

# **Data-driven approaches to physical modelling (in CFD)**

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# (Turbulence) modelling in the age of data

*[Data] has historically been used to calibrate simple engineering models... with the availability of large and diverse datasets, researchers have begun to explore methods to systematically inform turbulence models with data.*

– (Duraisamy, Iaccarino, and Xiao 2019)

## Open question

How can we exploit large high-resolution data-sets to improve the physical understanding and modelling of the physics (of turbulence)?



Amorphous data



Physical understanding

## Basic problem statement: Regression

DETERMINISTICALLY:

- ▶ Inputs/features  $x_i \in \mathbb{R}^{N_x}$  known at  $M$
- ▶ Outputs/data  $y \in \mathbb{R}^{N_y}$
- ▶ Find  $q : \mathbb{R}^{N_x} \rightarrow \mathbb{R}^{N_y}$  minimizing the *residual sum-of-squares*:

$$\mathcal{L}(q) := \frac{1}{M} \sum_{k=1}^M (y_i - q(x_i))^2$$

STATISTICALLY:

- ▶ Random variables  $X : \Omega \rightarrow \mathbb{R}^{N_x}$  and  $Y : \Omega \rightarrow \mathbb{R}^{N_y}$  with joint density  $\mathbb{P}(X, Y)$
- ▶ Find  $q : \mathbb{R}^{N_x} \rightarrow \mathbb{R}^{N_y}$  minimizing the *expected prediction error*:

$$\mathbb{E}_{X,Y}(Y - q(X))^2 := \int (y - q(x))^2 d\mathbb{P}(X, Y)$$

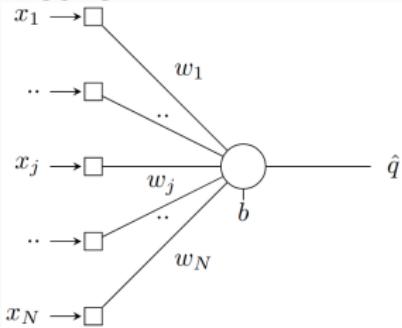
- ▶ With exact solution  $q(x) = \mathbb{E}(Y | X = x)$

## **Method 1: Physics-Informed Neural Networks (PINNs)**

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# Neural Networks - Definition

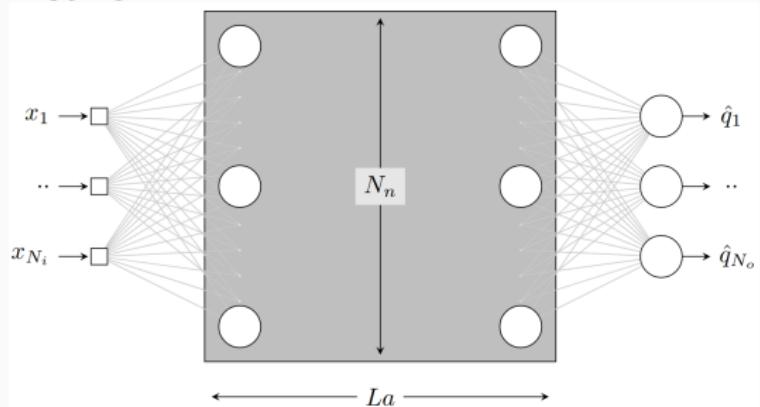
## Neuron



$$\sigma(x) : \mathbb{R} \rightarrow \mathbb{R}$$

$$\hat{q} := \sigma \left( \sum_{i=1}^N w_i x_i + b \right)$$

## Network



Single “layer”  $\ell \in \{1, \dots, L\}$ :

$$\mathbf{x}^\ell := \sigma \left( W^\ell \cdot \mathbf{x}^{\ell-1} + \mathbf{b}^\ell \right)$$

$$\mathbf{x}^{\ell-1}, \mathbf{x}^\ell, \mathbf{b}^\ell \in \mathbb{R}^N \quad W^\ell \in \mathbb{R}^{N \times N}$$

Network:

$$\hat{\mathbf{q}} := \sigma(W^L \sigma(W^{L-1} \sigma(\dots) + \mathbf{b}^{L-1}) + \mathbf{b}^L) \quad 5$$

# Neural Networks - Fitting/training/learning

## Standard linear (aka *sane*) regression

Function representation ( $P$  basis functions  $\varphi_p(\cdot)$ ):

$$\hat{q}_{\text{LIN}}(\mathbf{x}) := \sum_{p=1}^P \theta_p \varphi_p(\mathbf{x})$$

Solve, given  $M$  data-pairs  $(\mathbf{x}_k, y_k)$ :

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^P} \sum_{k=1}^M |y_k - \hat{q}_{\text{LIN}}(\mathbf{x}_k)|^2$$

Quadratic optimization problem  $\implies A^T A \boldsymbol{\theta} = A^T \mathbf{y}$ .

Neural networks, solve:

$$\min_{\substack{W^0, \dots, W^L \in \mathbb{R}^{N \times N}; \\ b^0, \dots, b^L \in \mathbb{R}^N}} \sum_{k=1}^M |y_k - \hat{q}_{NN}(\mathbf{x}_k)|^2$$

# Physics informed Neural Networks (PINNs)

Given a nonlinear PDE (e.g. Navier-Stokes) in  $\mathbf{x} \in \Omega \subset \mathbb{R}^3$ ,

$$\mathcal{N}(u) = (\mathbf{u} \cdot \nabla)u + \nabla p - \nu \nabla^2 u = 0,$$

with Dirichlet boundary-conditions  $u = u_{\partial\Omega}$  on the boundary of  $\Omega$ .

Then represent  $u$  as a NN  $\hat{u}(\mathbf{x})$ , and solve:

$$\min_{\substack{W^0, \dots, W^L \in \mathbb{R}^{N \times N}; \\ b^0, \dots, b^L \in \mathbb{R}^N}} \|\hat{u} - u_{\partial\Omega}\|_{\partial\Omega}^2 + \|\mathcal{N}(\hat{u})\|_{\Omega}^2$$

or approximately:

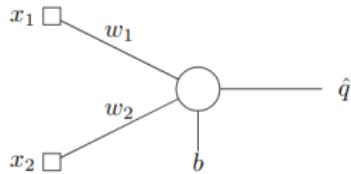
$$\min_{\substack{W^0, \dots, W^L \in \mathbb{R}^{N \times N}, \\ b^0, \dots, b^L \in \mathbb{R}^N}} \sum_{i=1}^{N_D} |\hat{u}(\mathbf{x}_i) - u_{\partial\Omega,i}|^2 + \sum_{j=1}^{N_C} |\mathcal{N}(\hat{u})_j|^2$$

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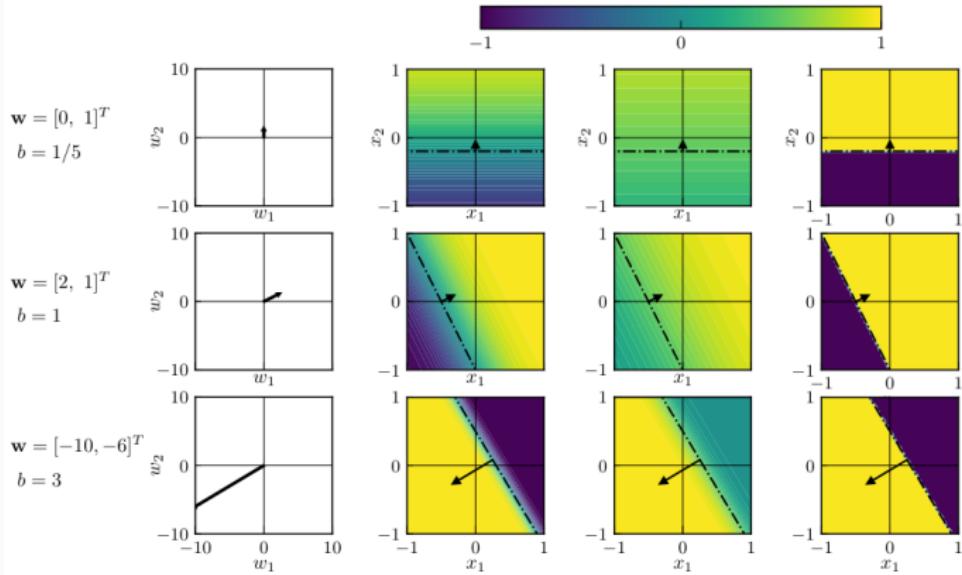
M. Raissi, P. Perdikaris, and G.E. Karniadakis (2019). "Physics-informed neural networks". In: *Journal of Computational Physics* 378, pp. 686–707.

ISSN: 0021-9991. DOI: 10.1016/j.jcp.2018.10.045

# Action of a single neuron



(a) Single artificial neuron with two inputs,  $\mathbf{w} = [w_1, w_2]$  and bias  $b$



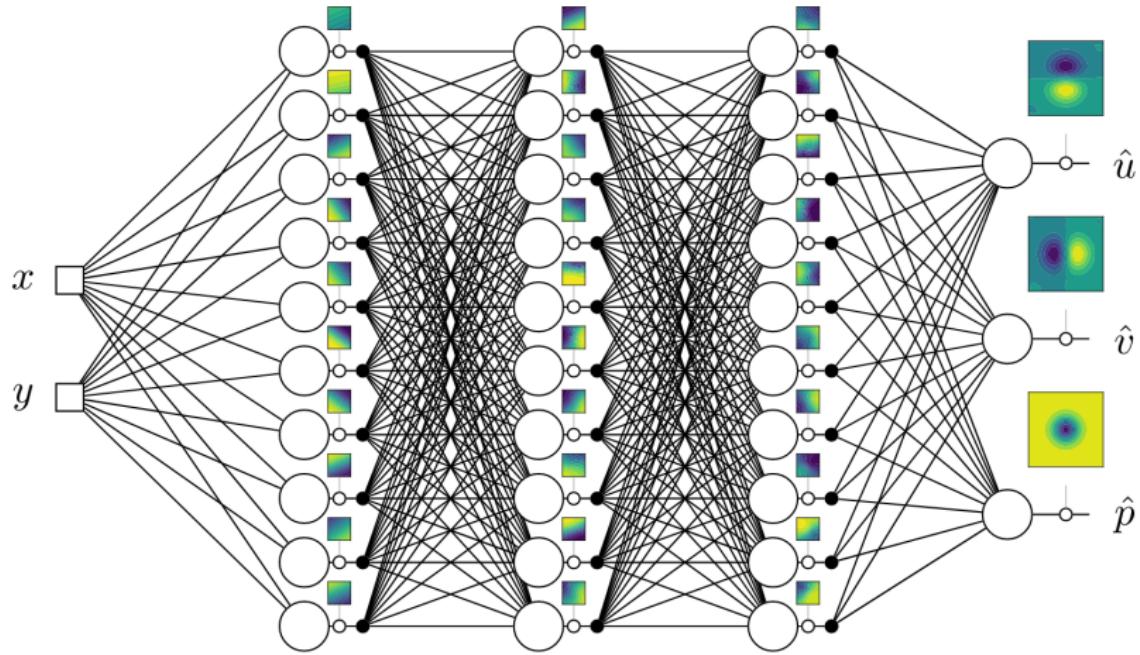
(b) weights and biases

(c)  $\sigma = \tanh$

(d)  $\sigma = 1/(1 + e^{-s})$

(e) step function

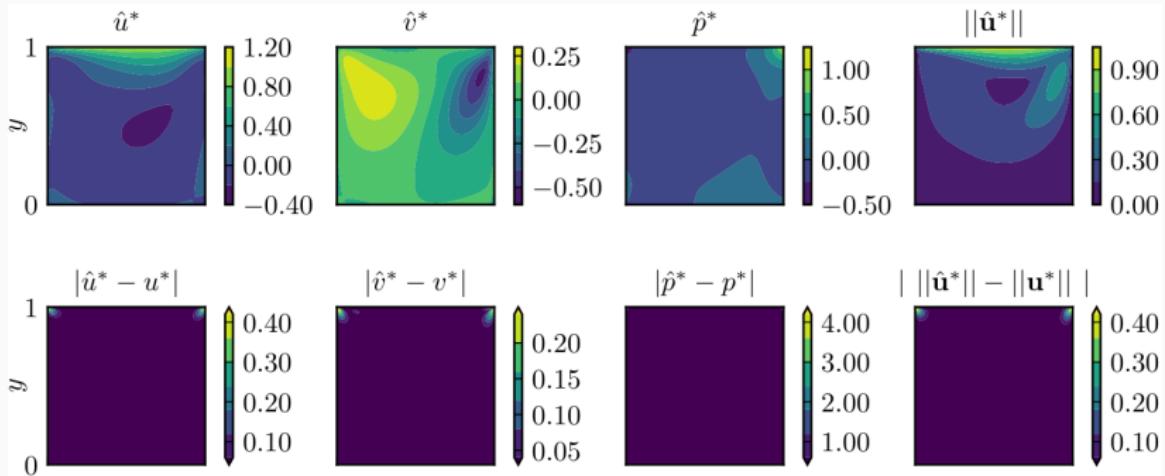
# Action of a network



N. Terleth (2019). "Artificial Neural Networks for Flow Field Inference".  
MA thesis. TU Delft [http://resolver.tudelft.nl/uuid:  
d69a58c4-91ea-4590-9153-c6fa35f374e5](http://resolver.tudelft.nl/uuid:d69a58c4-91ea-4590-9153-c6fa35f374e5)

## Example: Lid-driven cavity

- ▶ 3-layer, 10-neural fully-connected network, tanh activation
- ▶  $N_C = 1000$  collocation points in interior,  $N_D = 200$  boundary points
- ▶ Error computed with respect to OpenFOAM.



# PINNs - Prognosis

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## Excellent:

- ▶ Very flexible framework for eqns + data (data-assimilation!)
- ▶ Always gives a solution!
- ▶ Fun!

## Gloomy:

- ▶ Which equation do you want to solve? (Can't do all!)
- ▶ Always gives a solution!
- ▶ Inherits all the problems of Least-squares finite-elements
- ▶ Training is significantly harder than standard losses
- ▶ Much slower than a standard solver

## **Method 2: Sparse Identification of Nonlinear Dynamical systems (SINDy)**

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# Sparse regression

## Standard linear regression

Model:  $\hat{q}_{\text{LIN}}(\mathbf{x}) := \sum_{p=1}^P \theta_p \varphi_p(\mathbf{x})$

Solve:  $\min_{\boldsymbol{\theta} \in \mathbb{R}^P} \sum_{k=1}^M |y_k - \hat{q}_{\text{LIN}}(\mathbf{x}_k)|^2 = \min_{\boldsymbol{\theta} \in \mathbb{R}^P} \mathcal{L}(\boldsymbol{\theta})$

Regularization (option A =  $L_2$ ):

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^P} [\mathcal{L}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_2^2], \quad \|\boldsymbol{\theta}\|_2^2 := \sum_{p=1}^P |\theta_p|^2$$

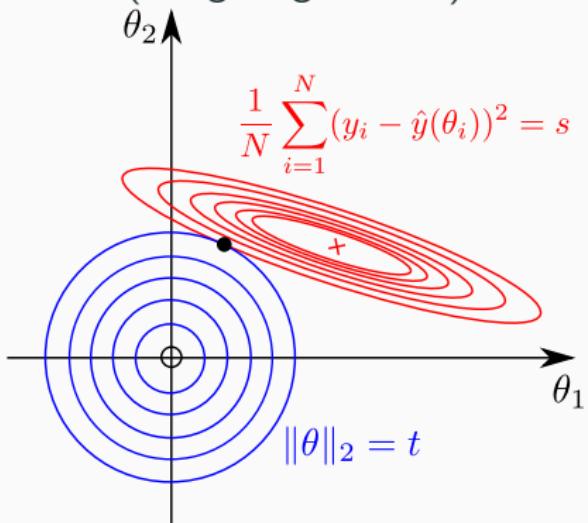
Regularization (option B =  $L_1$ ):

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^P} [\mathcal{L}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_1], \quad \|\boldsymbol{\theta}\|_1 := \sum_{p=1}^P |\theta_p|$$

## Sparse regression (interpretation)

$L_2$  regularized least-squares

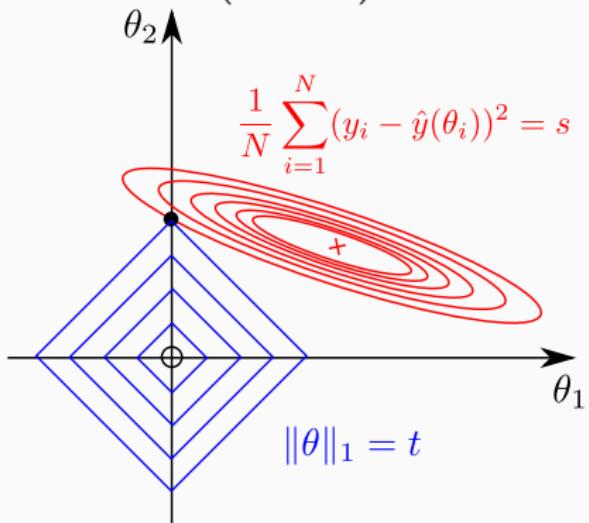
("ridge regression")



$$\min \mathcal{L}(\theta) \text{ s.t. } \|\theta\|_2^2 \leq t$$

$L_1$  regularized least-squares

("lasso")



$$\min \mathcal{L}(\theta) \text{ s.t. } \|\theta\|_1 \leq t$$

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Hastie, Tibshirani, and Friedman (2009). *The Elements of Statistical Learning*. Springer Series in Statistics

# Dictionary methods

## Dictionary methods

1. Generate *masses* of basis functions  $\varphi_p(\mathbf{x})$ ,  $P \gg 100$  in

$$\hat{q}(\mathbf{x}) := \sum_{p=1}^P \theta_p \varphi_p(\mathbf{x})$$

2. Solve

$$\min \mathcal{L}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_1$$

with sufficiently large  $\lambda$  so that most of the  $\theta_p = 0$ .

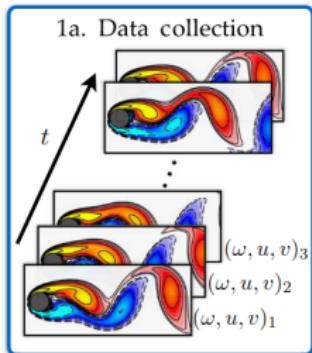
- Dictionary generation, e.g. given features  $(x_1, \dots, x_N)$ , and integers  $(Q_1, \dots, Q_N) \in \mathbb{N}^N$ , choose:

$$\varphi_p(\mathbf{x}) := x_1^{Q_1} \cdot x_2^{Q_2} \cdots x_N^{Q_N}$$

- Or also combined with fundamental functions sin, exp, etc.

# Sparse identification of nonlinear dynamical systems (SINDy)

Full data



$$\omega_t = \Theta(\omega, u, v)\xi$$

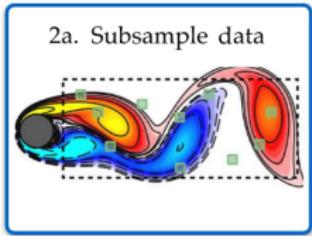
1b. Build nonlinear library of data and derivatives

$$\omega_t = \begin{bmatrix} 1 & 3 & u & \omega_x & \omega_y \\ \dots & \dots & \dots & \partial\omega_{xy} & \partial\omega_{yy} \\ \dots & \dots & \dots & \xi_1 & \xi_n \end{bmatrix}$$

1c. Solve sparse regression

$$\arg \min_{\xi} \|\Theta\xi - \omega_t\|_2^2 + \lambda \|\xi\|_0$$

Compressed data



$$\omega_t = \Theta(\omega, u, v)\xi$$

2b. Compressed library

$$\mathcal{C}\omega_t = \mathcal{C}\Theta(\omega, u, v)\xi$$

Sampling  $\mathcal{C}$

$$\mathcal{C}\Theta$$

2c. Solve compressed sparse regression

$$\arg \min_{\xi} \|\mathcal{C}\Theta\xi - \mathcal{C}\omega_t\|_2^2 + \lambda \|\xi\|_0$$

d. Identified dynamics

$$\omega_t + 0.9931u\omega_x + 0.9910v\omega_y = 0.0099\omega_{xx} + 0.0099\omega_{yy}$$

Compare to true Navier-Stokes ( $Re = 100$ )

$$\omega_t + (\mathbf{u} \cdot \nabla)\omega = \frac{1}{Re} \nabla^2 \omega$$

Rudy et al. (Apr. 2017). "Data-driven discovery of partial differential equations". In: *Science Advances* 3.4, e1602614. ISSN: 2375-2548. DOI: 10.1126/sciadv.1602614

## Excellent:

- ▶ Equations directly from data!
- ▶ Very low cost

## Gloomy:

- ▶ Need measurements of complete state
- ▶ Need ability to represent exact model in dictionary
- ▶ Sensitivity to noise
- ▶ Not really demonstrated outside of “toy” problems
- ▶ Not clear how to introduce *a priori* knowledge of equations

**Method 3: Field-Inversion  
Machine-Learning (FIML)**  
OR  
**Sparse regression of residuals  
(SpaRTA)**

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## Field-inversion

- ▶ Consider some PDE model e.g. conservation law

$$\mathcal{N}(u; \kappa(u)) = 0$$

with an unknown constitutive relationship  $\kappa(u)$ , solution  $u(\xi)$ .

- ▶ We have  $M$  (filtered/incomplete/noisy measurements) of the state  $y_i \simeq u(\xi_i)$  for some particular testcase.

### Field-inversion

1. Approximate  $\kappa(u) \simeq \beta(\xi)$  for this case,  $\xi \in \mathbb{R}^3$  (space)
2. Solve

$$\beta_{\text{best}}(\xi) := \arg \min_{\beta} \sum_{k=1}^M |y_i - u(\xi_i)|^2 \quad \text{s.t.} \quad \mathcal{N}(u; \beta(\xi)) = 0.$$

with  $\beta$  defined at (e.g.) every meshpoint.

## PDE-constrained optimization

This is a high-dimensional PDE-constrained optimization problem...

$$\min_q \sum_{k=1}^M |y_i - u(\xi_i)|^2 \quad \text{s.t.} \quad \mathcal{N}(u; \beta(\xi)) = 0.$$

... need  $d\mathcal{J}/d\beta$  to solve efficiently.

GRADIENT CALCULATION:

Get out your Lagrangian:

$$L(u, \lambda) := \sum_{k=1}^M |y_i - u(\xi_i)|^2 + \lambda \mathcal{N}(u; \beta(\xi))$$

and build an equation for the adjoint variable  $\lambda$

$$\frac{\partial \mathcal{N}^T}{\partial u} \lambda + \frac{\partial \mathcal{J}}{\partial u} = 0, \quad \Rightarrow \quad \frac{d\mathcal{J}}{d\beta} = \frac{\partial \mathcal{J}}{\partial \beta} + \lambda \frac{\partial \mathcal{N}}{\partial \beta}$$

## Example: Turbulence closure modelling

Reynolds decomposition  $u = U + u'(t)$  with averaging  $\langle \cdot \rangle$  substituted into N-S:

$$\mathcal{N}(U + u') = (U \cdot \nabla)U + \nabla p - \nu \nabla^2 U + \langle u'_i u'_j \rangle$$

with  $\langle u'_i u'_j \rangle$  is the *Reynolds stress tensor*.

### Turbulence closure problem

Model  $\langle u'_i u'_j \rangle$  in terms of resolved flow  $U$ .

E.g. “Boussinesq”:

$$\langle u'_i u'_j \rangle \simeq -\nu_T (\nabla U + \nabla U^T)$$

with some transport equation for  $\nu_T$

$$\mathcal{N}_T(U, \nu_T; \beta) = 0$$

## Example corrective fields (RANS turbulence closures)

- ▶ Partial correction of closure-model error -  $\beta(\xi)$



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Zeno Belligoli, RPD, and Georg Eitelberg (Mar. 2021). "Reconstruction of Turbulent Flows at High Reynolds Numbers Using Data Assimilation Techniques". In: *AIAA Journal* 59.3, pp. 855–867. ISSN: 1533-385X. DOI: 10.2514/1.j059474

## Prediction: Field-inversion Machine-learning

- So far no prediction!

**Idea: Model  $\beta$  in terms of  $u$**

- Standard regression problem where  $\beta(\xi)$  is the data:

$$\min_{\theta} \sum_{k=1}^M |\beta(\xi_k) - q(u_k; \theta)|^2$$

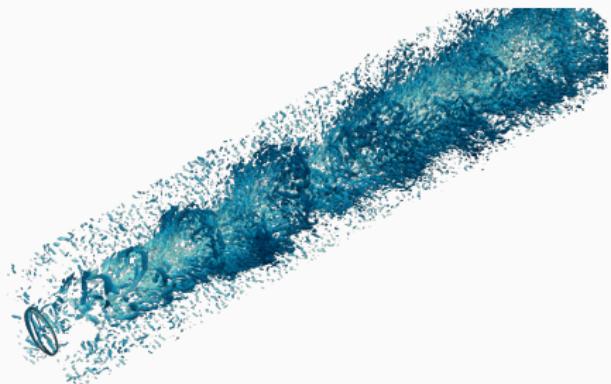
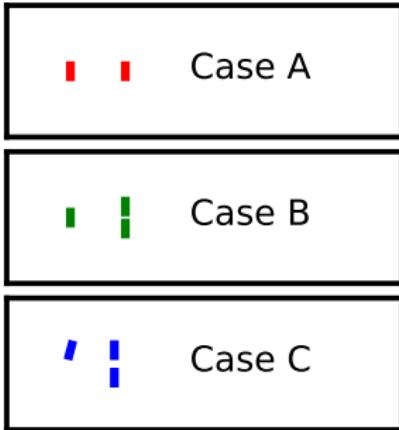
- $q(u; \theta_{\text{best}})$  is a new constitutive model  $\implies$  apply anywhere!

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Eric J. Parish and Karthik Duraisamy (Jan. 2016). “A paradigm for data-driven predictive modeling using field inversion and machine learning”. In: *Journal of Computational Physics* 305, pp. 758–774. ISSN: 0021-9991. DOI: 10.1016/j.jcp.2015.11.012

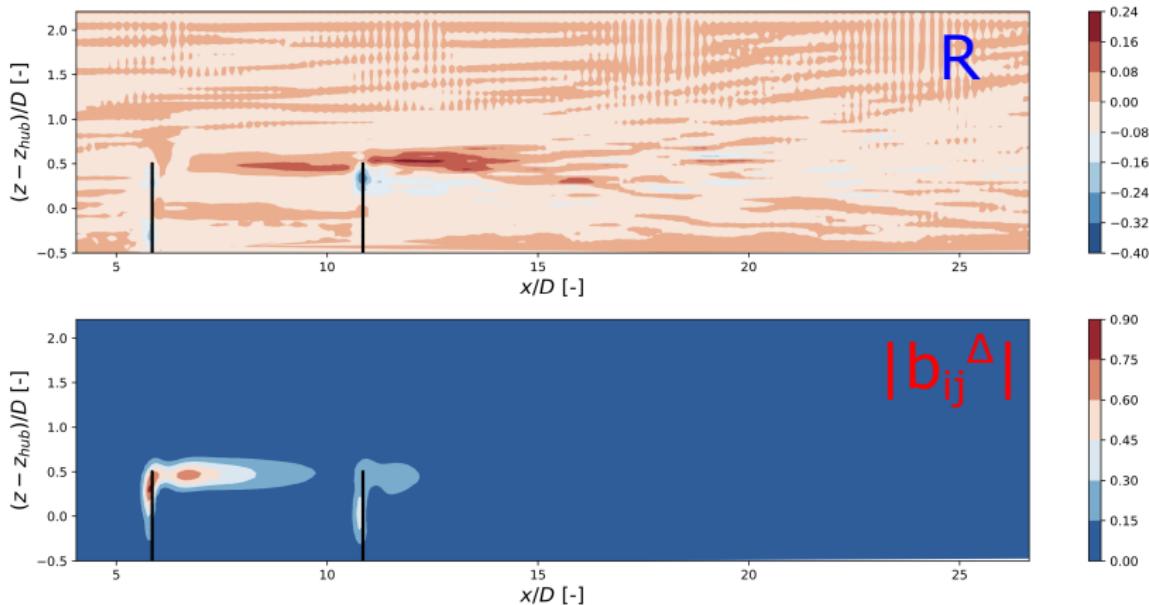
## Application: Wind-farm wake modelling

Training and test data - LES as ground-truth:



- ▶ OpenFOAM-6.0 with SOWFA-6 (from NREL)
- ▶ Neutral ABL based on precursor
- ▶ Turbine, inflow properties were taken from the wind-tunnel experiment of Chamorro and Porté-Agel (Chamorro and Porté-Agel 2010).

# Inverse problem: Optimal correction fields $\beta(\xi)$



Corrections:

- ▶  $R$  corrects turbulence kinetic energy budget
- ▶  $b^\Delta$  corrects the anisotropy of the Reynolds-stress

## Regressing corrections - $\beta(U)$

- ▶ Dictionary approach with elastic-net
- ▶ Result:

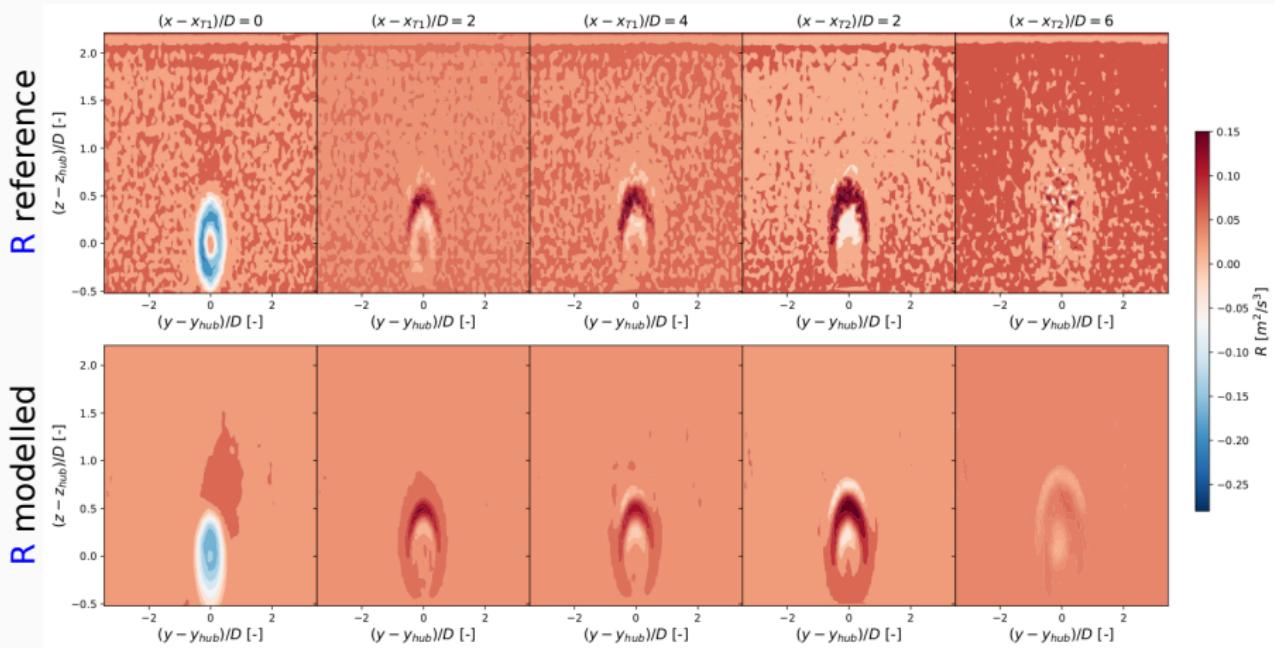
$$\hat{b}_{ij}^{\Delta}(\mathbf{q}) = [1.62 \cdot 10^{-1} \cdot q_{TI}^{1/2} \cdot q_F^{1/2} \\ + 4.84 \cdot 10^{-3} \cdot q_{TI}^{1/2} \cdot I_1^{1/2} \\ + 2.51 \cdot 10^{-2} \cdot q_F^{1/2} \\ + 2.00 \cdot 10^{-3} \cdot I_1^{1/2}] \cdot T_{ij}^{(1)}$$

$$\hat{R}(\mathbf{q}) = 8.06 \cdot 10^{-5} \cdot I_1^{1/2} \cdot q_{\nu}^3 \cdot k \cdot T_{ij}^{(1)} \partial_j u_i + \\ [-2.91 \cdot 10^1 \cdot q_{TI}^{1/2} \cdot q_F \cdot I_1^{1/2} \\ + 4.28 \cdot 10^{-1} \cdot q_{\perp}^2 \cdot q_F \cdot I_1^{1/2} \\ - 1.22 \cdot q_F \cdot q_{\gamma} \\ + 2.30 \cdot q_F^2 \cdot I_2] \cdot \epsilon$$

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Schmelzer, RPD, and Cinnella (2019). "Discovery of Algebraic Reynolds-Stress Models Using Sparse Symbolic Regression". In: *Flow, Turbulence and Combustion* 104.2-3, pp. 579–603. ISSN: 1573-1987. DOI: 10.1007/s10612-019-09832-1

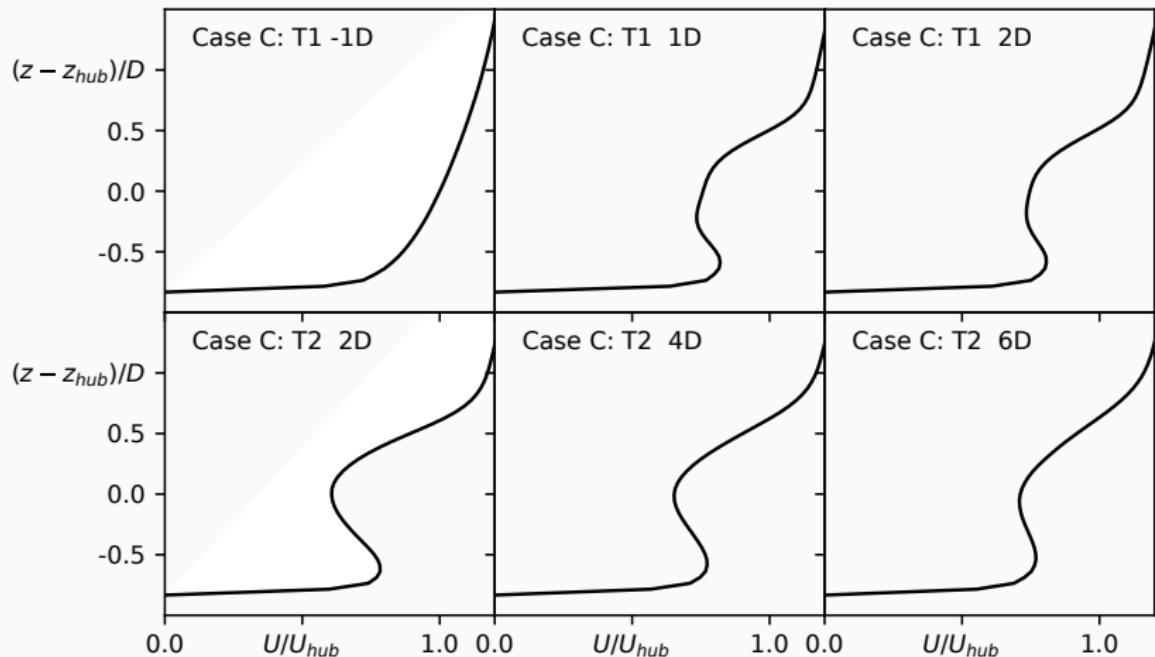
# Predictions of correction R (Train A,B; Test C)



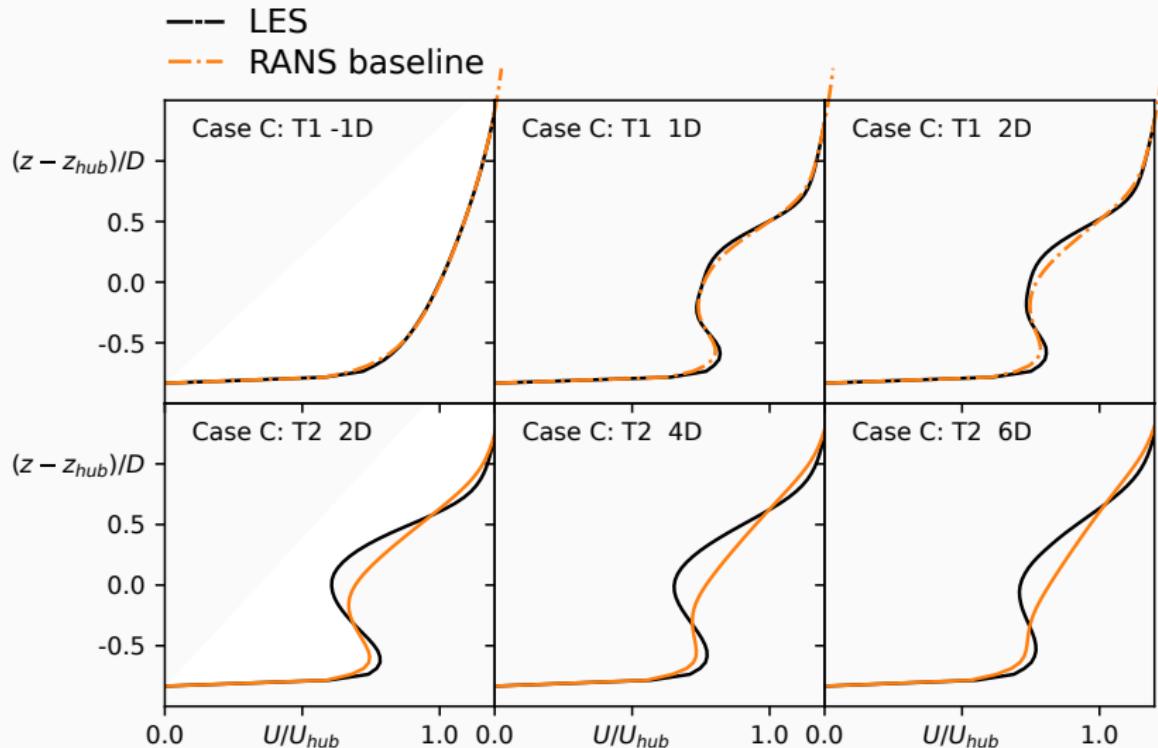
Steiner, RPD, and Viré (2020a). "Data-driven RANS closures for wind turbine wakes under neutral conditions". In: arXiv 2009.10816

# Predictions (Train A,B; Test C) - Mean $U$

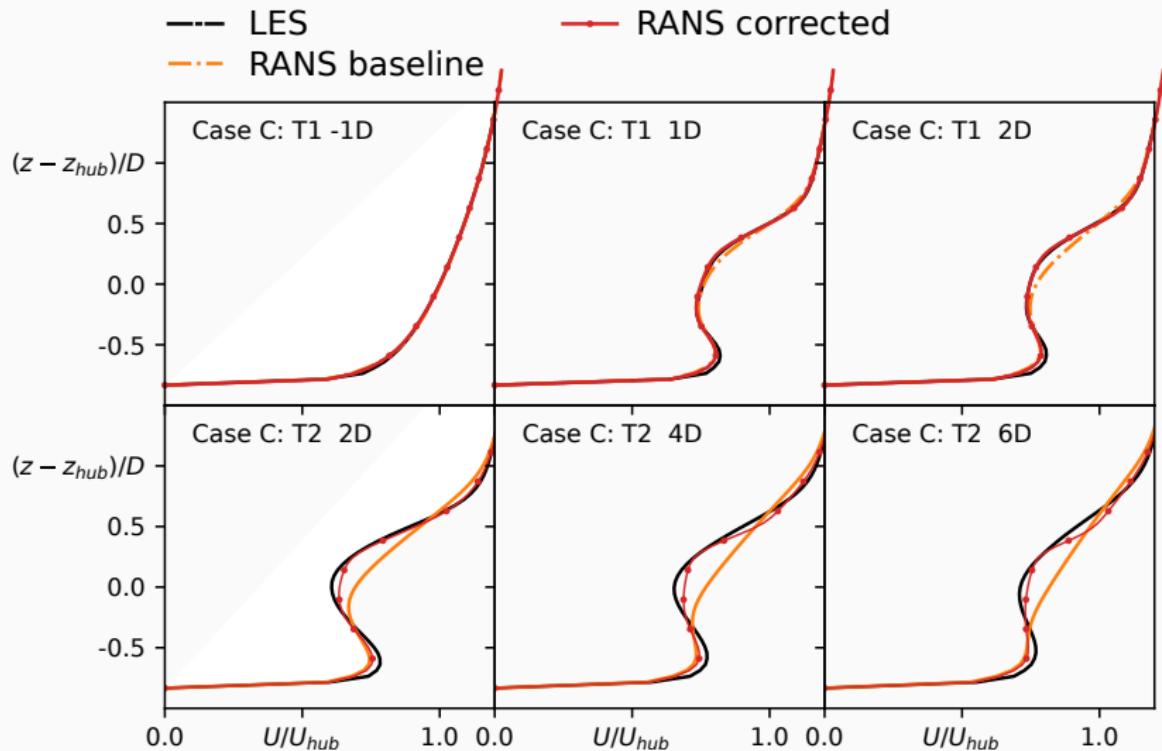
--- LES



## Predictions (Train A,B; Test C) - Mean $U$

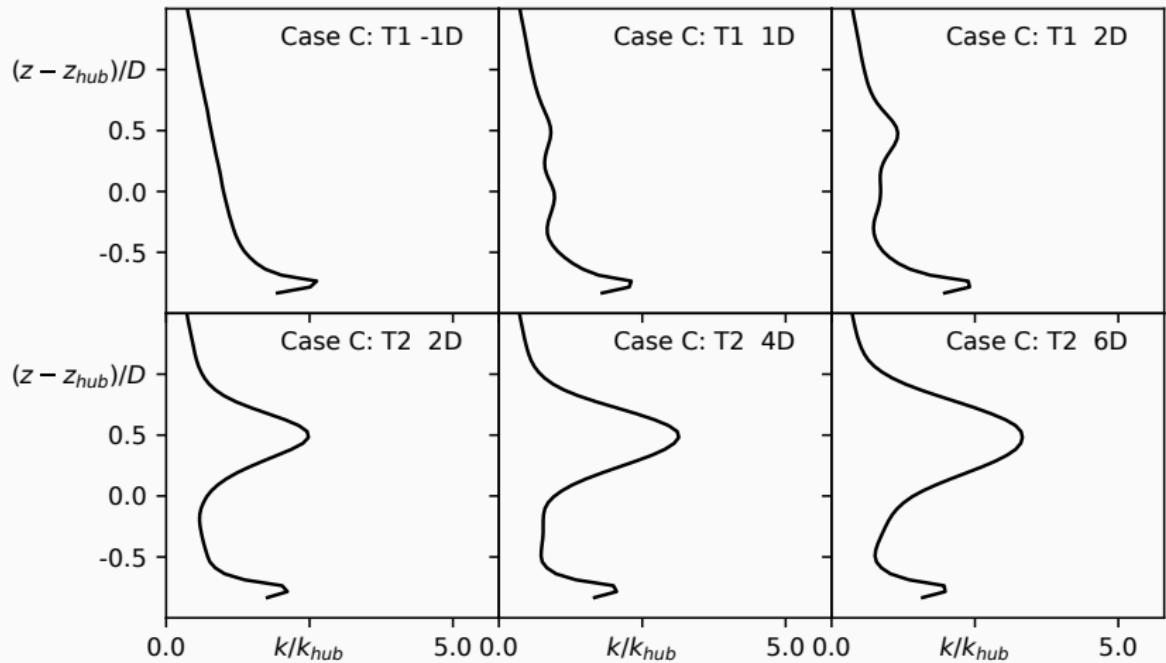


## Predictions (Train A,B; Test C) - Mean $U$

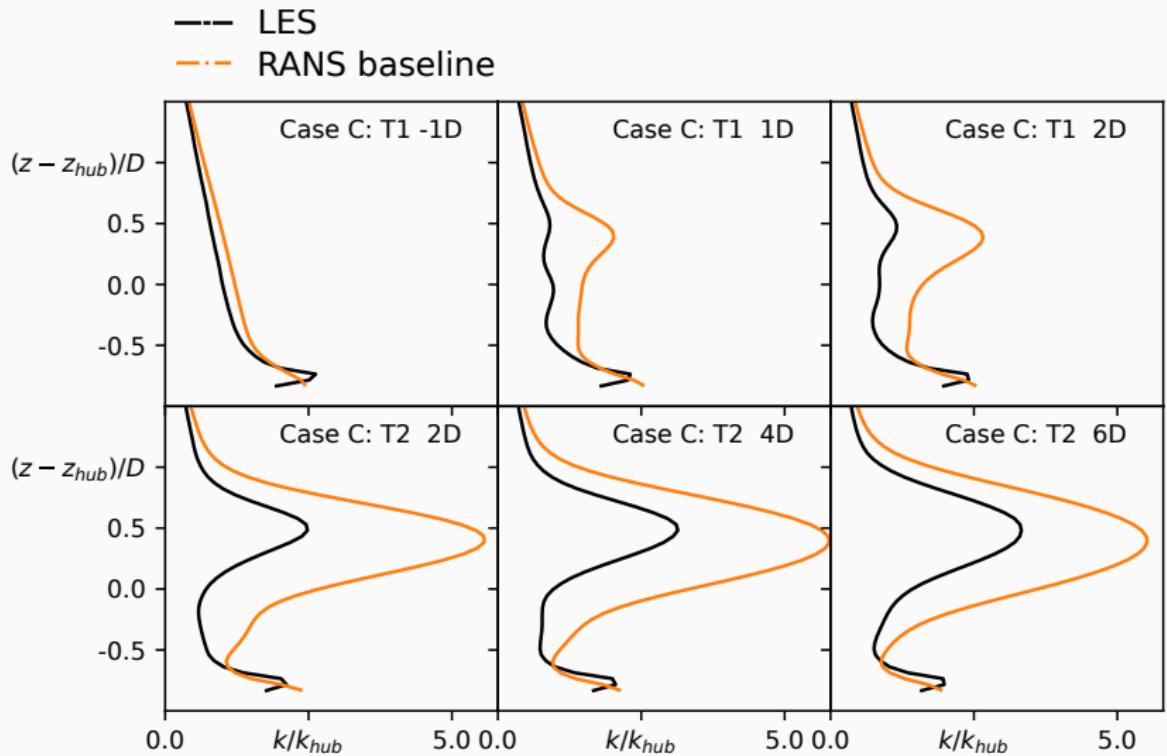


# Predictions (Train A,B; Test C) - T.K.E. $k$

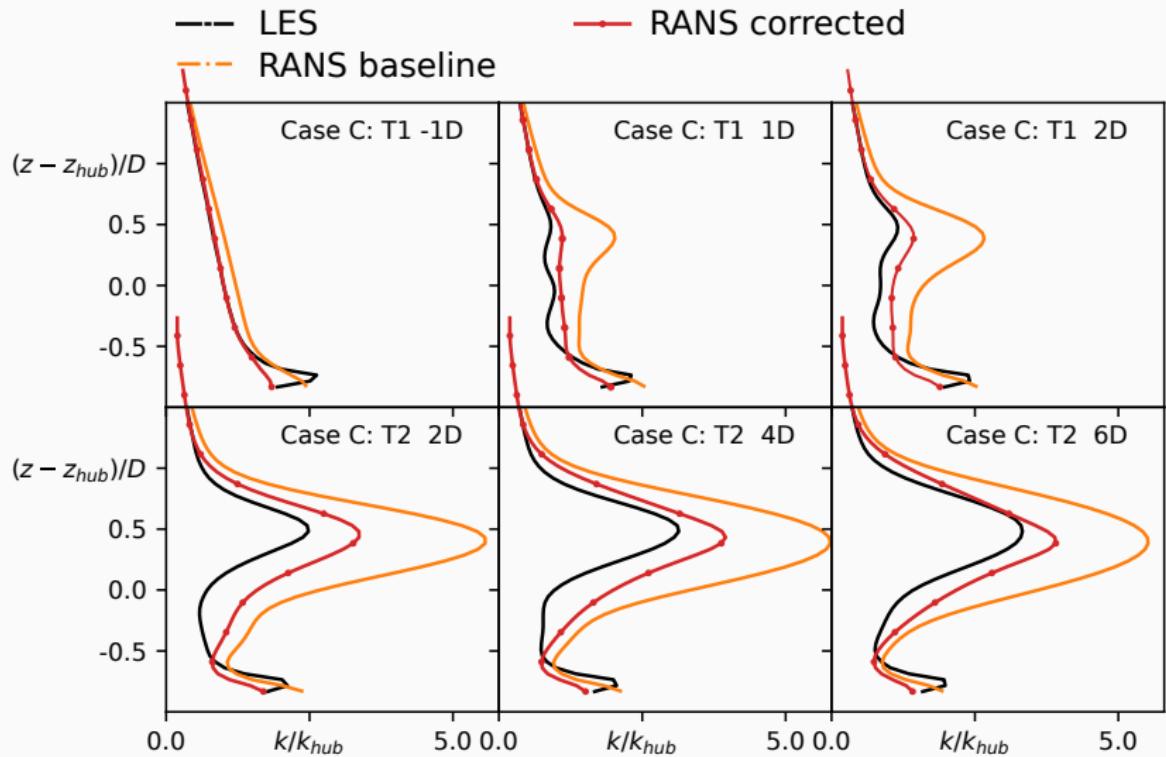
— LES



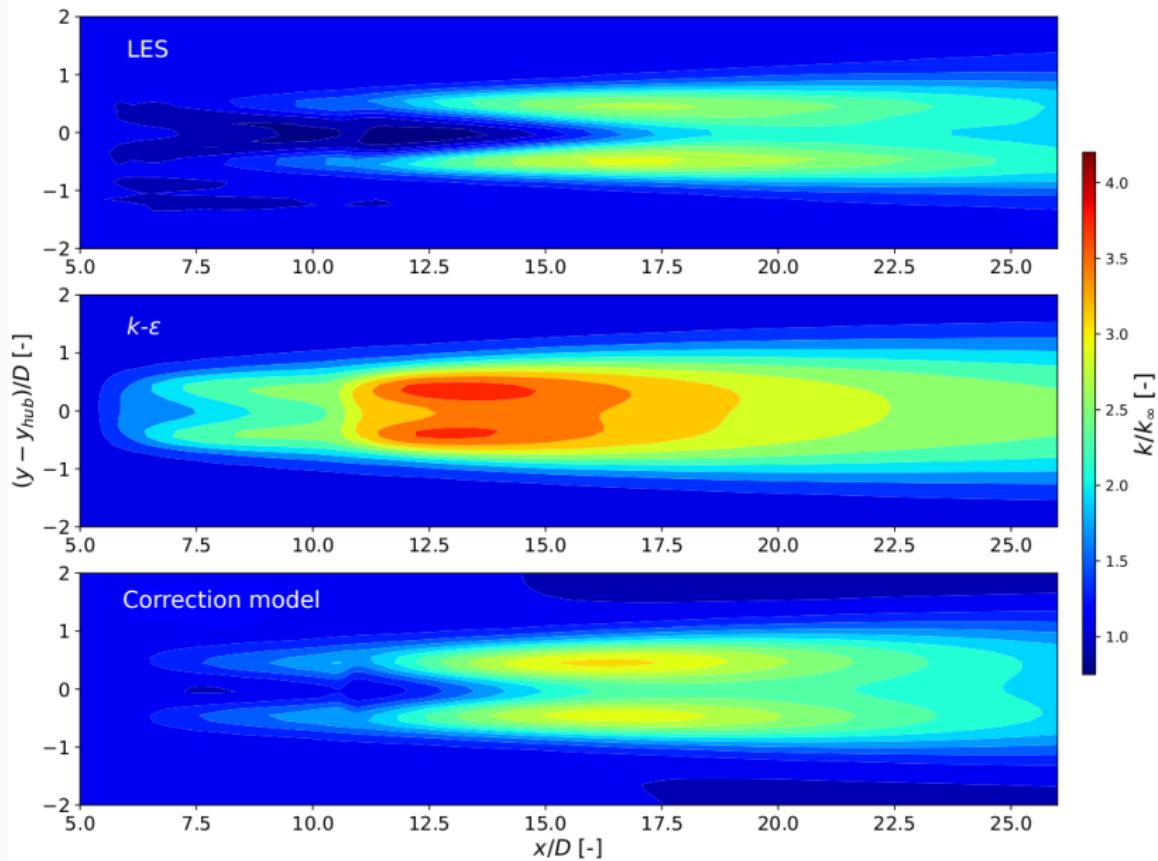
# Predictions (Train A,B; Test C) - T.K.E. $k$



# Predictions (Train A,B; Test C) - T.K.E. $k$



# Predictions (Train C; Test A) - T.K.E. $k$



# FIML - Prognosis

## Excellent:

- ▶ Formally complete/consistent
- ▶ Use any data!

## Gloomy:

- ▶ Data might be not informative
- ▶ Inverse problem is consistently a nightmare to solve

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Steiner, RPD, and Viré (2021). "Classifying regions of high model error within a data-driven RANS closure: Application to wind turbine wakes". In: *arXiv* 2106.15593

# Conclusions

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# References

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-  Belligoli, Zeno, RPD, and Georg Eitelberg (Mar. 2021). "Reconstruction of Turbulent Flows at High Reynolds Numbers Using Data Assimilation Techniques". In: *AIAA Journal* 59.3, pp. 855–867. ISSN: 1533-385X. DOI: [10.2514/1.j059474](https://doi.org/10.2514/1.j059474).
-  Brunton, Proctor, and Kutz (2016). "Discovering governing equations from data by sparse identification of nonlinear dynamical systems". In: *Proceedings of the National Academy of Sciences* 113.15, pp. 3932–3937. DOI: [10.1073/pnas.1517384113](https://doi.org/10.1073/pnas.1517384113).

## References ii

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-  Chamorro and Porté-Agel (2010). "Effects of Thermal Stability and Incoming Boundary-Layer Flow Characteristics on Wind-Turbine Wakes: A Wind-Tunnel Study". In: *Boundary-Layer Meteorology* 136.3, pp. 515–533. DOI: 10.1007/s10546-010-9512-1.
-  Duraisamy, Karthik, Gianluca Iaccarino, and Heng Xiao (2019). "Turbulence Modeling in the Age of Data". In: *Annual Review of Fluid Mechanics* 51.1, pp. 357–377. DOI: 10.1146/annurev-fluid-010518-040547.
-  Edeling, Cinnella, and RPD (2014). "Predictive RANS simulations via Bayesian Model-Scenario Averaging". In: *Journal of Computational Physics* 275, pp. 65–91.
-  Edeling, RPD, and Cinnella (2014). "Bayesian estimates of the parameter variability in the  $k - \varepsilon$  turbulence model". In: *Journal of Computational Physics* 258, pp. 73–94.

## References iii

-  Edeling, Schmelzer, et al. (2018). "Bayesian Predictions of Reynolds-Averaged Navier-Stokes Uncertainties Using Maximum a Posteriori Estimates". In: *AIAA Journal* 56.5, pp. 2018–2029. DOI: 10.2514/1.J056287.
-  Hastie, Tibshirani, and Friedman (2009). *The Elements of Statistical Learning*. Springer Series in Statistics.
-  Huijing, Jasper P., RPD, and Martin Schmelzer (July 2021). "Data-driven RANS closures for three-dimensional flows around bluff bodies". In: *Computers and Fluids* 225, p. 104997. ISSN: 0045-7930. DOI: 10.1016/j.compfluid.2021.104997.
-  Kumar, Schmelzer, and RPD (2018). "Stochastic turbulence modeling in RANS simulations via Multilevel Monte Carlo". In: *arXiv* 1811.00872.
-  Parish, Eric J. and Karthik Duraisamy (Jan. 2016). "A paradigm for data-driven predictive modeling using field inversion and machine learning". In: *Journal of Computational Physics* 305, pp. 758–774. ISSN: 0021-9991. DOI: 10.1016/j.jcp.2015.11.012.

## References iv

-  Porté-Agel, Fernando, Majid Bastankhah, and Sina Shamsoddin (2019). "Wind-Turbine and Wind-Farm Flows: A Review". In: *Boundary-Layer Meteorology* 174.1, pp. 1–59. ISSN: 1573-1472. DOI: 10.1007/s10546-019-00473-0.
-  Raissi, M., P. Perdikaris, and G.E. Karniadakis (2019). "Physics-informed neural networks". In: *Journal of Computational Physics* 378, pp. 686–707. ISSN: 0021-9991. DOI: 10.1016/j.jcp.2018.10.045.
-  Rudy et al. (Apr. 2017). "Data-driven discovery of partial differential equations". In: *Science Advances* 3.4, e1602614. ISSN: 2375-2548. DOI: 10.1126/sciadv.1602614.
-  Schmelzer, RPD, and Cinnella (2019). "Discovery of Algebraic Reynolds-Stress Models Using Sparse Symbolic Regression". In: *Flow, Turbulence and Combustion* 104.2-3, pp. 579–603. ISSN: 1573-1987. DOI: 10.1007/s10494-019-00089-x.

## References v

-  Steiner, RPD, and Viré (2020a). "Data-driven RANS closures for wind turbine wakes under neutral conditions". In: *arXiv* 2009.10816.
-  – (2020b). "Data-driven turbulence modeling for wind turbine wakes under neutral conditions". In: *Journal of Physics: Conference Series* 1618, p. 062051. ISSN: 1742-6596. DOI: 10.1088/1742-6596/1618/6/062051.
-  – (2021). "Classifying regions of high model error within a data-driven RANS closure: Application to wind turbine wakes". In: *arXiv* 2106.15593.
-  Terleth, N. (2019). "Artificial Neural Networks for Flow Field Inference". MA thesis. TU Delft.