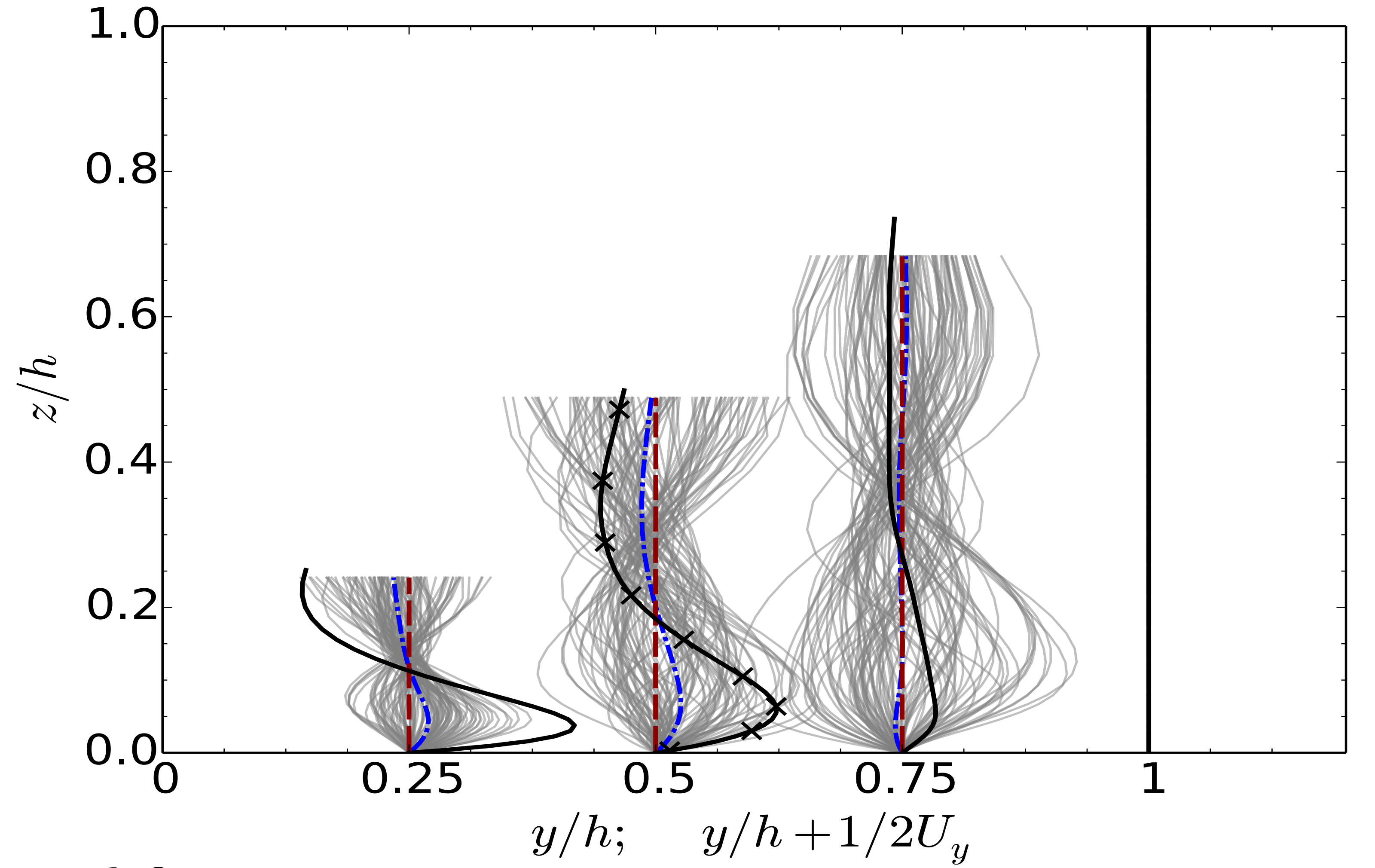
(b) U_x with informative $\sigma(x)$

Test Case II: Flow in a Square Duct



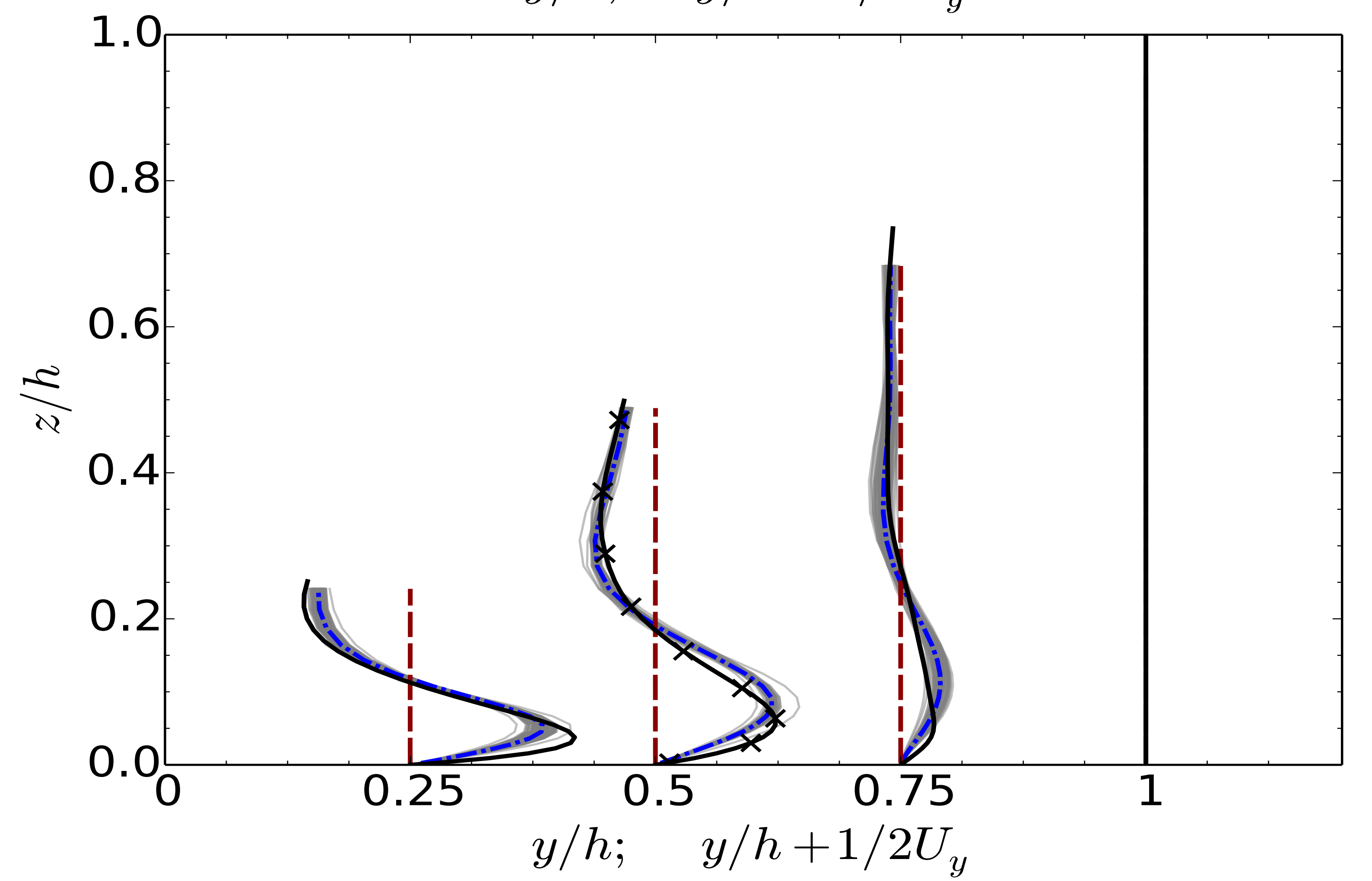
The flow features in-plane secondary flow vortexes, which cannot be predicted by standard RANS models.

Prior In-plane velocity:



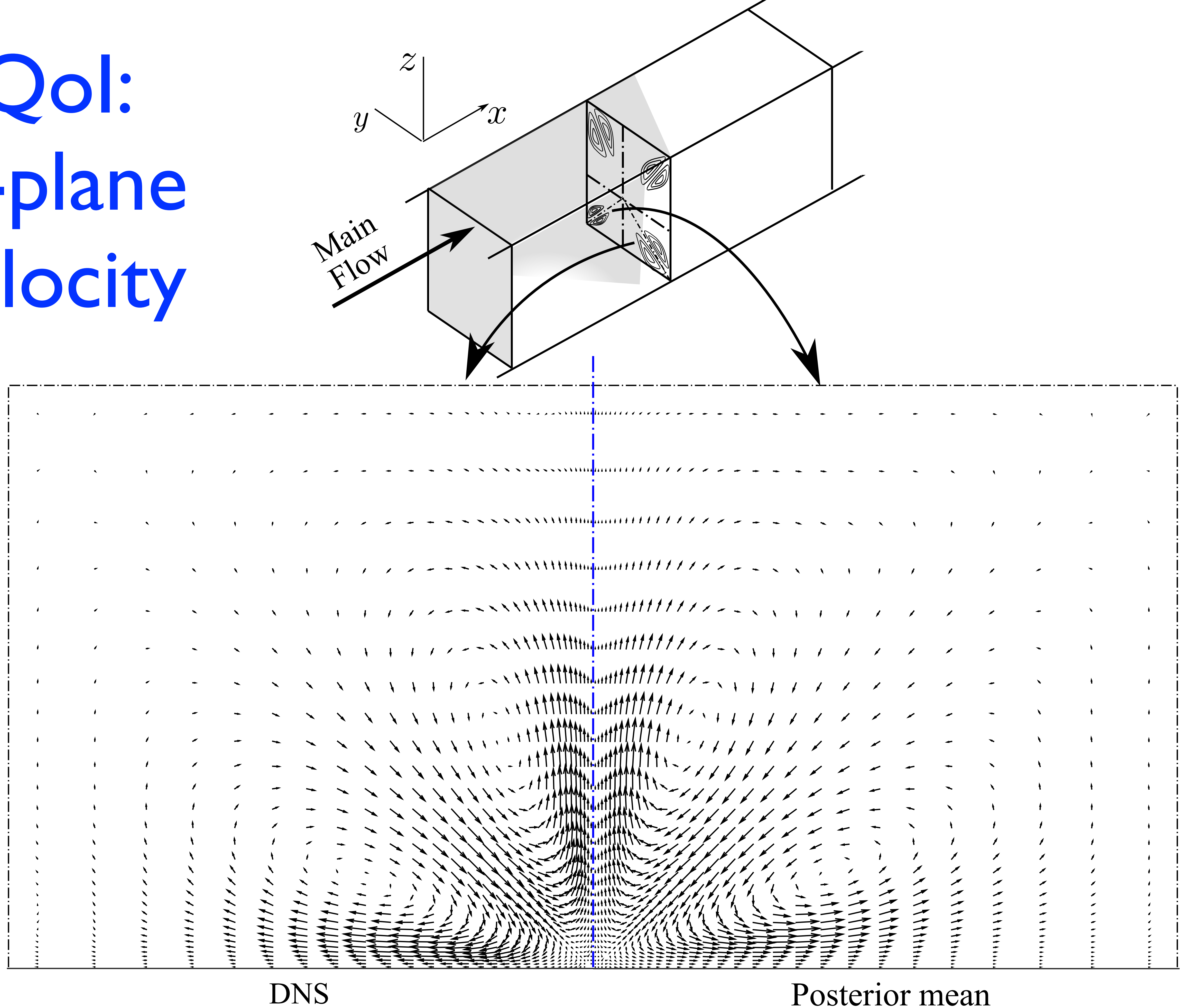
Black: DNS
Red: Baseline RAN
Blue: sample mean

Posterior In-plane velocity:

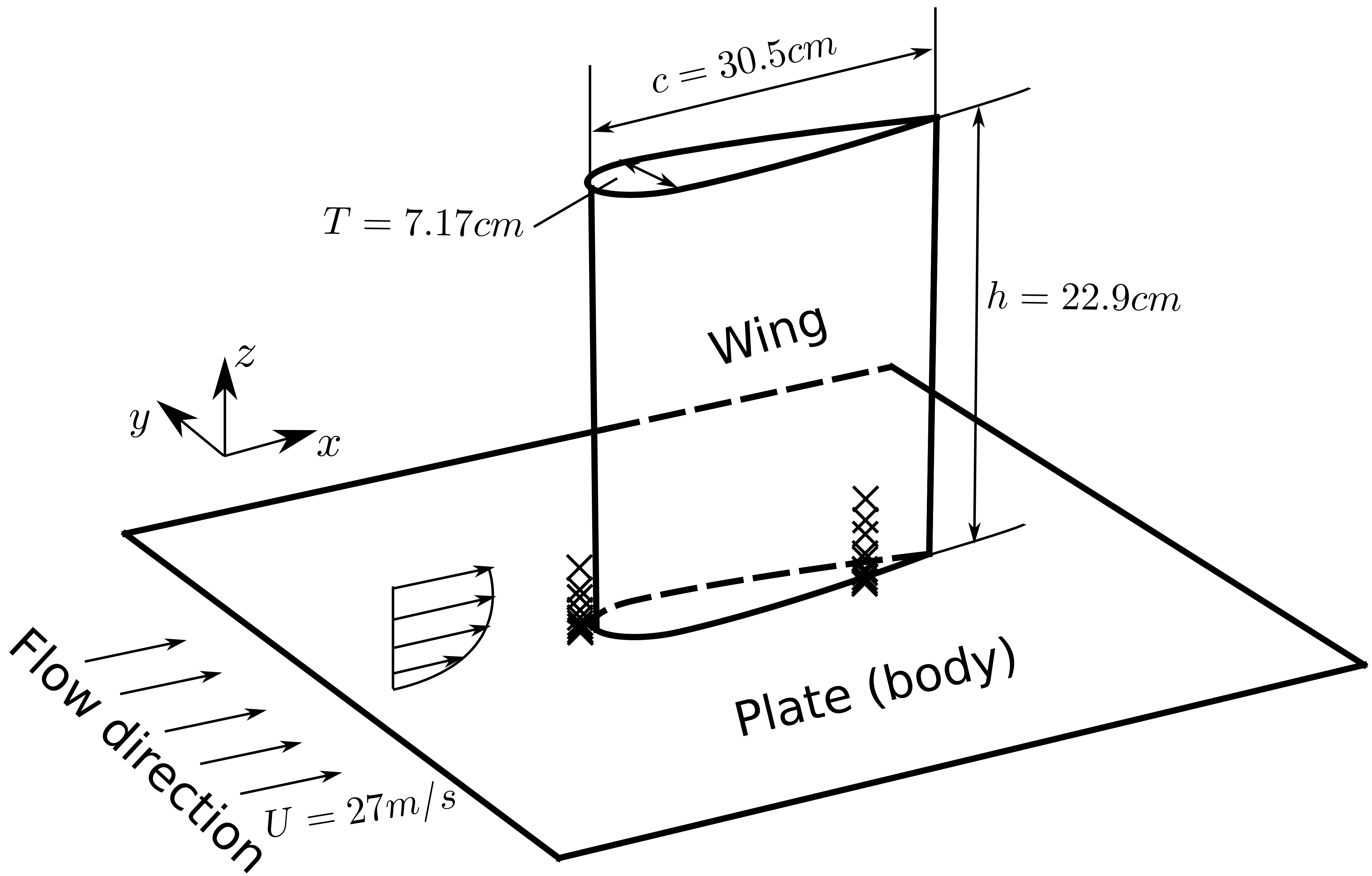


Prior scaled by a factor of 0.3 clarity

QoI: In-plane Velocity



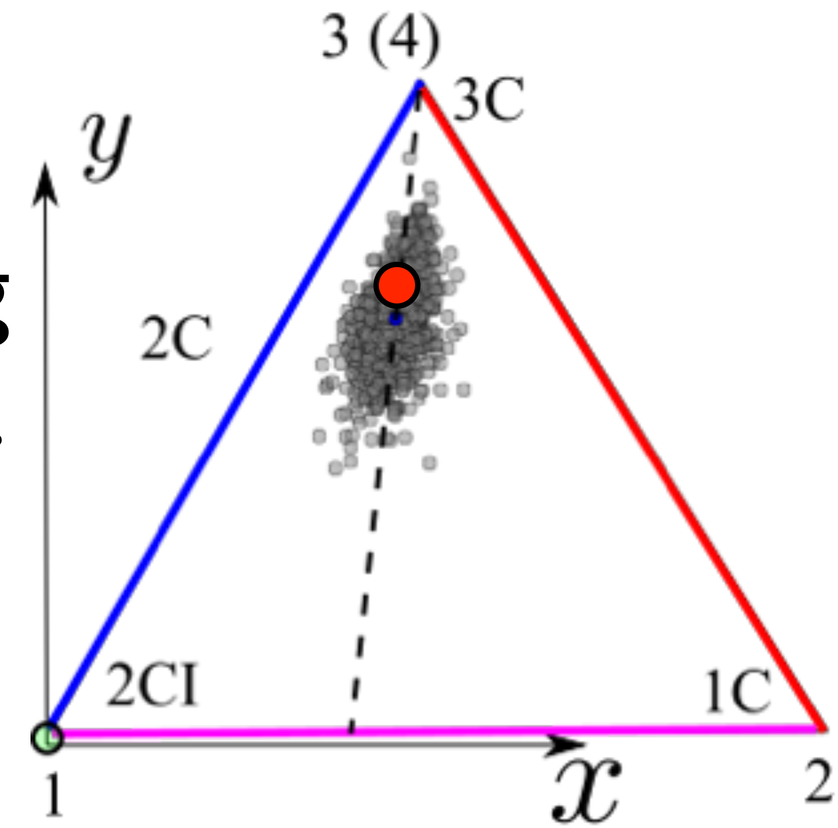
Test Case III: Wing-Body Junction Flow



[6] Wu, Wang, Xiao. Quantifying Model Form Uncertainty in RANS Simulation of Wing–Body Junction Flow. Submitted to FTC.

Computational Costs

- A baseline RANS simulation costs T. Each solve with perturbed Reynolds stress costs $0.1T$ (since we are starting at converged velocities in the baseline).



- 60 samples x 10 Kalman iterations = 600 forward evaluations

- Total computation CPU hours is $600 \times 0.1T = 60T$

- Samples evaluations are embarrassingly parallel: can run simultaneously on 60 processors. The wall time is still T !

Two Scenarios of Industrial CFD Simulations

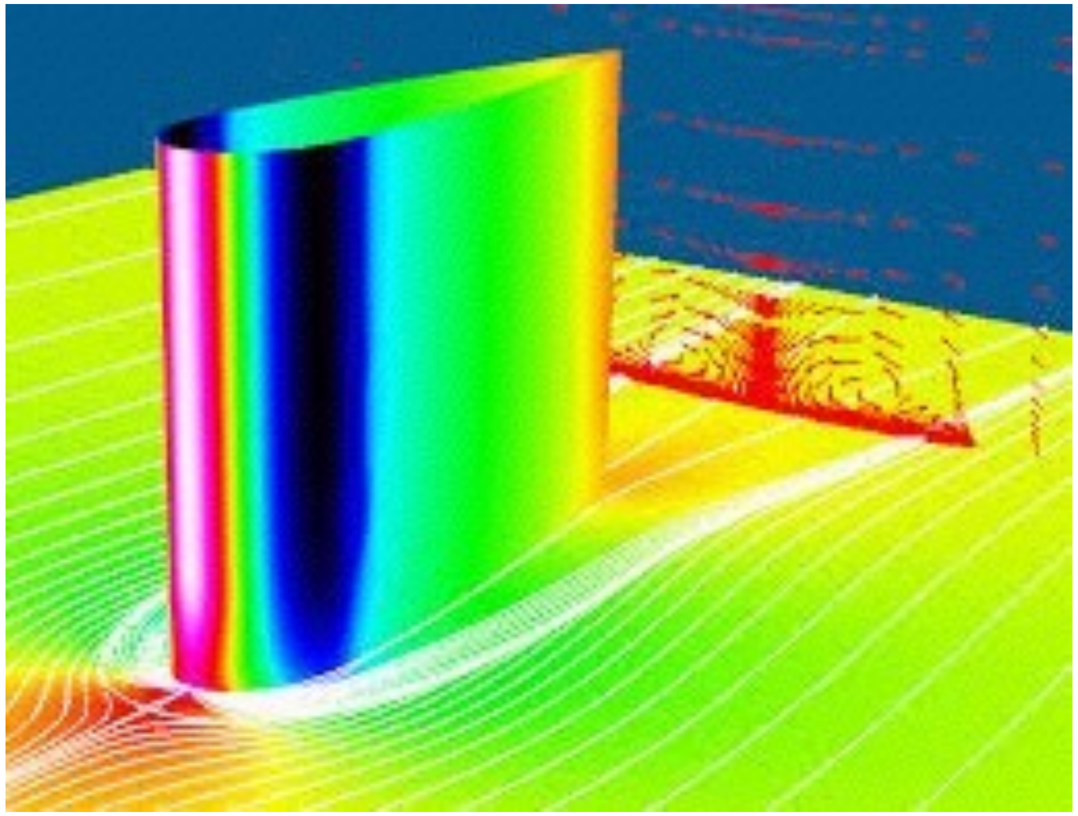
- Monitoring / Forecasting
- Support Design/Optimization

What If There Are No Data Available?

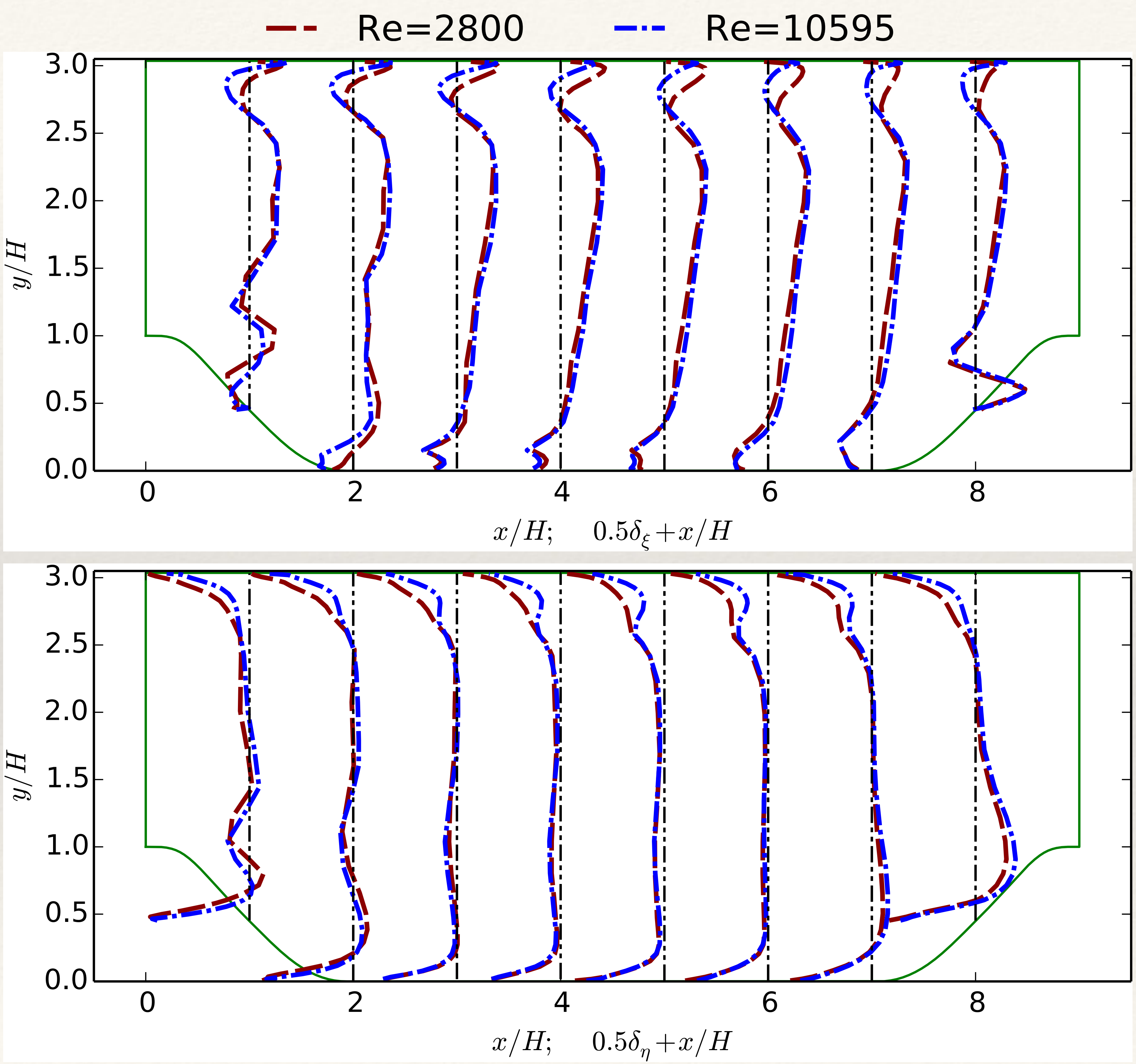
- Typical design cycle in civil aviation
- During engineering design (airplane etc.), the system has not been built yet: no data available!
- However, data may be available at a down-scaled model at a lower Reynolds number, or from a previous models of the same product line.

Vision for CFD in Support of Engineering Design and Optimization

Calibration Cases (w/ data)	Prediction Cases (w/o data)
A few configuration with data (DNS or measurements)	Similar configuration with different: • Twist • Sweep angles • Airfoil shape



Is The Discrepancy of Anisotropy Universal?



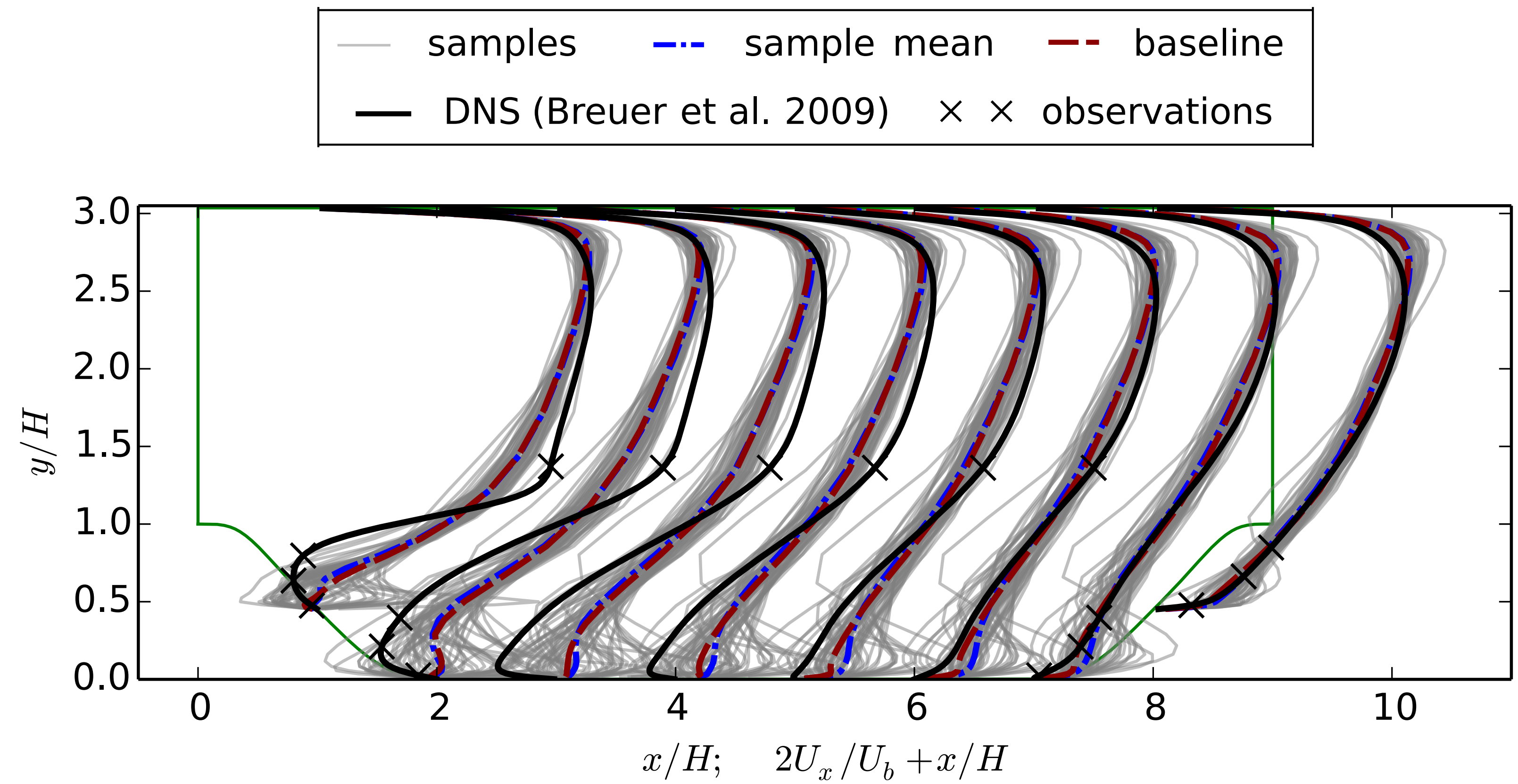
Probably!

δ^ξ

δ^η

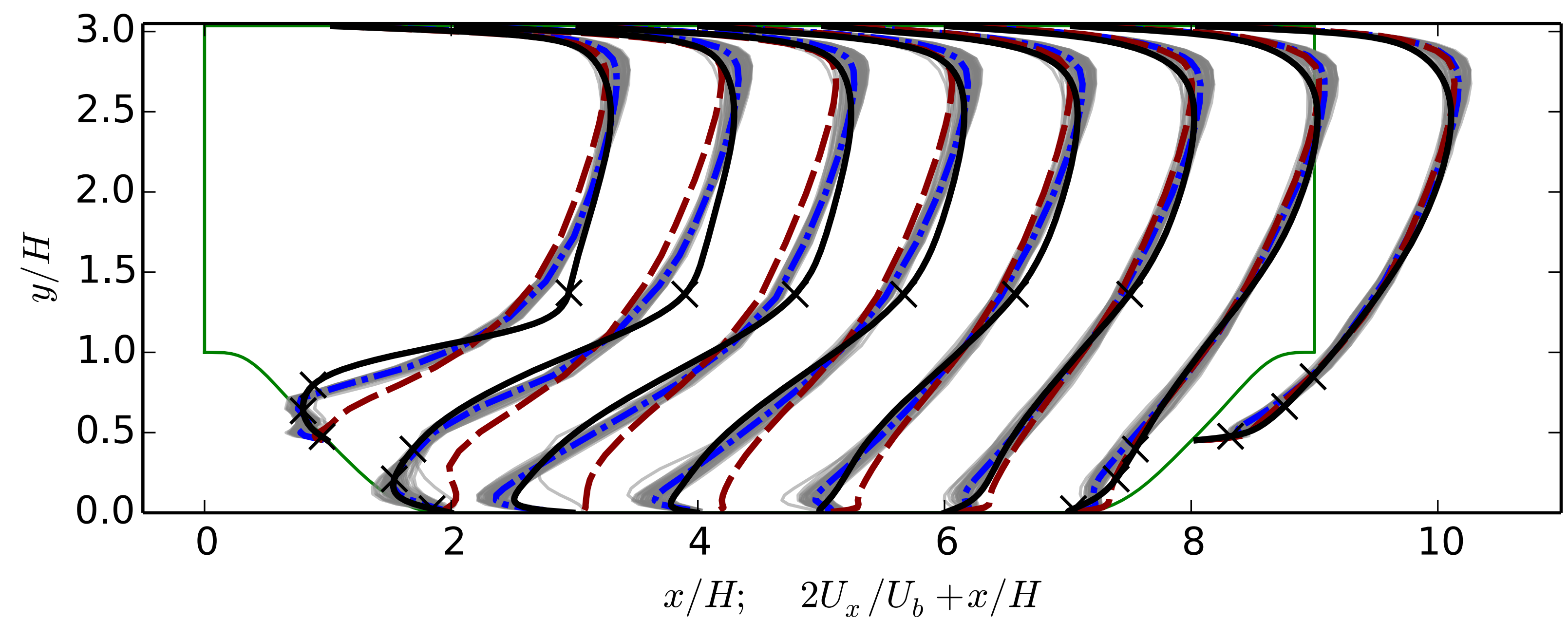
[3] J.-L. Wu, J.-X. Wang, and H. Xiao. A Bayesian calibration-prediction method for reducing model-form uncertainties with application in RANS simulations. *Flow, Turbulence and Combustion*, 2016.

Calibration at Re = 2800 (with Data)



(a) Prior ensemble of velocities

prior



(b) Posterior ensemble velocities

posterior

Prediction at Re=10595 (No Data)

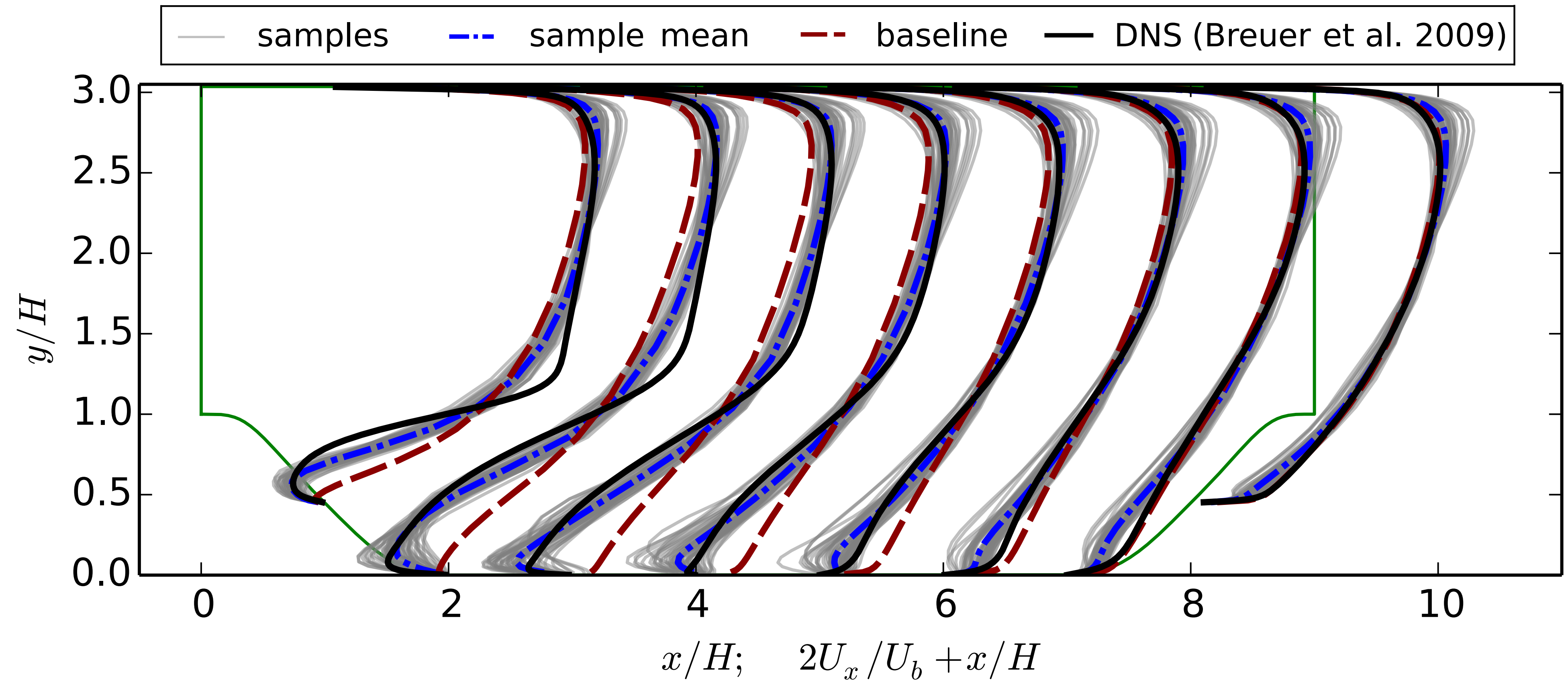
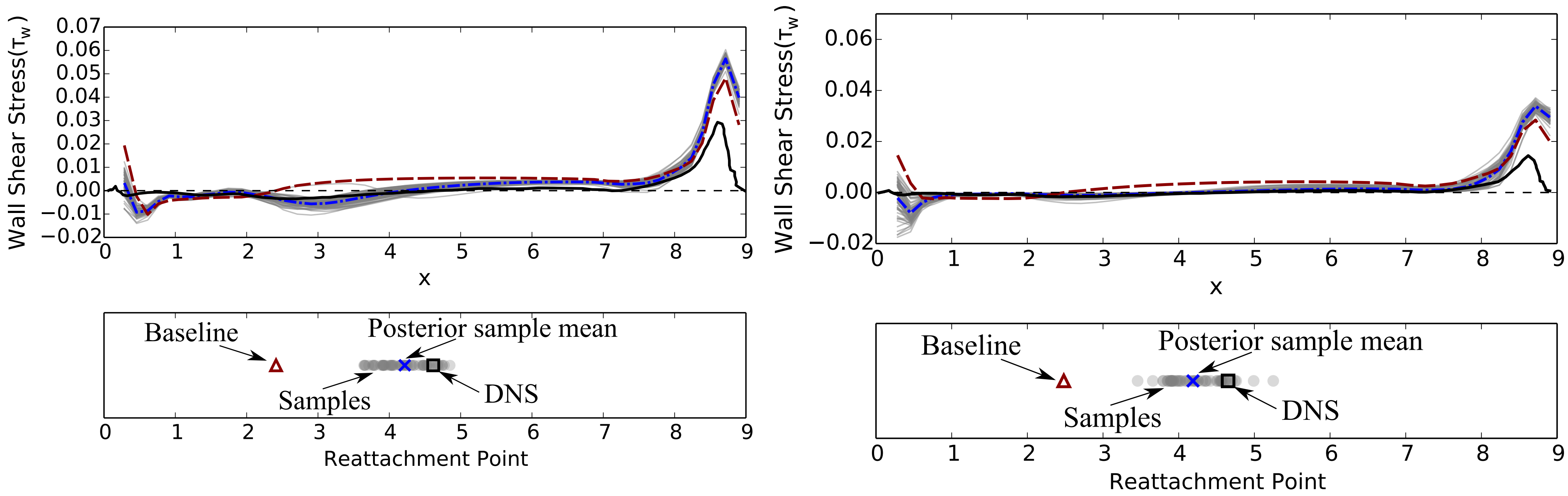


Figure 7: Ensemble of predicted velocity profiles of the flow over periodic hills of $Re = 10595$ at eight streamwise cross-sections $x/H = 1, 2, \cdots, 8$ compared with benchmark data and baseline results.

- Predictions still good even without data.



(a) Calibration of $Re = 2800$

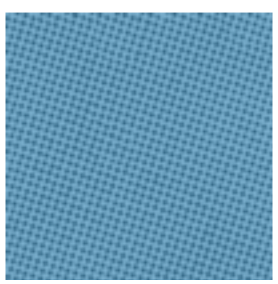
(b) Prediction of $Re = 10595$

Figure 5: The wall shear stress τ_w and reattachment point x_{attach} of flow over periodic hills of Re=10595. The extent of negative wall shear stress indicates the length of recirculation zone. The reattachment point is determined by the change of wall shear stress from negative to positive, which also indicates the end of recirculation zone. The greater opacity of markers indicates that there are more samples.

- Improvements for the predicted case.

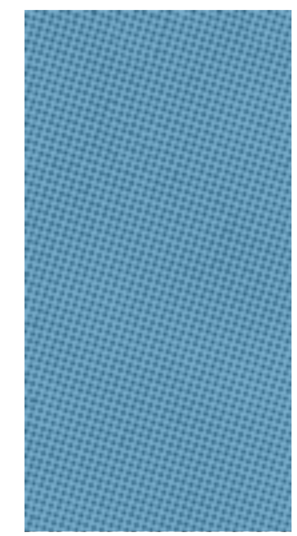
Another Illustrative Example

- Example for illustration: Calibrate Reynolds stress discrepancy in flow in square duct at Re $=10^4$; Predict: (1) a flow at higher Reynolds numbers and (2) a flow in a rectangular duct.



calibration:
square duct flow
@ low Re

prediction:
square duct flow
high Re

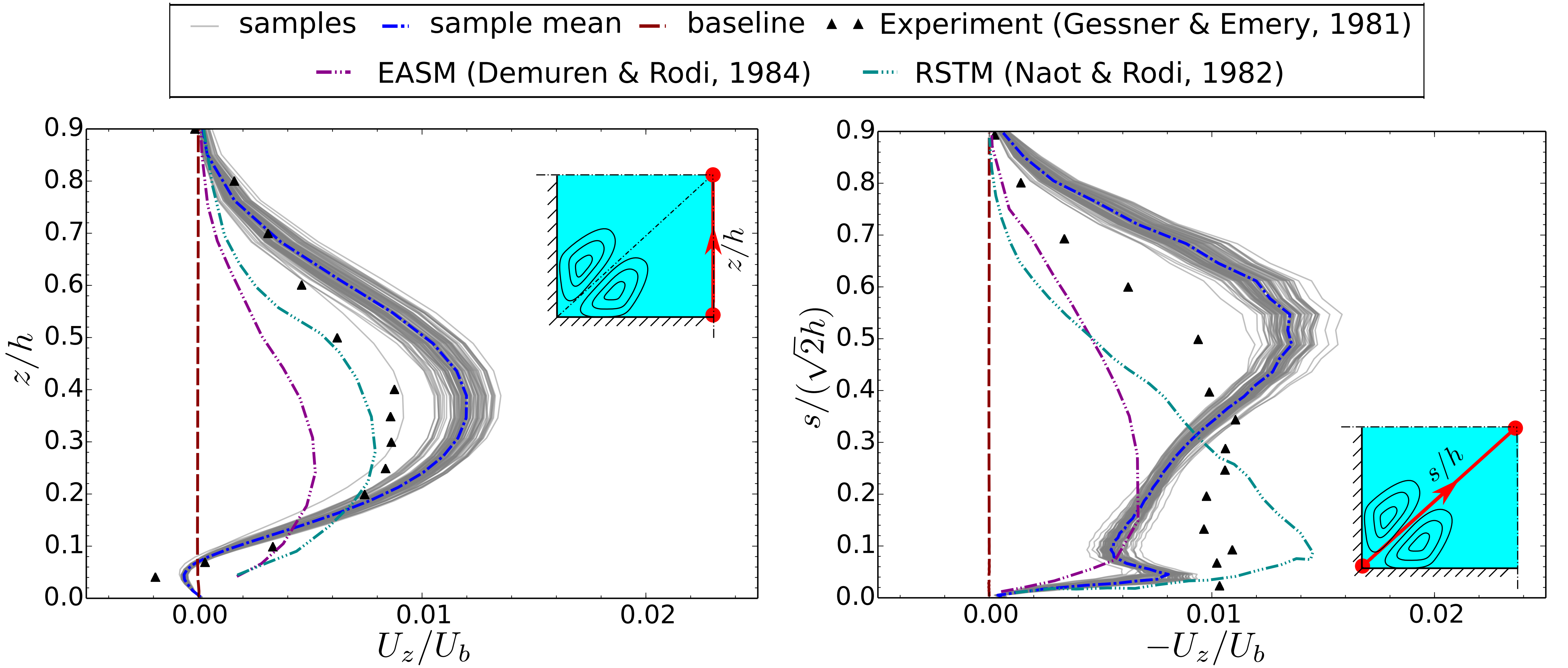


prediction:
rectangular duct
flow @ high Re

J.-L. Wu, J.-X. Wang, and H. Xiao. A Bayesian calibration-prediction method for reducing model-form uncertainties with application in RANS simulations. *Flow, Turbulence and Combustion*, 2016.

Prediction at High Reynolds Numbers

Calibrate Reynolds stress discrepancy at Re = 1 x 10^4; Extrapolate discrepancy to predict for Re = 2.5 x 10^5



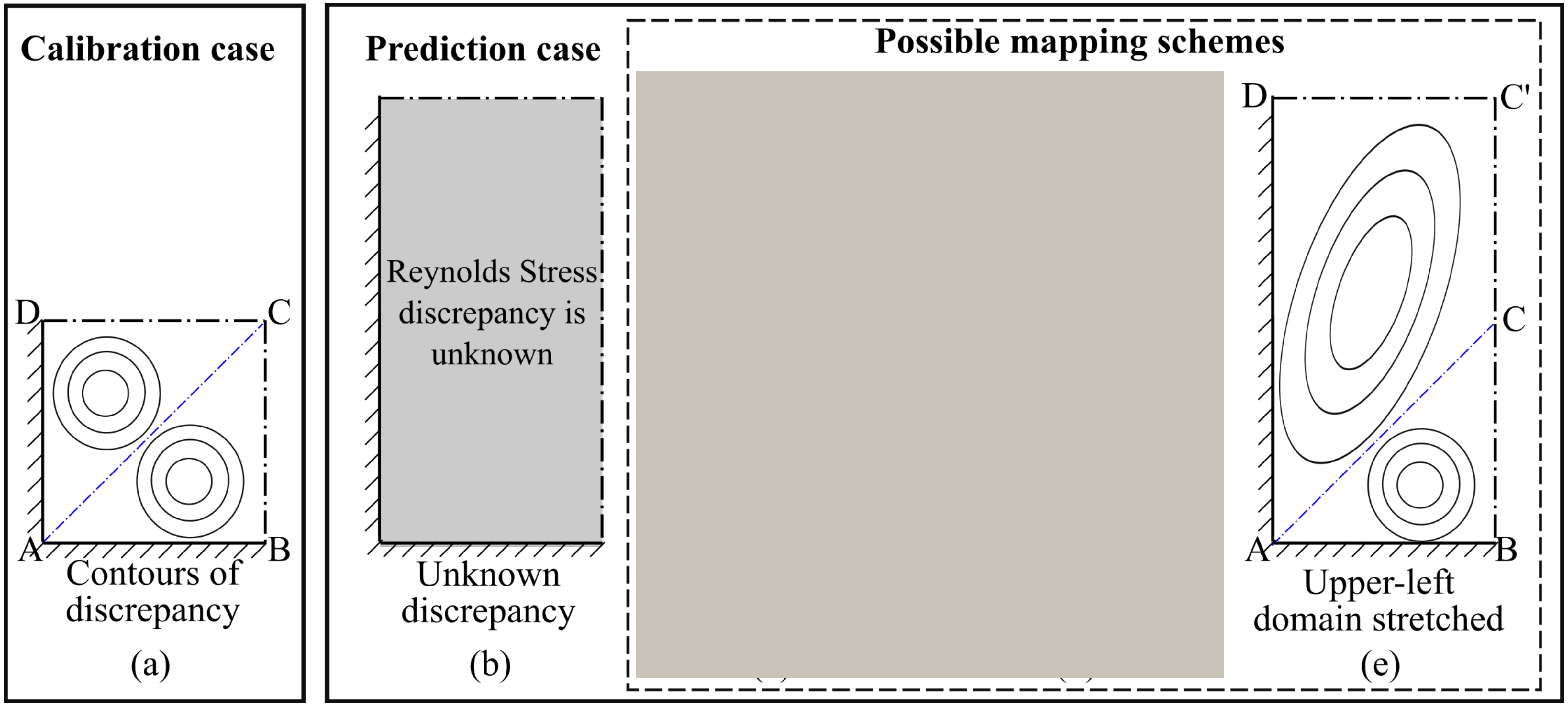
(a) Along vertical axis of symmetry

(b) Along diagonal

Figure 12: The comparison of predicted secondary velocity U_z at Reynolds number $Re = 2.5 \times 10^5$ with experimental data (denoted as ▲) and with predictions from advanced turbulence models including an explicit algebraic Reynolds stress model (EASM) and a Reynolds stress transport model (RSTM). Comparisons are shown (a) along the vertical axis of symmetry and (b) along the diagonal. Note that the prediction does not utilize observation data from the flow at $Re = 2.5 \times 10^5$.

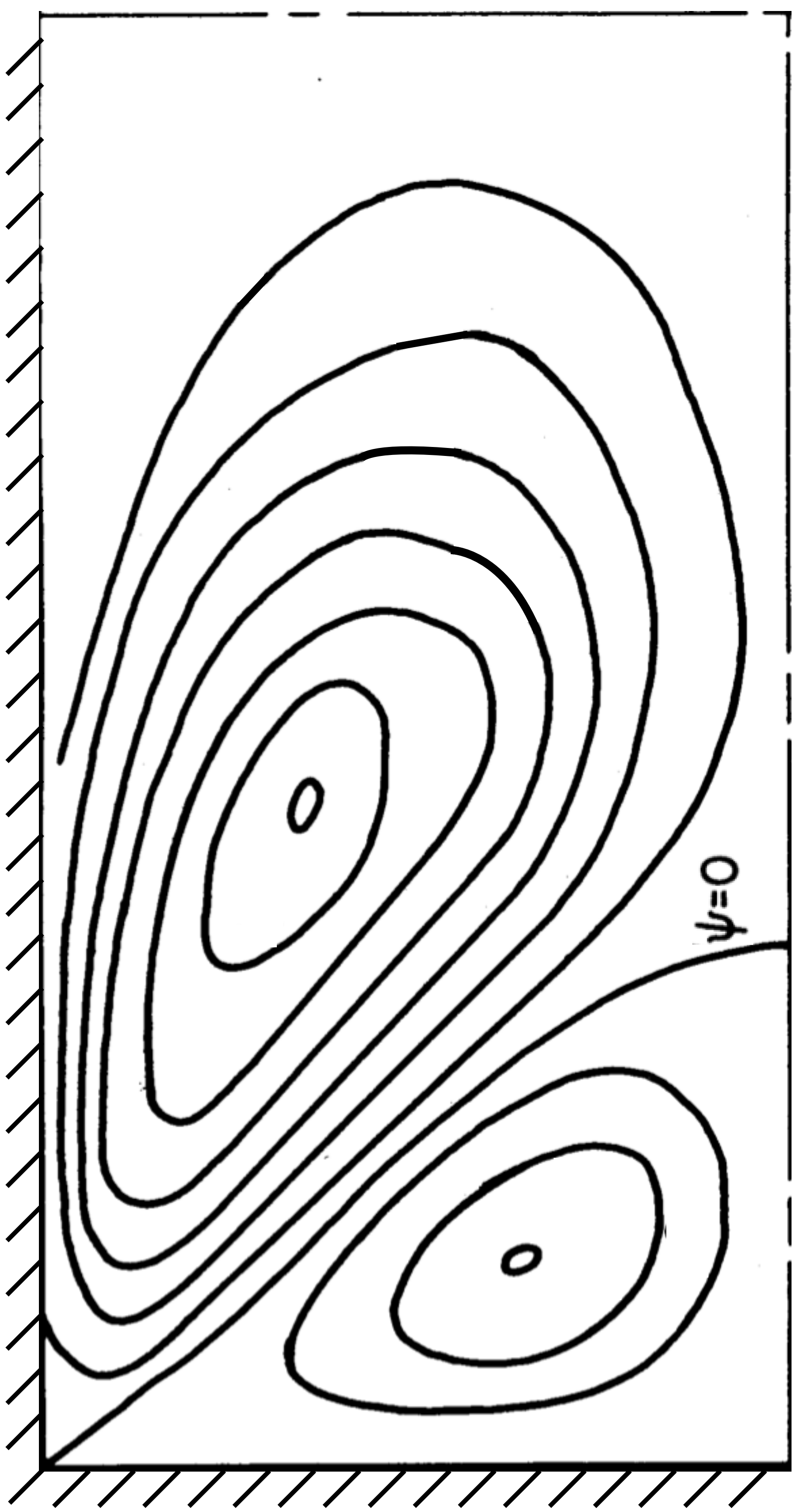
Extrapolation to Flow in a Different Geometry

The flow to be predicted has a different Reynolds number and different geometry than the calibration case.

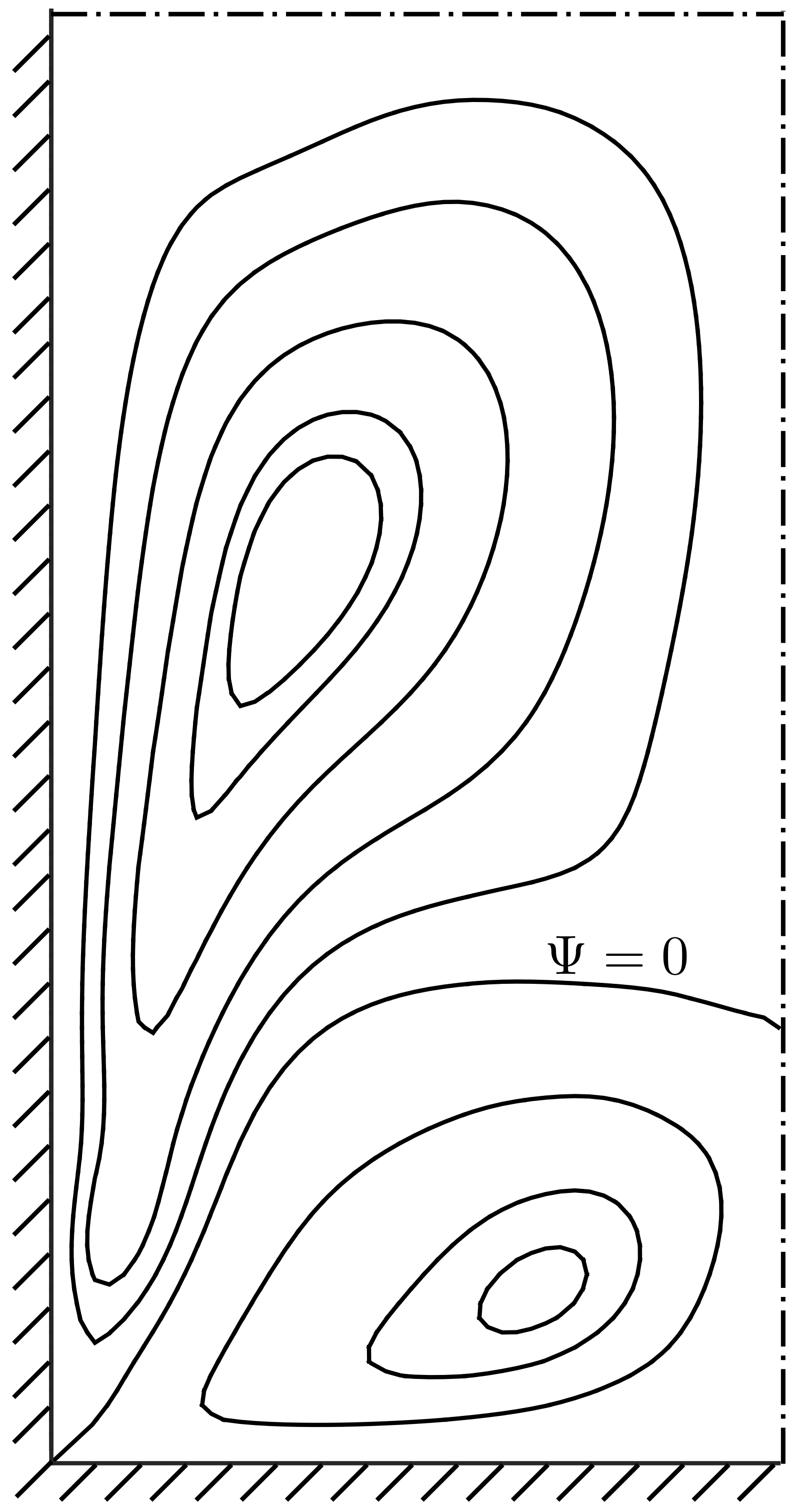


J.-L. Wu, J.-X. Wang, and H. Xiao. A Bayesian calibration-prediction method for reducing model-form uncertainties with application in RANS simulations. *Flow, Turbulence and Combustion*, 2016.

Predicted Streamlines



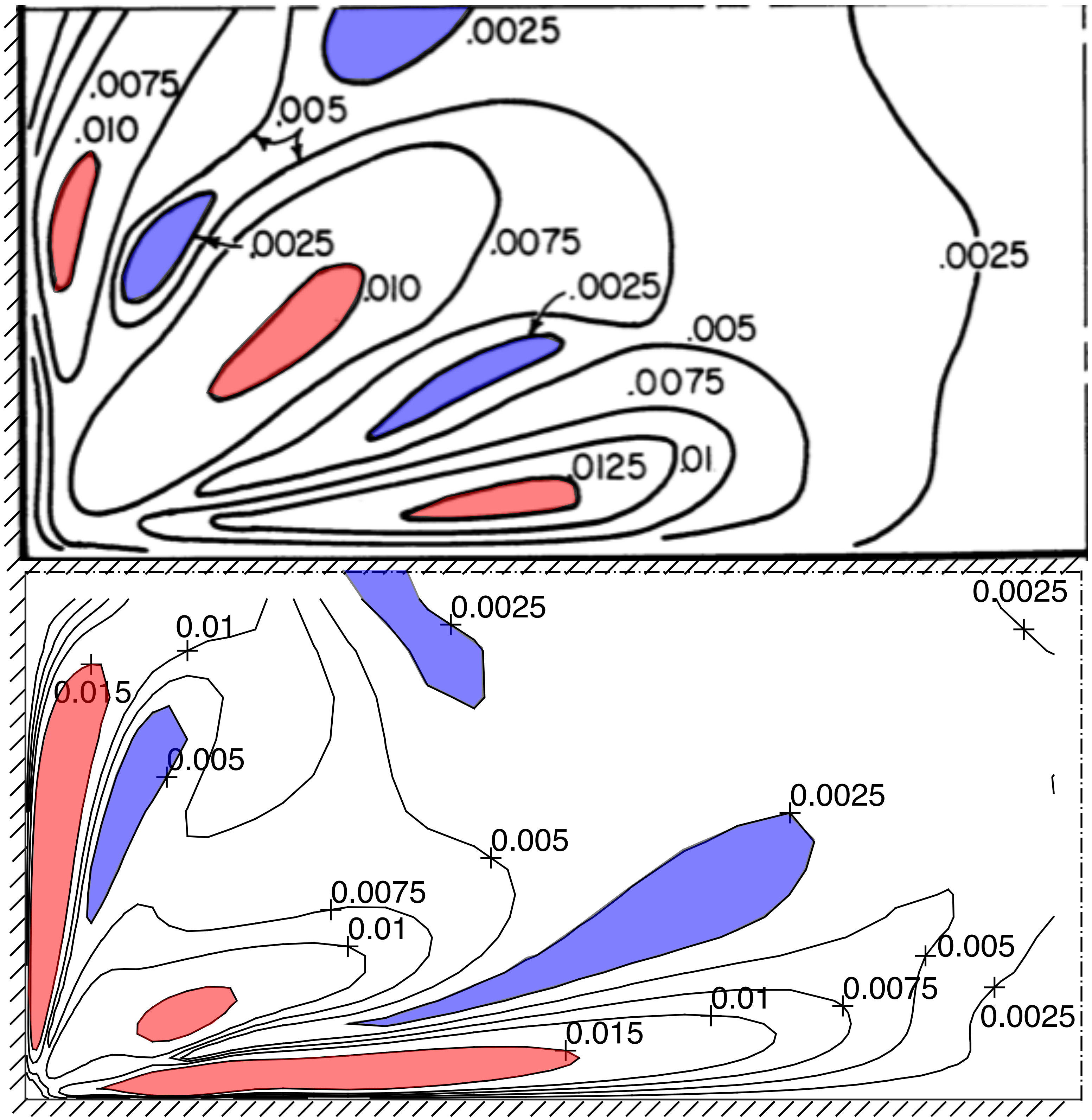
(a) Experiment [28]



(d) Scheme 3

(predicted posterior mean)

Predicted Secondary Flow Velocity Magnitude



Red: Peaks

Blue: Troughs

Assessment of Current Framework

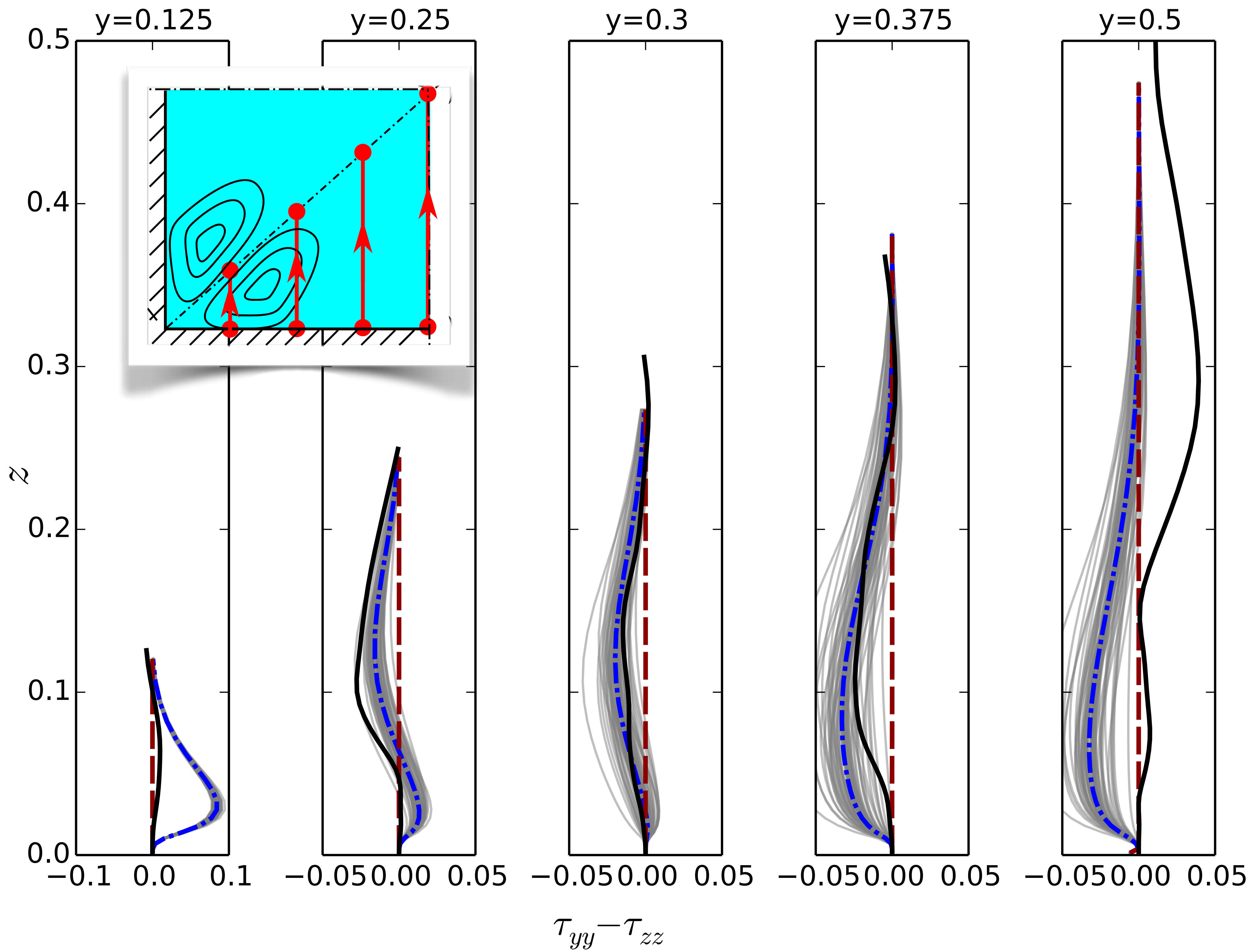
- + Bayesian inference utilizes disparate sources of information: physical constraints / empirical prior knowledge, observation data, and **numerical model**.
- + *Same formulation for different turbulence models: directly perturb Reynolds stresses.*
- + *Not constrained by the Boussinesq assumption.*
- + Inferred quantities (Reynolds stress) are physical and can be validated against benchmark. **We would know when we are wrong,** in contrast to inferring $\beta(x)$.

Inherited from Iaccarino et al.

Assessment of Current Framework

- +/– Has the potential for extrapolation to different flows (preliminary success shown; more work ongoing).
- – In currently assumed scenario (very sparse velocity data), inferred Reynolds stress are not accurate. **But:** a projection on a manifold is correct; possible to obtain accurate Reynolds stresses if given more data!
- * Adjoint model (as opposed to Ensemble Kalman filtering) may help retrieving better Reynolds stress.

Reynolds Stress Imbalance



Summary

- We developed a data-driven, physics-informed, Bayesian framework to quantify uncertainties in RANS models.
- The Bayesian framework incorporate all sources of information: **physical constraints + empirical prior knowledge, observation data, and numerical model.**
- Extended to cases without observation data (by extrapolating the inferred Reynolds stress discrepancy from a case with observation data).

Thank you for your attention!

Questions!