Ensemble Kalman method for learning turbulence models from indirect observation data

Xinlei Zhang[1], Heng Xiao[2], Xiaodong Luo[3], Guowei He[1]

[1]Institute of Mechanics, Chinese Academy of Sciences, China
[2]Department of Aerospace and Ocean Engineering, Virginia Tech, USA
[3]Norwegian Research Centre (NORCE), Norway

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Outline

1. Introduction
2. Data Assimilation: Field Inversion from Sparse Data
3. Unified Perspective (DA & ML) to Learn Models from Sparse Data
4. Results
5. Reflection
6. Conclusion

Learning Closure Model from Indirect Observation Data

Objective at a high level

We aim to learns *closure model* $\mathcal{M}_{\text{closure}} : x \mapsto y$

- Example: strain–stress relation, relative permeability curve – also called constitutive model or parameterization.
- Closure model can be algebraic relation or PDEs.

What does "indirect data" mean?

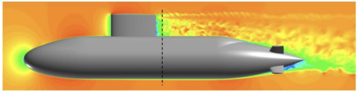
- We can directly learn from data $\{x_i, y_i\}_{i=1}^N$ independent of the solver, if such data y is available.
- However, typically we do not have direct data; rather, we have a physical solver $\mathcal{M}_{\text{physics}} : y \mapsto d$ that maps the output of the closure model y to an observable quantity d (e.g., displacement or velocity field, saturation field)
- These fields can be further post-processed to obtain integral quantities e.g., max deformation, lift/drag, or oil production

~~Machine Learning vs. Data Assimilation~~

- ML and DA have a lot of similarities:
  - optimize a cost function to improve predictions by using observation data
  - use (analytic or approximate) gradient-based optimization to find state/parameters/model
- How to combine ML and DA for better predictions?
  - DA respects the dynamic model more faithfully: physically consistent predictions
  - ML (neural networks) obtains analytic gradient (adjoint) more easily via back-propagation

RANS as Work-Horse tool for Turbulent Flow Simulations

- Turbulence is ubiquitous in natural and industrial flows (see examples below).
- RANS (Reynolds-Averaged Navier–Stokes) models are still the work-horse tool in industrial computational fluid dynamics (CFD) applications.
- High-fidelity methods such as LES (large eddy simulation) and DNS (direct numerical simulations) are still too expensive for practical flows.
- The drawback of RANS: poor performance in flows with separation, mean pressure gradient, mean flow curvature ... *Need to quantify and reduce model uncertainty.*



Source of Model Uncertainty in RANS Equations

- Incompressible Navier–Stokes equations:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} + \frac{1}{\rho} \nabla p &= 0 \end{aligned}$$

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- Reynolds Decomposition: $u_i = U_i + u_i'$ and $p = P + p'$

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$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} - \nu \nabla^2 \mathbf{U} + \frac{1}{\rho} \nabla P = \nabla \cdot \boldsymbol{\tau} \quad \text{where } \tau_{ij} = -\overline{u_i' u_j'}$$

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Reynolds stress $\boldsymbol{\tau}$ as source of model uncertainty in RANS equations

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\tau} - \nabla \cdot [(\nu_t + \nu) \nabla \boldsymbol{\tau}] = \mathsf{P} + \Phi + \mathsf{E}$$

☺ We can derive a transport PDE for the Reynolds stress $\boldsymbol{\tau}$.

☹ The PDE contains even more unclosed terms. $\longrightarrow$ closure problem

Data-Driven RANS Modeling Framework[1]

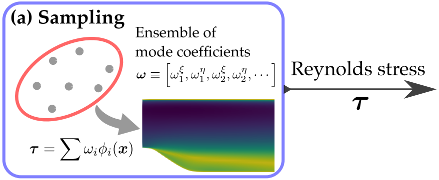
- Inject uncertainties in the Reynolds stress field: $\boldsymbol{\tau}(\boldsymbol{x}) = \sum_i \omega_i \phi_i(\boldsymbol{x})$
- Use sparse observation data y to reduce model uncertainties

Ensemble Kalman Filtering (EnKF)

EnKF Update

$$\boldsymbol{\omega}^{n+1} = \boldsymbol{\omega}^n + \mathsf{K}(\mathsf{y} - \mathcal{H}[\boldsymbol{\tau}])$$

K: Kalman gain
$\mathcal{H}$: RANS solver and observation operator



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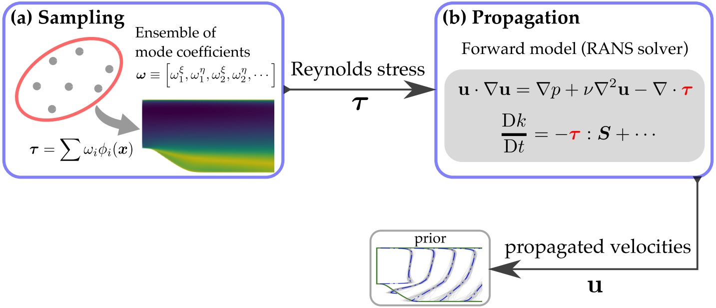

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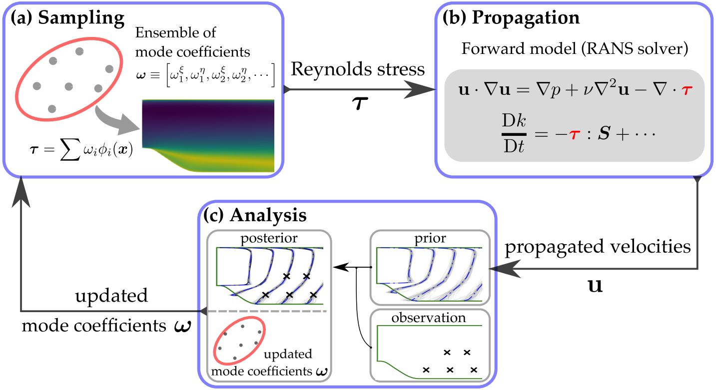

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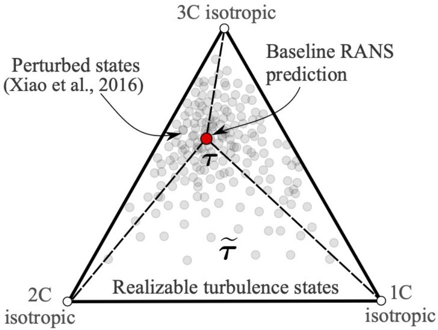
Enforcing Physical Constraints in Reynolds Stress Representation

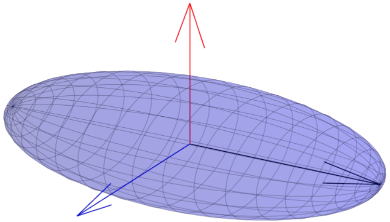
- $\boldsymbol{\tau}$ is a symmetric tensor field with *pointwise* physical realizability constraints

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

- Its magnitude and aspect ratio can be perturbed independently to ensure realizability within Barycentric triangle (similar to Lumley triangle); perturbing its orientations does not change its realizability.

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





Physics-Informed Parameterization of Reynolds Stress Field

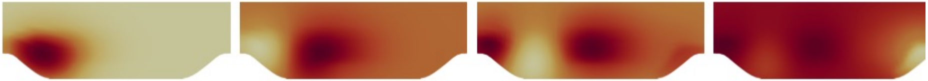
- Model the perturbation of Reynolds stress anisotropy (ξ, η) fields as *Gaussian random fields* with covariance kernel $\mathsf{C}(\boldsymbol{x}, \boldsymbol{x}')$ and RANS predictions ξ^{rans} as the mean, e.g.,:

$$\xi(\boldsymbol{x}) \sim \mathcal{GP}(\xi^{\text{rans}}, \mathsf{C}) \quad \text{with } \mathsf{C}\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \sigma(\boldsymbol{x})\sigma\left(\boldsymbol{x}'\right) \exp\left(-\|\boldsymbol{x} - \boldsymbol{x}'\|^2/\ell^2\right)$$

- The random fields are represented with Karhunen–Loève expansion:

$$\delta^{\xi}\left(\boldsymbol{x}; \theta^{\xi}\right) = \sum_{i=1}^{\infty} \omega_i^{\xi}|_{\theta^{\xi}} \phi_i(\boldsymbol{x}) \qquad \delta^{\eta}\left(\boldsymbol{x}; \theta^{\eta}\right) = \sum_{i=1}^{\infty} \omega_i^{\eta}|_{\theta^{\eta}} \phi_i(\boldsymbol{x})$$

- The basis functions $\phi_i(\boldsymbol{x})$ are eigenmodes of covariance kernel C.



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

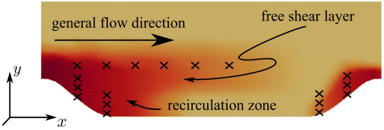
Physics-informed dimension reduction

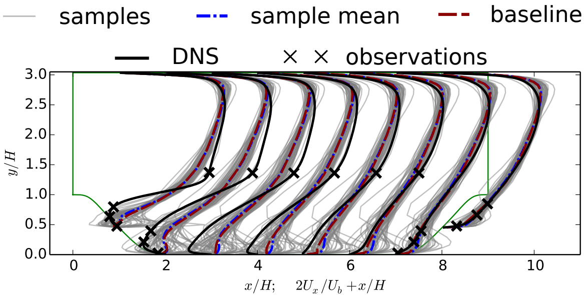
We used prior knowledge to simplify a field inference $\tau_{ij}(\boldsymbol{x})$ to random variables:

$$\boldsymbol{\omega} \equiv \left[\omega_1^{\xi}, \omega_1^{\eta}, \omega_2^{\xi}, \omega_2^{\eta}, \ldots,\right]$$

Case I: Flow Over Periodic Hills

Infer full velocity field from sparse data





- Observation data improves full-field velocity predictions
- Injected uncertainties into Reynolds stress anisotropy: preserved realizability and smoothness of $\boldsymbol{\tau}(\boldsymbol{x})$;
- Do not modify the velocity field directly: respect divergence-free constraints.

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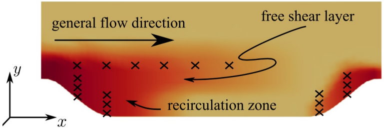

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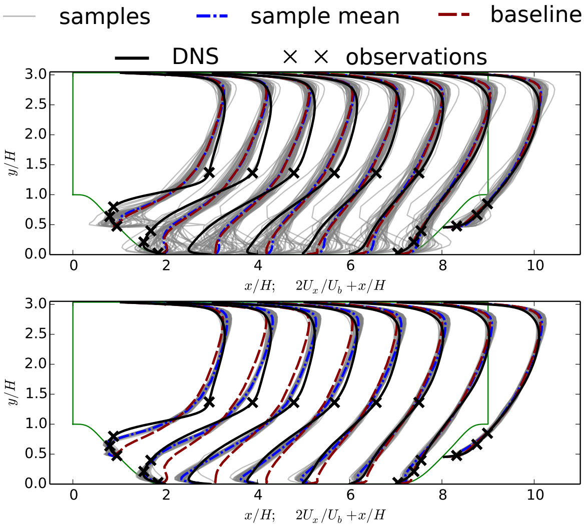
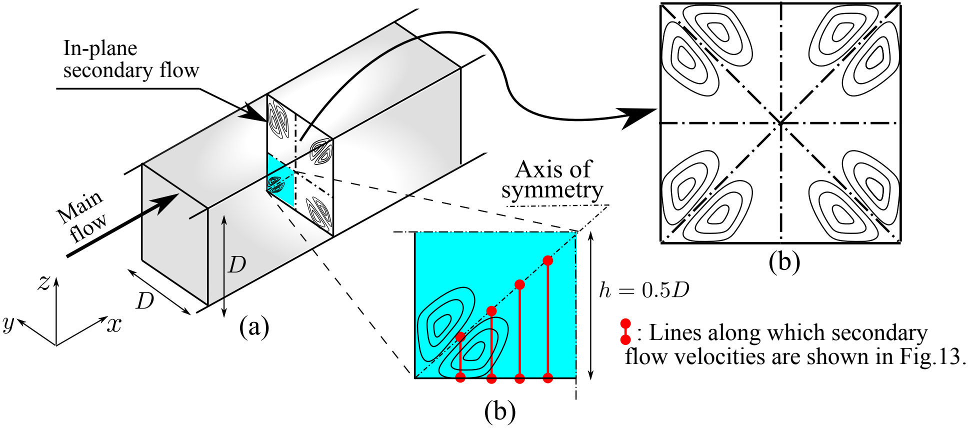


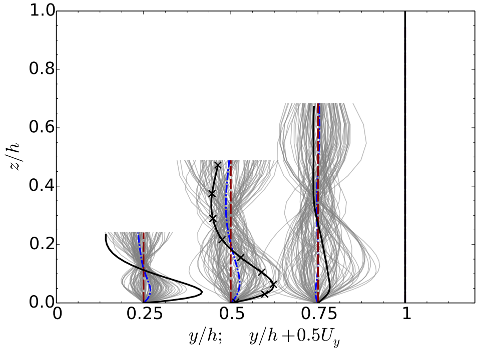
Case II: Secondary Flow in Turbulent Square Duct – Setup

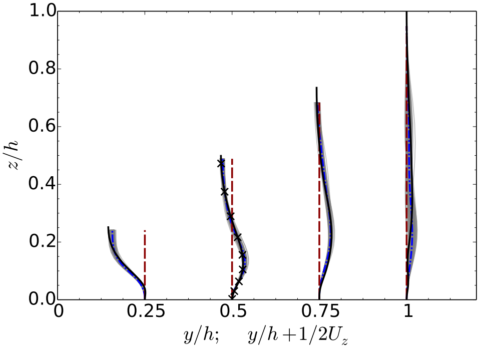
- Flow along a square duct (e.g., in draft pipes, rivers): a classical challenging test case for turbulence models.
- Features in-plane flows driven by normal Reynolds stress imbalance $\tau_{yy} - \tau_{zz}$
- Linear eddy viscosity models fail to predict mean flow due to lack of anisotropy in Reynolds stress tensor



Inferred In-plane Velocities (Seconary Flows)

- Velocities are observed on one station $y/h = 0.5$ only.
- The observation data improved in-plane velocities in the whole field.

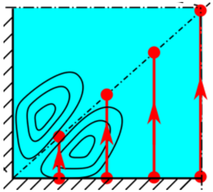




samples: ——— sample mean: -·-·-·-

baseline RANS: - - - - - - DNS: ———

Prior velocities scaled by a factor of 0.3 for clarity.



Data Assimilation for Turbulent Flow Simulations – Summary

- We combine sparse observation and low-fidelity model to achieve predictive capabilities.
- The physics-informed framework respect physics constraints of physical variables: realizability, smoothness, convection physics . . .

Application scenarios of data assimilation:

Complement system monitoring (CFD + Sensors): *one system only*, with online streamlined data from devices.

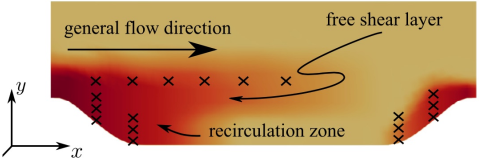
Need machine learning to learn underlying model from data

- Support design, analysis, and optimization
- With offline data; can be full-field data, on different but similar flows.

Learning (Closure)-Model from Sparse, Indirect Observations

What if only sparse data such as velocities ($\times$) or drag, lift are available, without Reynolds stresses!

$$\mathbf{U} \cdot \nabla \mathbf{U} - \nu \nabla^2 \mathbf{U} + \frac{1}{\rho} \nabla P = \nabla \cdot \boldsymbol{\tau}$$



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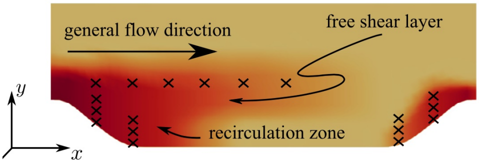


Unified Perspective to Adjoint, Data Assimilation and Machine Learning

All data-driven methods amounts to minimize the discrepancy J between model prediction[a] $\tilde{\mathrm{y}} = \mathcal{H}(\boldsymbol{\tau})$ and observation data y:

- Adjoint optimization (parameter tuning): find the parameters $\boldsymbol{\beta}$ in the turbulence models, so as to *minimize* the discrepancy $J = \|\mathrm{y} - \mathcal{H}[\boldsymbol{\beta}]\|^2$
- Data assimilation: find the Reynolds stress field $\boldsymbol{\tau}(\boldsymbol{x})$ to *minimize* the discrepancy $J = \|\mathrm{y} - \mathcal{H}[\boldsymbol{\tau}(\boldsymbol{x})]\|^2$
- Machine learning: find the turbulence model $\boldsymbol{\tau} = g_{\mathrm{nn}}(\nabla U; \boldsymbol{w})$ represented by a neural network $\boldsymbol{w}$ to *minimize* $J = \|\mathrm{y} - \mathcal{H}[\boldsymbol{w}]\|^2$

[a] Operator $\mathcal{H} : \boldsymbol{\tau} \mapsto \tilde{\mathrm{y}}$ is a composition of RANS solver and observation operator

Deep Learning of Turbulence Model from Sparse Data[2]

- Sensitivity of J w.r.t. Reynolds stress $\boldsymbol{\tau}$ is obtained as gradient of adjoint velocity: $\frac{\partial J}{\partial \boldsymbol{\tau}} = -\boldsymbol{\nabla}\hat{\boldsymbol{u}}$, where $\hat{\boldsymbol{u}}$ is solved from continuous adjoint:

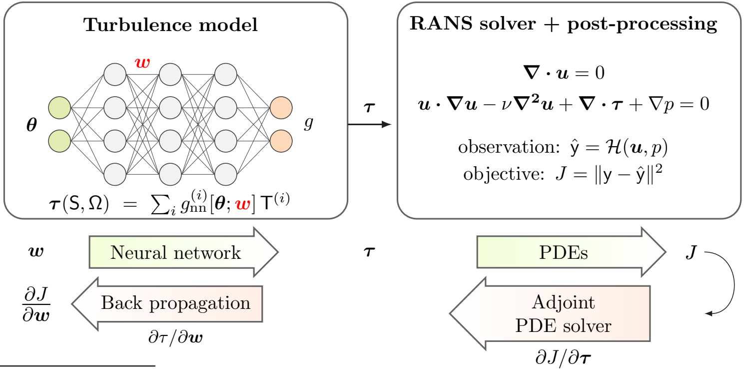
$$\boldsymbol{u} \cdot \boldsymbol{\nabla}\hat{\boldsymbol{u}} + \boldsymbol{\nabla}\hat{\boldsymbol{u}} \cdot \boldsymbol{u} + \nu \boldsymbol{\nabla}^2 \hat{\boldsymbol{u}} - \nabla \hat{p} = \frac{\partial J}{\partial \boldsymbol{u}}$$

- Adjoint based optimization. Gradient via chain rule: $\frac{\partial J}{\partial \boldsymbol{w}} = \frac{\partial J}{\partial \boldsymbol{\tau}} \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{w}}$

$$\frac{\partial J}{\partial \boldsymbol{w}} = \frac{\partial J}{\partial \boldsymbol{\tau}} \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{w}}$$

$\frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{w}}$: auto-diff

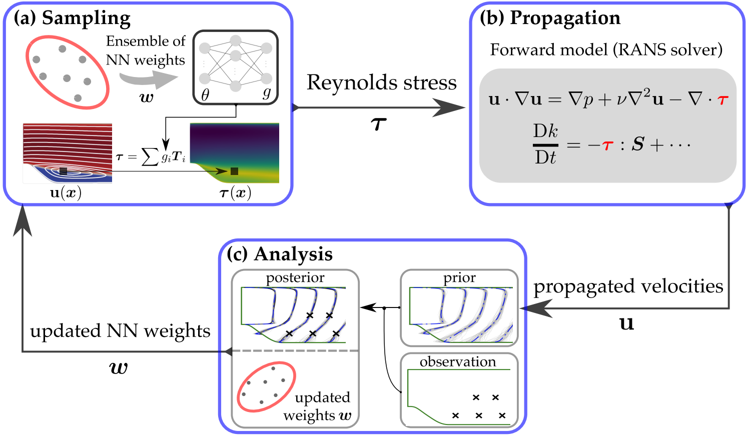
$$\frac{\partial J}{\partial \boldsymbol{\tau}} = -\boldsymbol{\nabla}\hat{\boldsymbol{u}}$$



[2] Michelén-Ströfer, Xiao. End-to-end differentiable learning of turbulence models from indirect observations. *Theo. Appl. Mech. Lett.* 11(4), 100280, 2021.

EnKF Learning of Turbulence Model from Sparse Data[3]

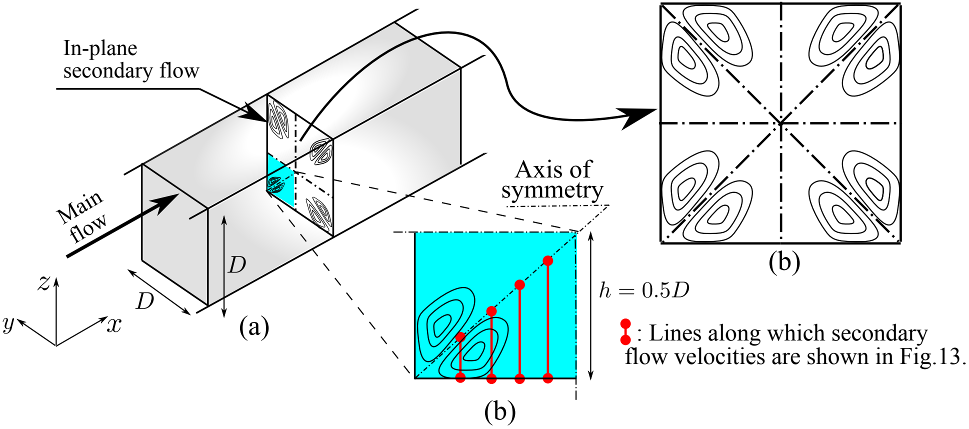
- EnKF is non-intrusive to the RANS solver: only requires an ensemble of forward simulations and not adjoint.
- Use analysis to update NN weights: $\boldsymbol{\omega}^{n+1} = \boldsymbol{\omega}^n + \mathsf{K}(\mathsf{y} - \mathcal{H}[\boldsymbol{\tau}])$



[3] Zhang, Xiao, Luo, He. Ensemble Kalman method for learning turbulence models from indirect observation data. Submitted to *J. Fluid Mech.* arXiv:2202.05122

Square Duct – Learn Turbulence Model from Velocity

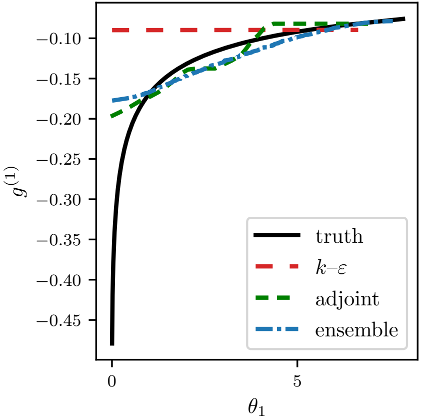
- Flow along a square duct
- Used Shih quadratic model as the synthetic truth

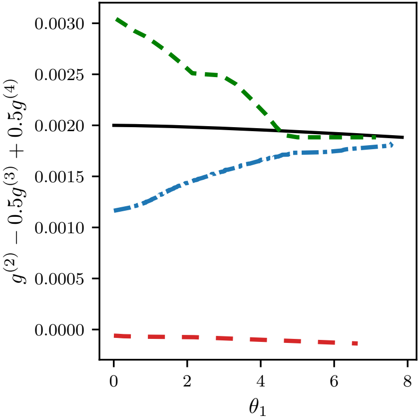


Learned Shih Quadratic Model from Synthetic Velocities

Shih model (cast into Pope's formulation)

$$g_1(\theta_1, \theta_2) = \frac{-2/3}{1.25 + \sqrt{2\theta_1} + 0.9\sqrt{2\theta_2}} \qquad g_2(\theta_1, \theta_2) = \frac{7.5}{1000 + (\sqrt{2\theta_1})^3}$$

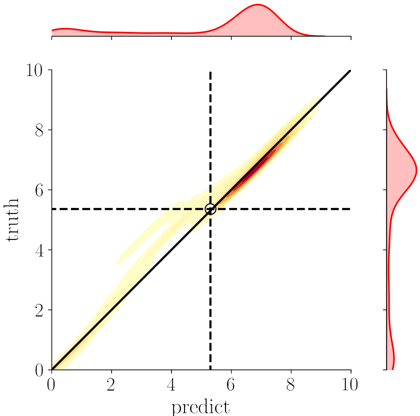


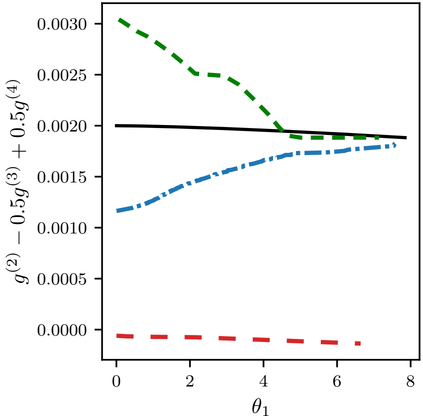


Learned Shih Quadratic Model from Synthetic Velocities

Remarks

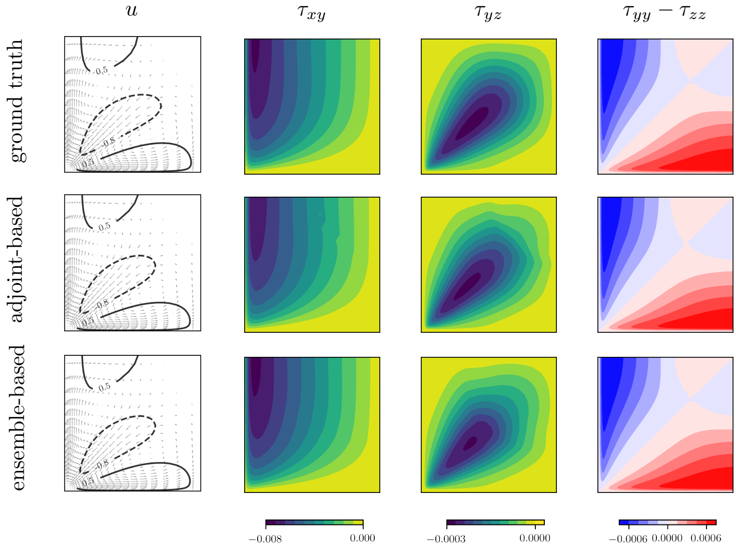
- Only a linear combination $g^{(2)} - 0.5g^{(3)} + 0.5g^{(4)}$ is informed by the in-plane velocities and thus can be learned
- The velocity is not sensitive to the Reynolds stresses in the duct center (small θ_1), so this part in parameter space is not learned well.





Performance Comparison: NN+Adjoint v.s. Ensemble Learning

- Learned nonlinear eddy viscosity model: $\boldsymbol{\tau}(\mathsf{S}, \Omega) = \sum_i g_{\mathrm{nn}}^{(i)}[\boldsymbol{\theta}; \boldsymbol{w}]\, \mathsf{T}^{(i)}$
- Almost identical results between NN+adjoint and EnKF.



Computational Cost: NN+Adjoint v.s. Ensemble Learning

- Most CPU time is spend on the RANS solver.
- RANS simulations in the ensemble method is parallel: 60 sampels on 60 cores.
- The faster convergence of the ensemble method is due to the use of Hessian and covariance inflation.

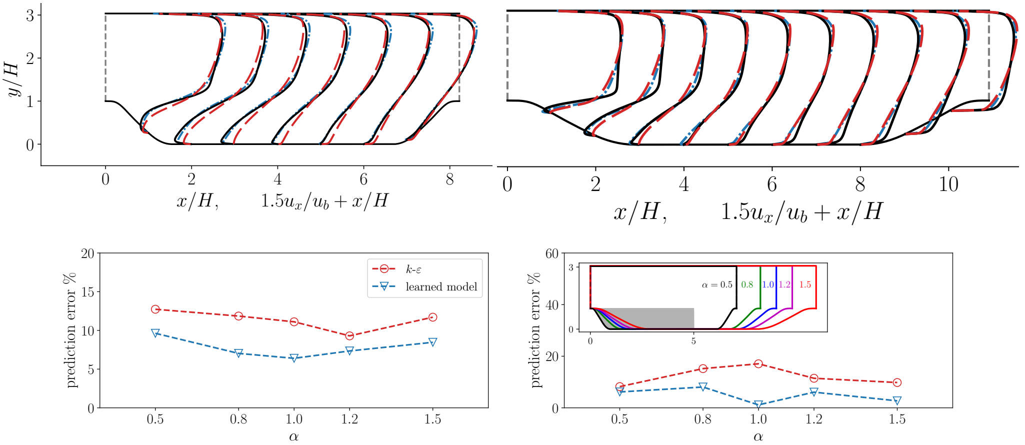
Comparison of computational costs (for square duct flow)

	Ensemble Method	NN + Adjoint
CPU time/step	8.3 min	7.2 min
Steps to converge	50	1000
Wall time	6 h	133 h

Ensemble Learning of Flow Over Periodic Hills: Extrapolation

A nonlinear eddy viscosity model learned with EnKF:

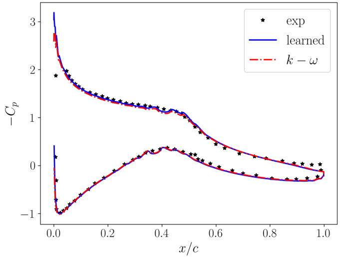
- Trained with velocity data (4 stations) from a periodic hill of slope 1.0
- Tested on $\alpha = 0.5$, 0.8 (left), 1.2, and 1.5 (right).

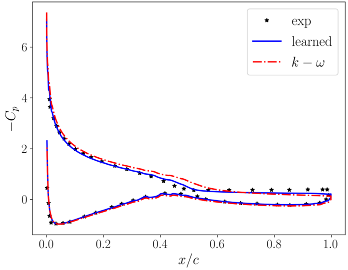


Training with Only Lift Coefficient

- Train model with integral data (lift coefficient) only
- Data from two flow conditions are used: angle of attack (AoA) 8° (attached) and 14° (separated)
- Improved estimation of lift force (C_l) and pressure distribution (C_p) by tuning the turbulence model

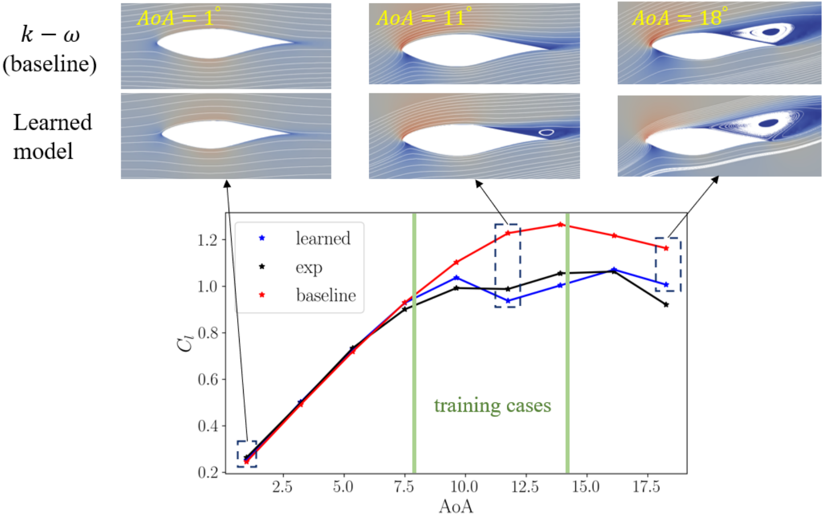
	k–ω	Learned	Experiment
C_l (AoA=14°)	1.25	1.07	1.05
C_l (AOA=8°)	0.97	0.94	0.95





Generalize to Different Flow Conditions (AoA)

- Improved preditions in the lift coefficient in all conditions (AoA $\in [1^\circ, 18^\circ]$)
- Recall that the model was trained on two AoAs (8° and 14°)



Can We Utilize (Free) Analytic Gradient of the Neural Network?

- The analytic gradient of the neural network $\partial \boldsymbol{\tau} / \partial w$ is not used!
- However, such gradient can be useful when we have both direct data (Reynolds stress) and indirect data (velocity, lift coefficient)
- Incorporate direct data as a regularization term in the cost function[4]

Learning from both direct and indirect data

- Cost function of regularized EnKF:

$$J = \| w^{\mathsf{a}} - w^{\mathsf{f}} \|_{\mathsf{P}}^2 + \| U^{\mathsf{DNS}} - \mathcal{H}[w^{\mathsf{f}}] \|_{\mathsf{R}}^2 + \| \tau^{\mathsf{DNS}} - \mathcal{G}[w^{\mathsf{f}}] \|_{\mathsf{Q}}^2$$

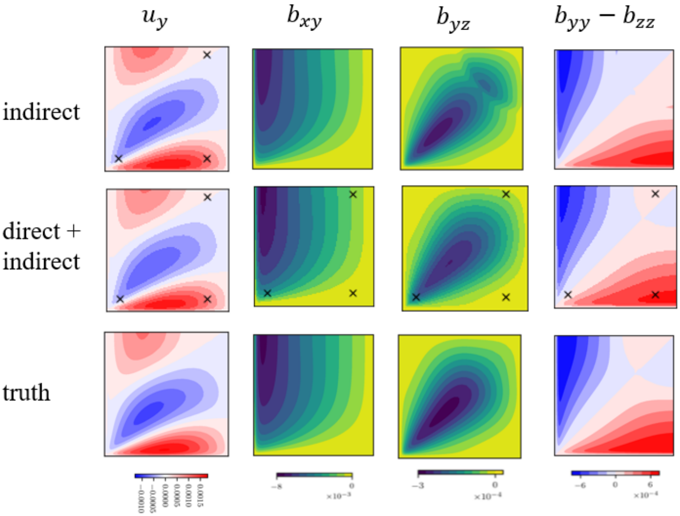
- Update scheme of regularized EnKF:

$$\tilde{w} = w^{\mathsf{f}} - \mathsf{P}\mathsf{G}'\mathsf{Q}^{-1}(\tau^{\mathsf{DNS}} - \mathcal{G}[w^{\mathsf{f}}]);$$
$$w^{\mathsf{a}} = \tilde{w} + \mathsf{P}\mathsf{H}^{\top}(\mathsf{H}\mathsf{P}\mathsf{H}^{\top} + \mathsf{R})^{-1}(U_j^{\mathsf{DNS}} - \mathcal{H}[\tilde{w}]).$$

[4] Zhang, Michelén-Ströfer, Xiao. Regularized ensemble Kalman methods for inverse problems. *J. Comput. Phys.*, 416, 109517, 2020.

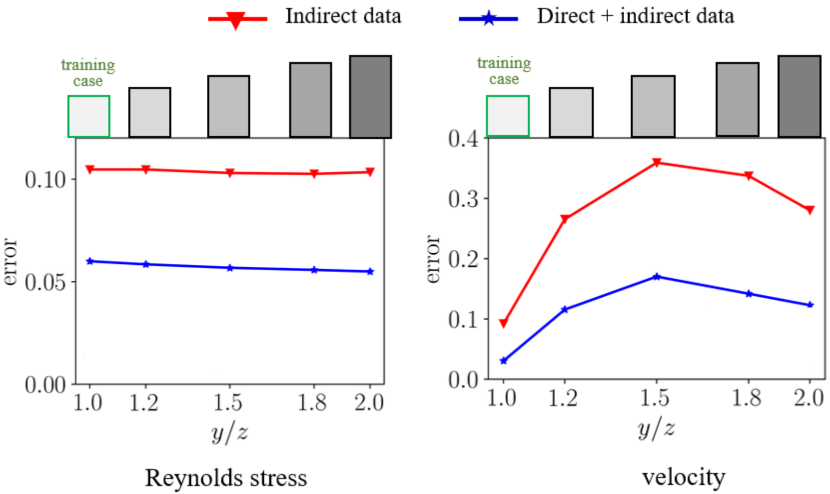
Joint Training with Direct and Indirect Data – Reconstruction

- Use indirect and direct data, but only at sparse locations ($\times$)
- Combination of the two data sources enhances the reconstruction of velocity and Reynolds stresses: reduces ill-conditioning.



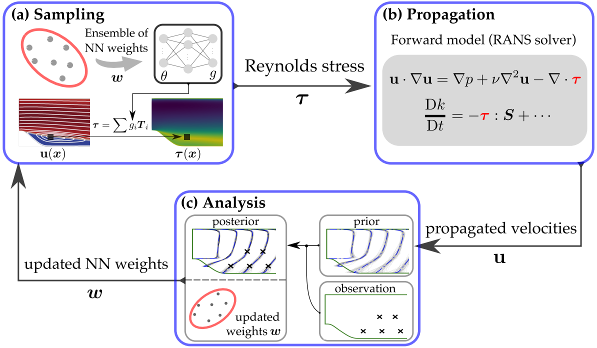
Joint Training with Direct and Indirect Data – Generalization

- Generlizable to different aspect ratios
- Provides improved predictions of velocities and Reynolds stresses



Conclusion

- Combined data assimilation, adjoint, and machine learning to learn turbulence models.
- Ensemble learning method is competitive compared to fully adjoint models.
- In the context of learning closure models from both indirect and direct data, this approach can have significant merits.



Reference

Details in the following preprint:

Zhang, Xiao, Luo, He. Ensemble Kalman method for learning turbulence models from indirect observation data. Submitted to *J. Fluid Mech.* arXiv:2202.05122