Regularized Ensemble Kalman Method for Inverse Problems

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Outline

Acknowledgment of Collaborators

Work presented here are performed in collaboration with my former Ph.D. students:

- Dr. Xin-Lei Zhang (currently at Institute of Mechanics, Chinese Academy of Sciences)
- Dr. Carlos Michelén-Ströfer (currently at Sandia National Lab.)

Dr. X.L. Zhang

Reference

- X.-L. Zhang, C. Michelén-Ströfer, H. Xiao. Regularization of ensemble Kalman methods for inverse problems. *Journal of Computational Physics*, 416, 109517, 2020

Outline

Turbulence Modeling with RANS

- 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*. We use data assimilation methods to achieve this goal.

Source of Model Uncertainty in RANS Equations

- Incompressible Navier–Stokes equations:

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

- Reynolds Decomposition: $u_i = U_i + u_i'$ and $p = P + p'$
- Reynolds-Averaged Navier-Stokes Equations:

$$\nabla \cdot \mathbf{U} = 0$$
$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} - \nu \nabla^2 \mathbf{U} + \frac{1}{\rho} \nabla P = \nabla \cdot \boldsymbol{\tau} \quad \text{where } \tau_{ij} = -\overline{u_i' u_j'}$$

Reynolds stress is the source of model uncertainty in RANS equations.

Hierarchy of RANS Turbulence Models[1]

Reynolds stress closure is the source of model uncertainty in RANS equations.

- Eddy viscosity models: compute eddy viscosity ν_t and use Boussinesq assumption: $\operatorname{dev}(\boldsymbol{\tau}) = \nu_t \left(\nabla \mathbf{U} + (\nabla \mathbf{U})^\top \right)$ to obtain $\boldsymbol{\tau}$
- Reynolds stress transport models: solve a transport PDE for the Reynolds stress tensor τ_{ij} to close RANS

RANS equations

$$\frac{D\bar{\mathbf{u}}}{Dt} + \frac{1}{\rho}\nabla \bar{p} - (\nabla \cdot \nu \nabla)\bar{\mathbf{u}} = \nabla \cdot \boldsymbol{\tau}$$

Eddy viscosity models

$$\boldsymbol{\tau} + \frac{2k}{3}\mathbf{I} = 2\nu_t \mathbf{S} \qquad \nu_t = C_\mu \frac{k^2}{\varepsilon}$$

$$\frac{Dk}{Dt} + \nabla \cdot T_k = P_k - \varepsilon$$

[1] Xiao and Cinnella. Quantification of model uncertainty in RANS simulations: A review. Progress in Aerospace Sciences. 108, 1-31, 2019.

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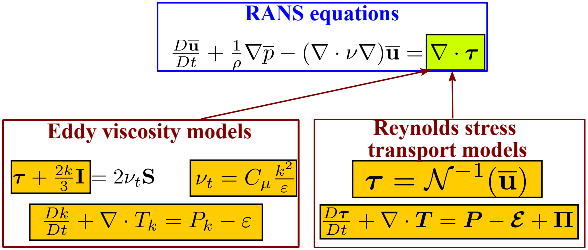

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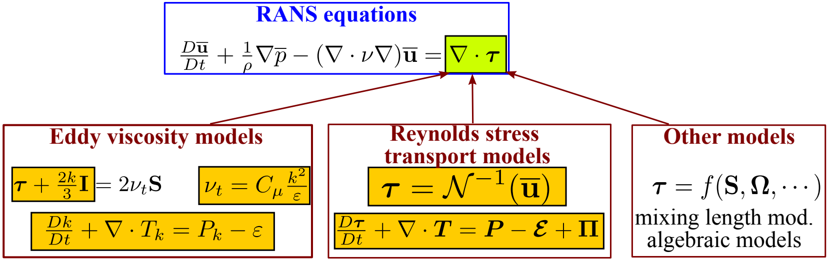


[1] Xiao and Cinnella. Quantification of model uncertainty in RANS simulations: A review. Progress in Aerospace Sciences. 108, 1-31, 2019.

Reducing RANS Model Uncertainty with Data[2]

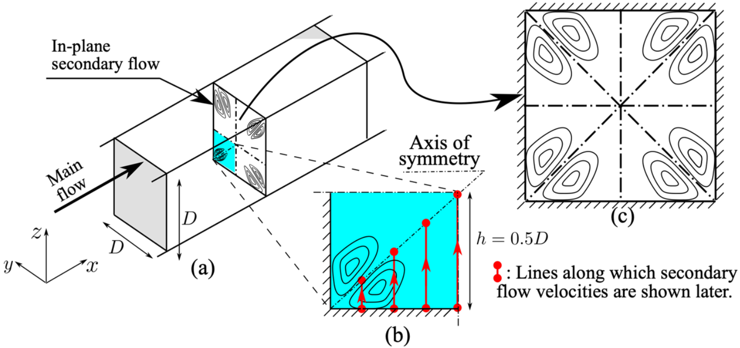
Using EnKF to quantity and reduce RANS model uncertainty:

- With data (e.g., sparse observation of velocities), one can reduce the uncertainties in the modeled Reynolds stresses.
- This can lead to an improved prediction of velocity fields in unobserved locations.

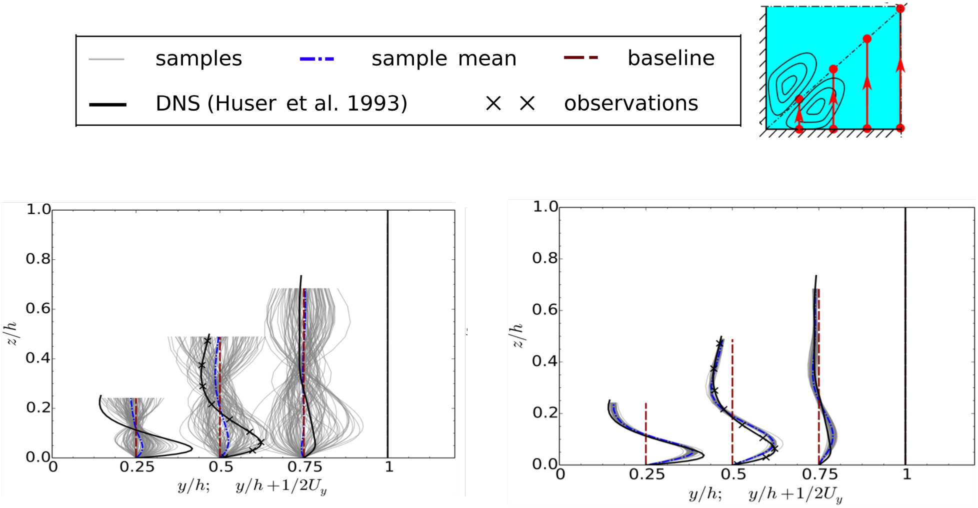
[2] Xiao, Wu, Wang, Sun, Roy. Quantifying and reducing model-form uncertainties in Reynolds-averaged Navier–Stokes simulations: A data-driven, physics-informed Bayesian approach. *J. of Computational Physics*, 115-136, 2016.

Example: Flow Reconstruction in Square Duct - Setup

- Flow in a square duct
- Features in-plane flows driven by normal Reynolds stress imbalance $\tau_{yy} - \tau_{zz}$



Second Flow Velocities in Square Duct



Prior

Posterior

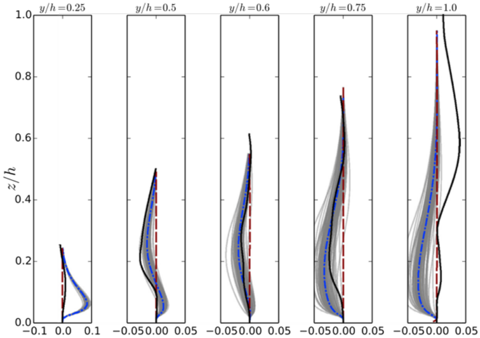
Ill-Posedness in Turbulent Field Inversion: Challenges

Can we infer Reynolds stresses?

- *Not yet, at least not with velocity data alone.*
- The mapping is highly non-unique: many Reynolds stress $\boldsymbol{\tau}(\boldsymbol{x})$ fields produce the same velocity U field, or at least when observed sparsely.
- Can only give the projection $\boldsymbol{\tau}(\boldsymbol{x})$ informed by the observed in-plane velocity:

$$\tau_{yy} - \tau_{zz}$$

Inferred $\tau_{yy} - \tau_{zz}$



Vorticity transport PDE:

$$\frac{D\omega_x}{Dt} = \nu\nabla^2\omega_x + \omega_x\frac{\partial U}{\partial x} + \omega_y\frac{\partial U}{\partial y} + \omega_z\frac{\partial U}{\partial z} + \frac{\partial^2\tau_{yz}}{\partial y^2} - \frac{\partial^2\tau_{yz}}{\partial z^2} - \frac{\partial^2}{\partial y\partial z}(\tau_{yy} - \tau_{zz})$$

Turbulent Field Inversion and Ill-Posedness: Ideas

Need to impose more physical constraints:

- Positive definiteness (realizability) - *similar to inferring permeability* κ
- Boundary conditions[3]
- Smoothness
- Representation with better basis (Karhunen–Loève modes): the field is governed by a transport PDE.[4]

Alternatively, we can simplify the problem by inferring eddy viscosity field ν_{t} and accepting the Boussinesq assumption $\mathrm{dev}(\boldsymbol{\tau}) = \nu_t \left(\nabla \mathbf{U} + (\nabla \mathbf{U})^\top\right)$.
But even inferring ν_{t} can be difficult . . .

[3] Michelén-Ströfer, Zhang, Xiao, Delgosha. Enforcing boundary conditions on physical fields in Bayesian inversion. *Computer Methods in Applied Mechanics and Eng.*, 367:113097, 2020.

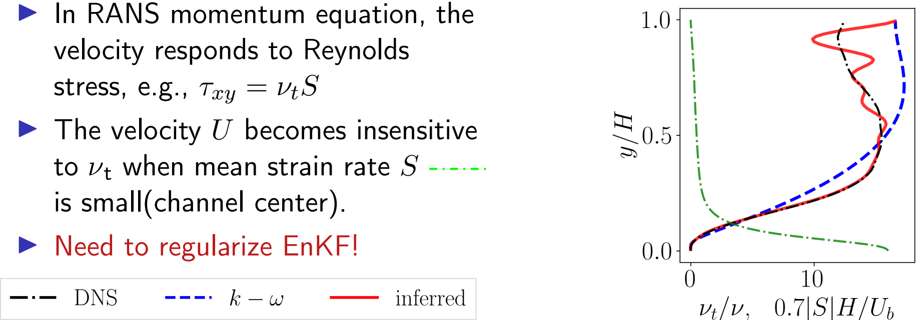
[4] Wu, Michelén-Ströfer, Xiao. Physics-informed covariance kernel for model-form uncertainty quantification with application to turbulent flows. *Computers & Fluids*, 193:104292, 2019.

Ill-Posedness in Turbulence Field Inversion

Given velocity measurement, find the eddy viscosity field or Reynolds stress field that give the best agreement with data.

- Such a field inversion problem is essential in shed light in turbulence modeling
- Eddy viscosity ν_t is not a physical quantity in general flows; Reynolds stress field $\boldsymbol{\tau}$ is difficult to measure.

- In RANS momentum equation, the velocity responds to Reynolds stress, e.g., $\tau_{xy} = \nu_t S$
- The velocity U becomes insensitive to ν_t when mean strain rate S -·-·- is small(channel center).
- Need to regularize EnKF!



Outline

Background: Regularization in Adjoint Methods

Formulation of inversion

$$\mathrm{x}^{\mathrm{opt}} = \arg\min_{\mathrm{x}} J \quad \text{with} \quad J(\mathrm{x}) = \left\| \mathrm{x} - \mathrm{x}^{\mathrm{f}} \right\|^2_{\mathrm{P}^{-1}} + \| \mathcal{H}[\mathrm{x}] - \mathrm{y} \|^2_{\mathrm{R}^{-1}}$$

Regularization

- For ill-posed problem: introducing a constraint $\mathcal{G}[\mathrm{x}] = 0$ into the cost function (e.g., smoothness, sparsity, prior). See, for example, Dow and Wang (2011)
- Regularization in adjoint based optimization (e.g., variational data assimilation) is straightforward: add a regularization (penalty) term $\mathcal{G}[\mathrm{x}] = 0$ into the objective function:

$$J(\mathrm{x}) = \|\mathrm{x} - \mathrm{x}^{\mathrm{f}}\|^2_{\mathrm{P}^{-1}} + \|\mathcal{H}[\mathrm{x}] - \mathrm{y}\|^2_{\mathrm{R}^{-1}} + \lambda \|\mathcal{G}[\mathrm{x}]\|^2_{\mathrm{Q}^{-1}}$$

Equivalence between Adjoint and Ensemble Methods

$$J(\mathrm{x}) = \left\|\mathrm{x} - \mathrm{x}^{\mathrm{f}}\right\|^2_{\mathrm{P}^{-1}} + \|\mathcal{H}[\mathrm{x}] - \mathrm{y}\|^2_{\mathrm{R}^{-1}} + \|\mathcal{G}[\mathrm{x}]\|^2_{\mathrm{Q}^{-1}}$$

- The update scheme of EnKF is derived by maximizing the *a posteriori* probability
- Therefore, this maximization is implicit in the Kalman update scheme.
- Objective: modify the filtering scheme in EnKF to achieve the same regularization as in adjoint method.

$J(x) = \|H\mathcal{F}(x) - d\|^2_R + \|x - x_0\|^2_P$	$J(x) = \|H\mathcal{F}(x) - d\|^2_R + \|x - x_0\|^2_P + \|G(x)\|^2_W$
$\vdots$	$\vdots$
$x_{post} = x_{prior} + K\left(d - H\mathcal{F}(x_{prior})\right)$	$x_{post} = x_{prior} + K\left(d - H\mathcal{F}(x_{prior})\right) + K_2 G(x_{prior})$

Regularized Ensemble Kalman Filter[5] (1/2)

- Can we derive an analysis that is equivalent to the regularization term in adjoint methods?

$$J(\mathsf{x}_j) = \|\mathsf{x}_j - \mathsf{x}_j^{\mathsf{f}}\|^2_{\mathsf{P}^{-1}} + \|\mathcal{H}[\mathsf{x}_j] - \mathsf{y}_j\|^2_{\mathsf{R}^{-1}} + \|\mathcal{G}[\mathsf{x}_j]\|^2_{\mathsf{Q}^{-1}}.$$

$$\mathsf{P}^{-1}(\mathsf{x}_j^{\mathsf{a}} - \mathsf{x}_j^{\mathsf{f}}) + (\mathcal{H}'[\mathsf{x}_j^{\mathsf{a}}])^\top \mathsf{R}^{-1}(\mathcal{H}[\mathsf{x}_j^{\mathsf{a}}] - \mathsf{y}_j) + \mathcal{G}'[\mathsf{x}_j^{\mathsf{a}}]^\top \mathsf{Q}^{-1}\mathcal{G}[\mathsf{x}_j^{\mathsf{a}}] = 0.$$

- Assumptions for simplification

$$\mathcal{H}[\mathsf{x}_j^{\mathsf{a}}] \approx \mathcal{H}[\mathsf{x}_j^{\mathsf{f}}] + \mathcal{H}'[\mathsf{x}_j^{\mathsf{f}}](\mathsf{x}_j^{\mathsf{a}} - \mathsf{x}_j^{\mathsf{f}}),$$
$$\mathsf{H} \equiv \mathcal{H}'[\mathsf{x}_j^{\mathsf{a}}] \approx \mathcal{H}'[\mathsf{x}_j^{\mathsf{f}}]$$
$$\mathcal{G}[\mathsf{x}^{\mathsf{f}}] \approx \mathcal{G}[\mathsf{x}^{\mathsf{a}}], \qquad \mathcal{G}'[\mathsf{x}^{\mathsf{f}}] \approx \mathcal{G}'[\mathsf{x}^{\mathsf{a}}]$$

- Kalman gain matrix: $\mathsf{K} = \mathsf{P}\mathsf{H}^\top(\mathsf{R} + \mathsf{H}\mathsf{P}\mathsf{H}^\top)^{-1}$

[5] Zhang, Michelén-Ströfer, Xiao. Regularized ensemble Kalman methods for inverse problems. *J. Computational Physics*, 416, 109517, 2020.

Regularized Ensemble Kalman Filter (2/2)

- Derived analysis scheme:

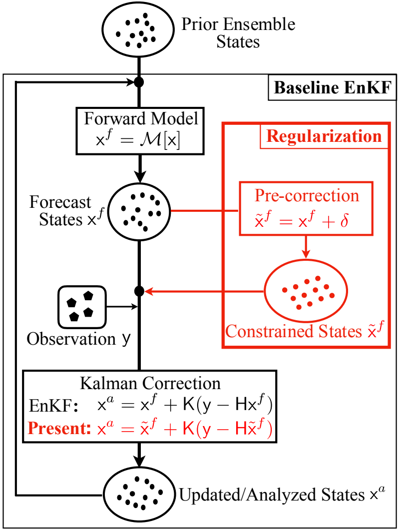
$$\mathrm{x}_j^a = \mathrm{x}_j^f \underbrace{- \mathrm{P}(I + \mathrm{H}^\top \mathrm{R}^{-1}\mathrm{HP})^{-1} \mathcal{G}'^\top \mathrm{Q}^{-1}\mathcal{G}}_{\text{regularization term}} \underbrace{+ \mathrm{PH}^\top(\mathrm{R} + \mathrm{HPH}^\top)^{-1}(\mathrm{y}_j - \mathrm{Hx}_j^f)}_{\text{Kalman correction}}$$

- Re-written to a pre-correction form:

$$\boxed{\tilde{\mathrm{x}}_j^f = \mathrm{x}_j^f + \delta}, \quad \text{with } \delta = -\mathrm{P}\mathcal{G}'^\top \mathrm{Q}^{-1}\mathcal{G}$$

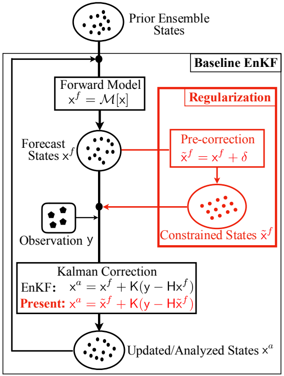
$$\mathrm{x}_j^a = \tilde{\mathrm{x}}_j^f + \mathrm{K}(\mathrm{y}_j - \mathrm{H}\tilde{\mathrm{x}}_j^f)$$

- This is similar to the baseline EnKF except for the correction (boxed)



Regularized Ensemble Kalman Filter: Implementation

- Built general constraints into EnKF
- Derived regularization for ensemble methods equivalent to that in adjoint methods
- Bridges the gap between regularization in adjoint- and ensemble-based methods
- Requires only minor algorithmic modifications



Open-source implementation in Python[6]. Code: github.com/xiaoh/DAFI

[6] Michelén-Ströfer, Zhang, Xiao. DAFI: An open-source framework for ensemble-based data assimilation and field inversion. *Comm. Computational Physics*, 29, 1583-1622, 2021.

Test 1: Demonstration on Toy Problem - Setup

- State: $\boldsymbol{\omega} = [\omega_1, \omega_2]^\top$
- Model (adopted from Wu et al. 2019):

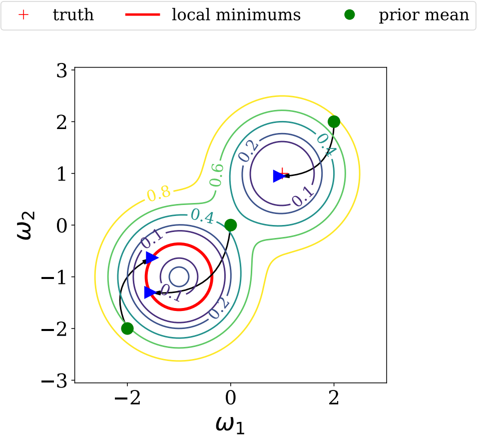
$$\mathbf{z} = \begin{bmatrix} \exp(-(\omega_1+1)^2 - (\omega_2+1)^2) \\ \exp(-(\omega_1-1)^2 - (\omega_2-1)^2) \end{bmatrix}$$

- Observation mapping:

$$\mathrm{y} = H\mathbf{z}, \;\; H = [-1.5, -1.0]$$

- Truth $\boldsymbol{\omega} = (1.0, 1.0)$
- Local minima (circle):

$$(\omega_1+1)^2 + (\omega_2+1)^2 = \log 1.5$$



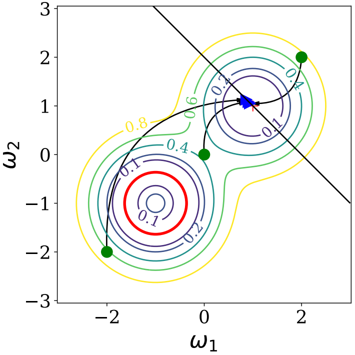
EnKF inference results depends on the prior initial states.

Test 1: Demonstration on Toy Problem - Results

Test 1: Equality constraint

$$h_{\text{eq}}[\boldsymbol{\omega}] = \omega_1 + \omega_2 - 2 = 0$$

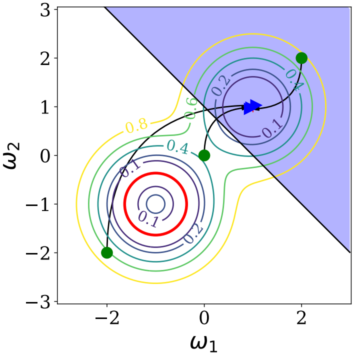
$$\mathcal{G}(\boldsymbol{\omega}) = h_{\text{eq}}[\boldsymbol{\omega}]$$



Test 2: Inequality constraint

$$h_{\text{in1}}[\boldsymbol{\omega}] = -\omega_1 - \omega_2 + 1 < 0$$

$$\mathcal{G}(\boldsymbol{\omega}) = \max\left(0, (h_{\text{in}}[\boldsymbol{\omega}])^2\right)$$



Test 2: Inferring Diffusivity From Temperature - Setup

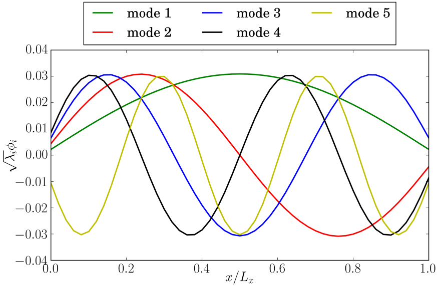
- Objective: infer diffusivity field $\mu[x]$ from observations of temperature u

$$-\frac{d}{dx}\left(\mu[x]\frac{du}{dx}\right) = f[x]$$

$$f[x] = 100\sin(2\pi x/L_x)$$

$$u|_{x=0} = u|_{x=L_x} = 0$$

- Synthetic truth: only first 3 modes are nonzero
- Observation data at $x/L = 0.1, 0.2, \ldots, 0.9$

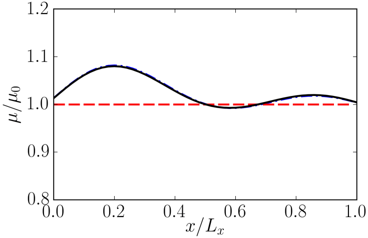


Karhunen–Loève Modes

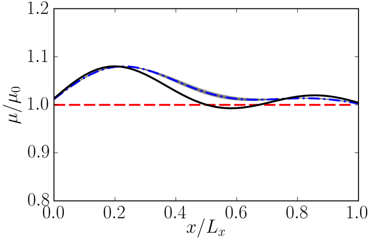
Penalty function: $\mathcal{G}[\boldsymbol{\omega}] = \boldsymbol{\omega}$
Weight matrix: $\mathsf{Q}^{-1} = \mathrm{diag}\left(\frac{1}{n}, \frac{2}{n}, \frac{3}{n}, \ldots, \frac{n-1}{n}, 1\right)$

Test 2: Inferring Diffusivity From Temperature - Results

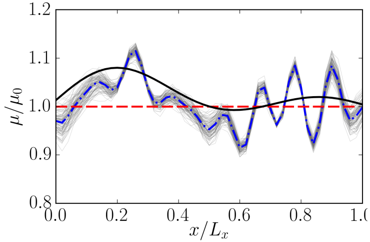
Baseline, 3 modes:



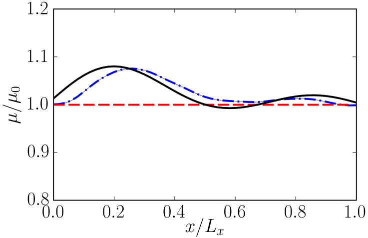
Regularized, 3 modes:



Baseline, 20 modes:

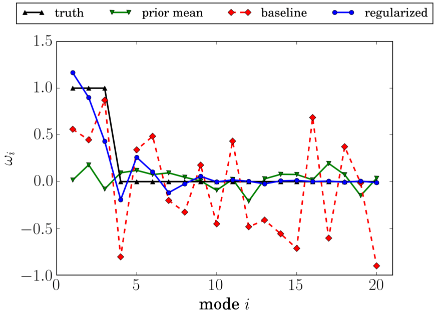


Regularized, 20 modes:

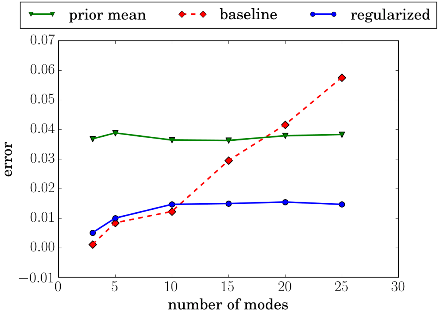


Test 2: Inferring Diffusivity From Temperature - Error

$$-\frac{d}{dx}\left(\mu[x]\frac{du}{dx}\right) = f[x]$$



Inferred Coefficients

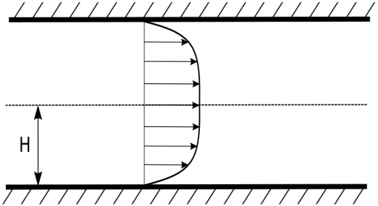


Error vs. no. of Modes

Outline

Inversion of Eddy Viscosity in Channel Flows: Setup[7]

- Observation: streamwise velocity U
- Inferred quantity: eddy viscosity $\nu_{\mathrm{t}}(\mathrm{x})$



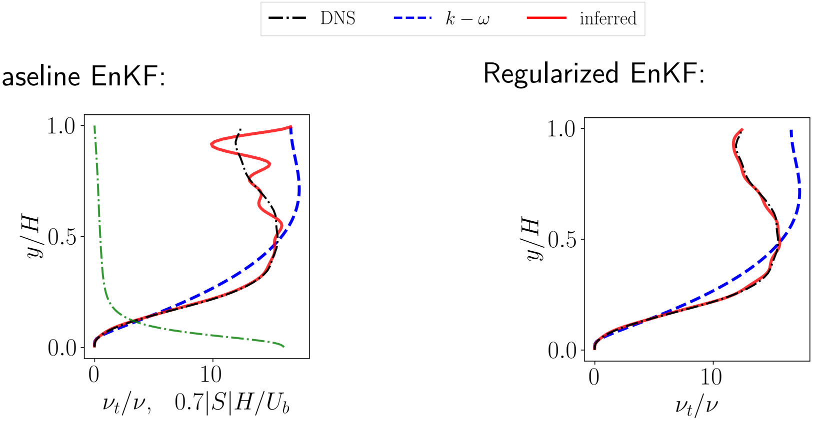
[7] Zhang, Xiao, He. Regularized ensemble Kalman inversion of turbulence quantity fields. *Submitted*.

Inversion of Eddy Viscosity in Channel Flows: Results

- Smoothness regularization is essential in recovering ν_t in the channel center
- Baseline EnKF cannot obtain accurate inversion due to the ill-conditioning in channel center

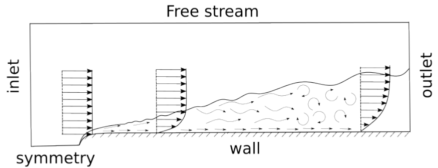
Baseline EnKF:

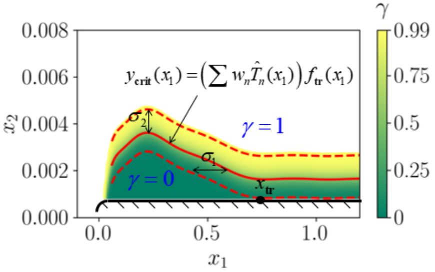
Regularized EnKF:



Inferring Laminar-Turbulent Intermittency: Setup

- The intermittency is an indicator of the larminar region and the turbulent region. ($\gamma = 0$: laminar region; $\gamma = 1$: turbulent region)
- Parameterization of the intermittency field with sigmod function (transition from ($\gamma = 0$ to $\gamma = 1$
- Regularization on the prior value of the transition point
- Regularization on the sparsity of the Chebyshev mode

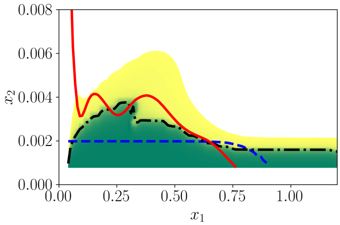




Inferring Laminar-Turbulent Intermittency: Results γ

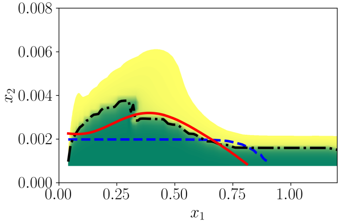
- Regularization leads to smooth intermittency field
- The inferred field is close to the results of Langtry-Menter transition model

Baseline, Level $\gamma = 0.5$



initial — Langtry-Menter — inferred

Regularize, Level $\gamma = 0.5$

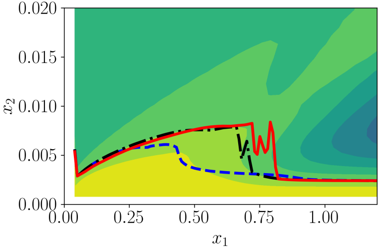


Inferring Laminar-Turbulent Intermittency: Results ν_t

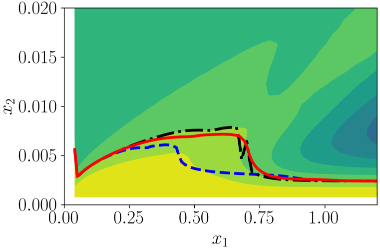
Regularization leads to better agreements with synthetic truth (Langtry-Menter).

Background is the contour for γ

Baseline, Level $\nu_t/\nu = 6.7$



Regularize, Level $\nu_t/\nu = 6.7$



Conclusion

- We used observation data to quantify and reduce model uncertainty in RANS simulations.
- Inferring latent field $(\nu_{\mathrm{t}}, \boldsymbol{\tau})$ is ill-conditioned and need regularization
- To this end, we proposed a regularized EnKF method to enforce constraints, with preliminary success in application of turbulence field inversion

Additional:

- Preliminary efforts in combining data assimilation and machine learning.

Outline

1. Background: Ill-Posedness in Turbulence Modeling
2. Regularization of EnKF
3. Application to Turbulence Field Inversion
4. Data Assimilation for Learning Physical Models
5. Conclusion

From Field Inversion to Model Learning (1/2)

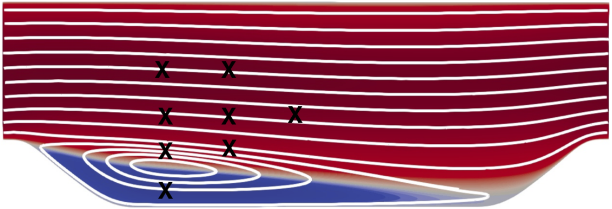
Scenario: Inferring Reynolds stress from velocity

Consider the Reynolds averaged Navier-Stokes equation

$$\mathbf{U} \cdot \nabla \mathbf{U} - \nu \nabla^2 \mathbf{U} + \frac{1}{\rho} \nabla P = \nabla \cdot \boldsymbol{\tau} \quad \text{or concisely,} \quad \mathcal{N}[\mathbf{u}] = \nabla \cdot \boldsymbol{\tau}$$

Assume:

- Reynolds stress field $\boldsymbol{\tau}(\mathbf{x})$ is the only known quantity (field)
- Sparse observations velocities are available in the domain ($\times$)



From Field Inversion to Model Learning (2/2)

Data Assimilation

- What is the Reynolds stress field $\boldsymbol{\tau}(\mathbf{x})$ that, after feeding to the physical solver, would give the best agreement with observed velocity?

$$\mathcal{N}[\mathbf{U}] = \nabla \cdot \boldsymbol{\tau}(\mathbf{x})$$

- Specific to this configuration. The field inferred from this observation cannot be generalized to different systems (configurations).

Machine Learning

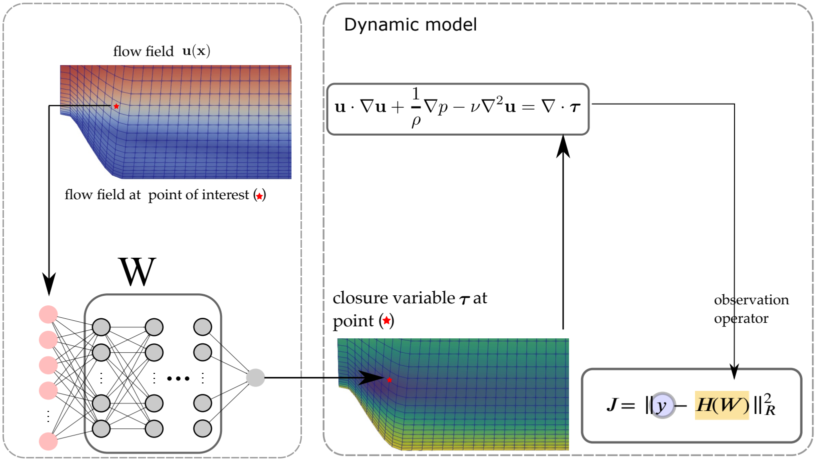
(from sparse observations)

- What is the closure model $\boldsymbol{\tau} = f(\mathbf{U}; W)$ that give the Reynolds stress field that in turn leads to best agreement with observed velocity?

$$\mathcal{N}[\mathbf{U}] = \nabla \cdot \boldsymbol{\tau}(\mathbf{U}; W)$$

- Should be universal, at least generalizable to similar configurations.

From Field Inversion to Model Learning[8] (3/3)

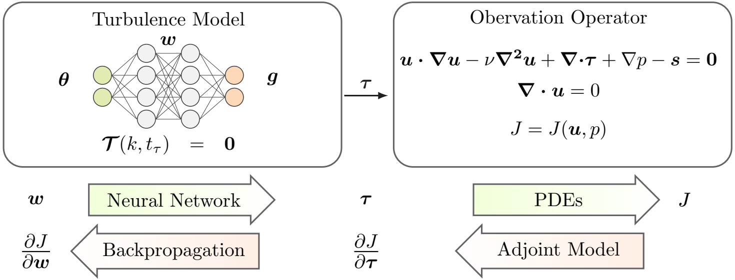


[8] Michelén-Ströfer, Zhang, Xiao. Ensemble gradient for learning turbulence models from indirect observations, 2021. Submitted. Available at: arxiv: 2104.07811

Combining Neural Networks and Adjoint for Model Learning[9]

- Learn neural-network-based turbulence model from observed velocities
- Adjoint based optimization. Gradient w.r.t. $\boldsymbol{\omega}$ via chain rule:

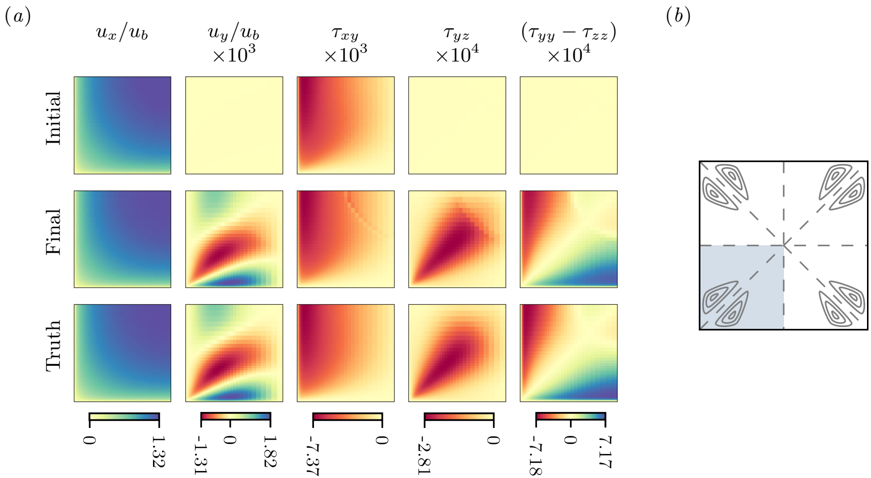
$$\frac{\partial J}{\partial \boldsymbol{w}} = \frac{\partial J}{\partial \boldsymbol{\tau}} \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{w}}$$



[9]Michelén-Ströfer, Xiao. End-to-end differentiable learning of turbulence models from indirect observations. *Theoretical and Applied Mechanics Letters*. arxiv: 2104.04821

Differential Framework for Model Learning

Learn Reynolds stress from velocity observations: square duct



Using Ensemble to Compute Gradient

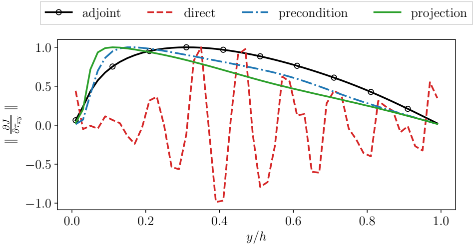
- Fully differential framework is desirable, but adjoint can be expensive to develop
- Propose using ensemble simulations to compute gradient

$$\nabla_\tau J = \left((\Delta\tau^\top \Delta\tau + \lambda \mathsf{I})^{-1} \Delta\tau^\top \right)^\top \left(\Delta U^\top \mathsf{R}^{-1} \left(\mathcal{H}(\tau) - \mathsf{y} \right) \right)$$

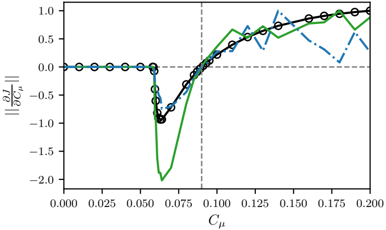
  - State representation: $\tau = \overline{\tau} + \beta \Delta\tau$
  - Chain rule to compute gradient: $\nabla_\tau J = \nabla_\beta J \cdot \nabla_\tau \beta$
  - $\nabla_\beta J = \Delta U^\top \mathsf{R}^{-1} \left(\mathcal{H}(\tau) - \mathsf{y} \right)$
  - $\nabla_\tau \beta = (\Delta\tau^\top \Delta\tau + \lambda \mathsf{I})^{-1} \Delta\tau^\top$

Ensemble Gradient vs. Adjoint Gradient

- Ensemble method provides a smooth estimation of the sensitivity and give the same gradient direction as the adjoint method.
- Sensitivity to C_μ with ensemble method has different magnitude, but the ensemble gradients result in the same sign and same zero as from the adjoint in the search region near the true value.



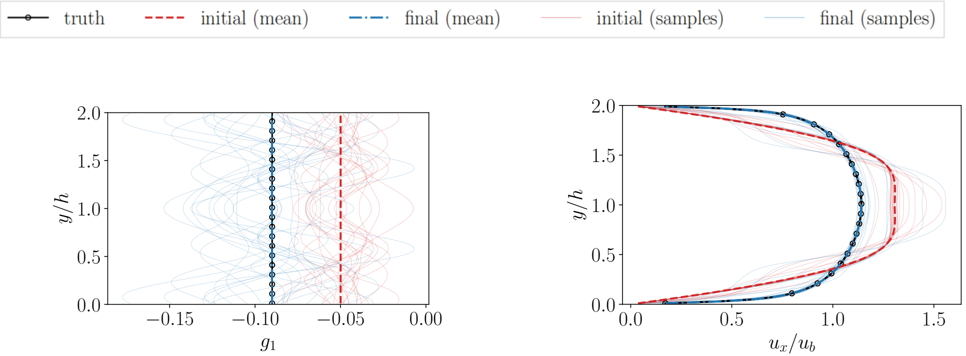
Gradient



Gradient vs. C_μ

Ensemble Gradient for Learning Eddy Viscosity Model

- Use the observation of velocity to learn the eddy viscosity
- The trained model not only results in the correct velocity but learns the true underlying model for $g_1 (= -C_\mu)$



Learned coefficient $(-C_\mu)$

Learned velocity U

Outline

1. Background: Ill-Posedness in Turbulence Modeling
2. Regularization of EnKF
3. Application to Turbulence Field Inversion
4. Data Assimilation for Learning Physical Models
5. Conclusion

Conclusion (again)

- We used observation data to quantify and reduce model uncertainty in RANS simulations.
- Inferring latent field $(\nu_{\mathrm{t}}, \boldsymbol{\tau})$ is ill-conditioned and need regularization
- To this end, we proposed a regularized EnKF method to enforce constraints, with preliminary success in application of turbulence field inversion
- Preliminary efforts in combining data assimilation and machine learning.

References

1. EnKF-based mean velocity construction:
   - Xiao, Wu, Wang, Sun, Roy. Quantifying and reducing model-form uncertainties in Reynolds-averaged Navier–Stokes simulations: A data-driven, physics-informed Bayesian approach. *J. of Computational Physics*, 115-136, 2016.
2. Regularization of EnKF:
   - Zhang, Michelén-Ströfer, Xiao. Regularized ensemble Kalman methods for inverse problems. *J. of Computational Physics*, 416, 109517, 2020.
3. Python implementation:
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4. Enforcing boundary conditions and PDE-informed covariance:
   - Michelén-Ströfer, Zhang, Xiao, Delgosha. Enforcing boundary conditions on physical fields in Bayesian inversion. *Computer Methods in Applied Mechanics and Eng.*, 367:113097, 2020.
   - Wu, Michelén-Ströfer, Xiao. Physics-informed covariance kernel for model-form uncertainty quantification with application to turbulent flows. *Computers & Fluids*, 193:104292, 2019.
5. Application to turbulence modeling:
   - Zhang, Xiao, He. Regularized ensemble Kalman inversion of turbulence quantity fields. *Submitted*.

Thank you

Thank you for you attention.
Questions and comments are appreciated!

Projection Method: EnKF with Constraints

- After Kalman filtering, the projection method projects the updated state onto a constrained surface by solving a constrained optimization problem:

$$\mathsf{x}^{\mathsf{a}} = \arg\min J(\mathsf{x}^{\mathsf{a}} - \hat{\mathsf{x}}^{\mathsf{f}})^{\top} \hat{\mathsf{P}}^{-1} (\mathsf{x}^{\mathsf{a}} - \hat{\mathsf{x}}^{\mathsf{f}}) \quad \text{s. t.} \quad \mathsf{G}\hat{\mathsf{x}}^{\mathsf{a}} = \mathsf{z}$$

- Problem solved with the Lagrange multiplier method:

$$L = (\mathsf{x}^{\mathsf{a}} - \hat{x}^{\mathsf{f}})^{\top} \hat{\mathsf{P}}^{-1} (\mathsf{x}^{\mathsf{a}} - \hat{\mathsf{x}}^{\mathsf{f}}) + 2\lambda^{\top} (\mathsf{G}\hat{\mathsf{x}}^{\mathsf{a}} - \mathsf{z})$$

- This method imposes a hard constraint

Projection Method: EnKF with Constraints

- Taking the first order derivatives w.r.t state and the Lagrange multiplier λ to be zero yields:

$$\frac{\partial L}{\partial \mathsf{x}^{\mathsf{a}}} = \hat{\mathsf{P}}^{-1}(\mathsf{x}^{\mathsf{a}} - \hat{\mathsf{x}}^{\mathsf{f}}) + \mathsf{G}^{\top}\lambda = 0,$$

$$\frac{\partial L}{\partial \lambda} = \mathsf{G}\hat{\mathsf{x}}^{\mathsf{a}} - \mathsf{z} = 0$$

- This leads to

$$\boldsymbol{\lambda} = (\mathsf{G}\hat{\mathsf{P}}\mathsf{G}^{\top})^{-1}(\mathsf{G}\hat{\mathsf{x}}^{\mathsf{f}} - \mathsf{z})$$

$$\mathsf{x}^{\mathsf{a}} = \hat{\mathsf{x}}^{\mathsf{f}} - \hat{\mathsf{P}}\mathsf{G}^{\top}(\mathsf{G}\hat{\mathsf{P}}\mathsf{G}^{\top})^{-1}(\mathsf{G}\hat{\mathsf{x}}^{\mathsf{f}} - \mathsf{z})$$

Pseudo Observation Method: EnKF with Constraints

- Augment the observation with the constraints:

$$\begin{bmatrix} \mathsf{y} \\ \mathsf{z} \end{bmatrix} = \begin{bmatrix} \mathsf{H} \\ \mathsf{G} \end{bmatrix} \mathsf{x} + \begin{bmatrix} \epsilon \\ 0 \end{bmatrix}$$

$$\tilde{\mathsf{R}} = \begin{bmatrix} \mathsf{R} & 0 \\ 0 & 0 \end{bmatrix}$$

- Extended to enforce soft constraints by adding noise in the constraint function and modified the error covariance matrix
- The observation augmentation method is equvalent to projection method (Simon, 2010)
- No change in Kalman updating, but observation matrix can be large – expensive for matrix inversion.
- Cannot handle inequality constraints.