Towards generalizable RANS modelling using invariance recovery

December 2023

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Customized data-driven (turbulence) modelling

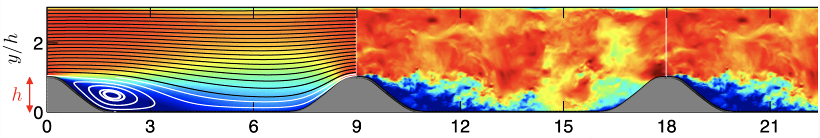
Exact (incompressible) N-S equations are:

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \nu \nabla^2 \boldsymbol{u}, \quad \nabla \cdot \boldsymbol{u} = 0.$$

Multi-scale problem: separate mean from fluctuating velocity:
$\boldsymbol{u} = \boldsymbol{U} + \boldsymbol{u}'(t)$ where $\boldsymbol{U} := \bar{\boldsymbol{u}}$ gives:

$$(\boldsymbol{U} \cdot \nabla)\boldsymbol{U} = -\nabla p + \nu \nabla^2 \boldsymbol{U} - \nabla \cdot \overline{\boldsymbol{u}'\boldsymbol{u}'}$$

with $\tau_{ij} := \overline{\boldsymbol{u}'_i \boldsymbol{u}'_j}$ the *Reynolds stress tensor*.

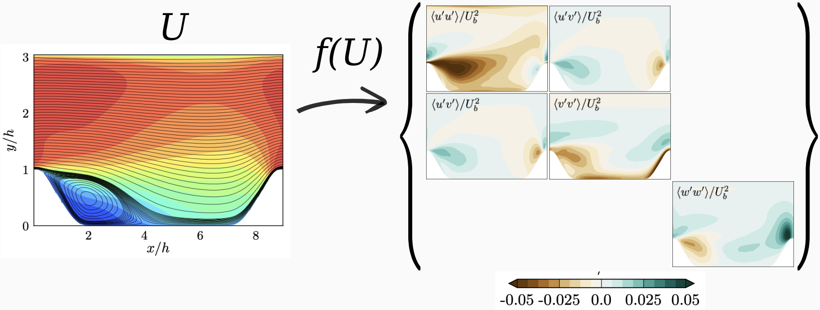


Data-driven (turbulence) modelling

Data-driven modelling - Naïve/optimistic idea

1. The only missing term is τ_{ij}, so...
2. Given DNS/LES, solve RANS with *prescribed* τ_{ij}^{DNS}
3. Generalize by finding map $\tau_{ij} \approx f(U^{\mathrm{RANS}})$

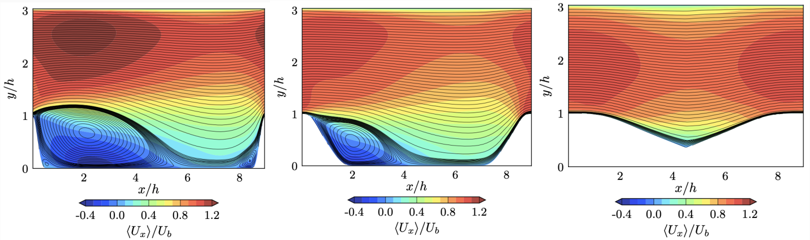
$$\min_{f} \|\tau^{\mathrm{DNS}} - f(\boldsymbol{U}^{\mathrm{RANS}})\|^2$$



One-shot optimization

Single-LES optimization (one-shot)

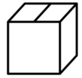
1. Run **one** LES at the *initial design* ($\phi = 1$).
2. Train a custom RANS model for the flow using this LES. This should *correlate* well with the LES locally (in the design space).
3. Perform the optimization with RANS (cheap).



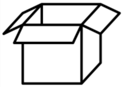
Symbolic regression

Supervised learning problem: Regress data $\{(\boldsymbol{U}^{(k)}, \tau^{(k)}) \mid k = 1, \ldots, N\}$

- ANN, random-forest, other highly-parameterized regressor.

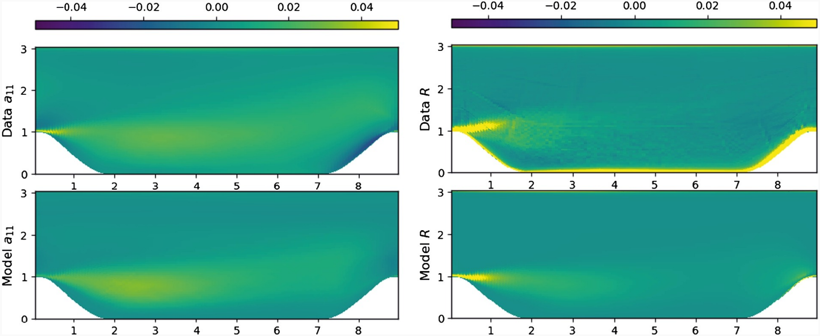


- Symbolic regression
  - Genetic programming (GP)
  - Gene-expression programming (Weatheritt and Sandberg 2016)
  - Sparse regression (Schmelzer, RPD, and Cinnella 2019)



Symbolic closure model training for $\psi = 1$

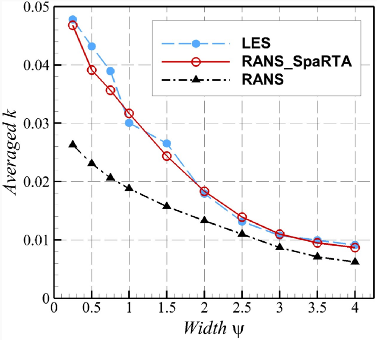
Corrective fields b_{ij}^{Δ} and R:



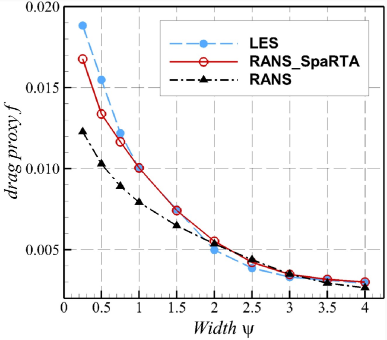
Symbolic regression model:

$$b_{ij}^{\Delta} \simeq 2.8\, T_{ij}^{(2)},$$
$$R \simeq 0.4\, T_{ij}^{(1)} \cdot 2k \partial U_i / \partial x_j.$$

SR *predictions* of $\bar{k}$ and f ($\psi \neq \psi_0$)



(a) averaged turbulence kinetic energy



(b) drag f

Zhang and RPD et al. (2021). "Customized data-driven RANS closures for bi-fidelity LES–RANS optimization". In: *JCP* 432. DOI: 10.1016/j.jcp.2021.110153

Bi-fidelity optimization

Bi-fidelity LES optimization (multi-shot)

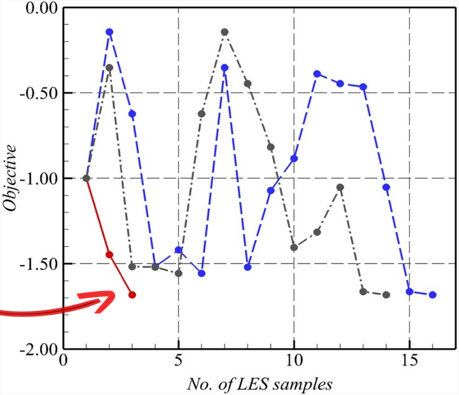
1. ...
2. Build surrogate with multi-fidelity Bayesian optimation.
3. Update closure with new LESs as they are obtained.

Three optimizations:

LES single-fidelity optimization

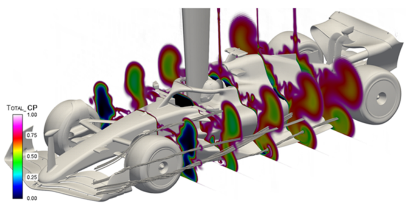
Bi-fidelity with baseline RANS

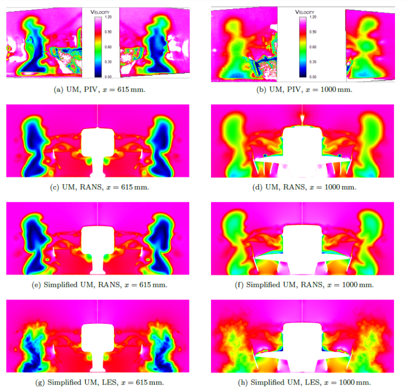
Bi-fidelity with custom RANS



Out-of-distribution generalization

Problem #1: Real flows have a large amount of structure...



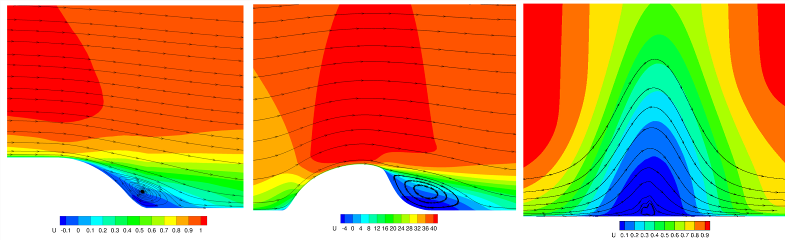


Jonas Pangerl (June 2023). "High Fidelity CFD Simulation of sub-scale Race Car Wing and Wheel Configurations". In: *AIAA AVIATION 2023 Forum*. American Institute of Aeronautics and Astronautics. DOI: 10.2514/6.2023-3762

Out-of-distribution generalization

Problem #2: We want models that for constitutive laws that are independent of geometry/boundary-conditions.

- Training flows *always* conflate multiple effects.
- Universal physics may be hidden by specific conditions.



Empirical Risk Minimization

Framework: Consider multi *environments*:

- Training environments $e \in \mathcal{E}_{\text{train}}$
- Test environments $e \in \mathcal{E}_{\text{test}}$
- $\mathcal{E}_{\text{all}} = \mathcal{E}_{\text{train}} \cup \mathcal{E}_{\text{test}}$

A natural idea:

***Empirical* Risk Minimization**

Minimize average/total risk over all training environments $e \in \mathcal{E}_{\text{train}}$, i.e. solve:

$$\min_f \sum_{e \in \mathcal{E}_{\text{train}}} \|\boldsymbol{y}^e - f(\boldsymbol{x}^e)\|^2$$

Example #1: Model problem

Example (Arjovsky)

$$X_1 \leftarrow \mathcal{N}(\mu(e), 1)$$
$$Y \leftarrow X_1 + \mathcal{N}(0, 1)$$
$$X_2 \leftarrow \beta(e) Y + \mathcal{N}(0, 1)$$

Training: $\mathcal{E}_{\mathrm{train}} = \{(\mu = 1, \beta = 10), (\mu = 2, \beta = 20)\}$

Test environment: $\mathcal{E}_{\mathrm{test}} = \{(\mu = 3, \beta = 30)\}$

- Best model (over all environments): $y = x_1$
- over $\mathcal{E}_{\mathrm{train}}$: $y = \alpha_1 x_1 + \alpha_2 x_2$, $\alpha_1 \neq 1, \alpha_2 \neq 0$
  - Increasingly poor model as $\mu, \beta \to \infty$

Martin Arjovsky (2021). *Out of Distribution Generalization in Machine Learning*. arXiv: 2103.02667 [stat.ML]

Invariant Risk Minimization

Split model into two pieces: $f(\boldsymbol{x}) = w \circ \Phi(\boldsymbol{x})$

- $\Phi(x)$: compute invariants from features.
- $w(\Phi)$: regress target y using invariants.

Invariant Risk Minimization (ideal)

Solve for w, Φ such that w is seperately optimal in each envionment:

$$\min_{w,\Phi} \sum_{e' \in \mathcal{E}_{\text{train}}} \|\boldsymbol{y}^{e'} - w \circ \Phi(\boldsymbol{x}^{e'})\|^2$$

$$\text{s.t.} \quad w = \arg\min_{w'} \|\boldsymbol{y}^{e} - w' \circ \Phi(\boldsymbol{x}^{e})\|^2, \ \forall e \in \mathcal{E}_{\text{train}}$$

Invariant Risk Minimization

Split model into two pieces: $f(\boldsymbol{x}) = w \circ \Phi(\boldsymbol{x})$

- $\Phi(x)$: compute invariants from features.
- $w(\Phi)$: regress target y using invariants.

Invariant Risk Minimization (tractable)

Set $w = 1$ and solve for Φ such that model is insensitive to w:

$$\min_{f} \sum_{e' \in \mathcal{E}_{\mathrm{train}}} \left\{ \|\boldsymbol{y}^{e'} - w \circ \Phi(\boldsymbol{x}^{e'})\|^2 + \lambda \cdot \|\nabla_w [w \circ \Phi(\boldsymbol{x}^{e'})]\|^2 \right\}$$

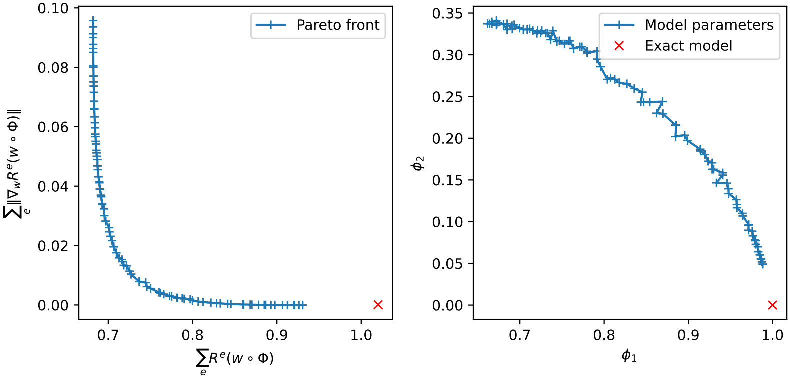
Martin Arjovsky (2021). *Out of Distribution Generalization in Machine Learning*. arXiv: 2103.02667 [stat.ML]

Invariant Risk Minimization

For model problem (with $Y = 1 \cdot X_1 + 0 \cdot X_2$ "exact" solution):

$$X_1 \leftarrow \mathcal{N}(\mu(e), 1);\;\; Y \leftarrow X_1 + \mathcal{N}(0,1);\;\; X_2 \leftarrow \beta(e) Y + \mathcal{N}(0,1)$$

Pareto front with NSGA-II (Deb et al. 2002)



Recovery of physical invariants

Require: Models must respect physical invariances.

Navier-Stokes is:

- **Rotationally invariant**

  Scalar $y \in \mathbb{R}$, matrix $A \in \mathbb{R}^{3\times 3}$, vector $\boldsymbol{v} \in \mathbb{R}^3$:

$$y = f(A, \boldsymbol{v}, c) \iff y = f(QAQ^T, Q\boldsymbol{v}, c), \quad \forall QQ^T = I.$$

$\implies$ only *tensor-invariants* may be used ($\operatorname{tr} A$, $\det A$, etc.)

- **Galilean invariant**

$$y = f(\boldsymbol{U}) \iff y = f(\boldsymbol{U} + \boldsymbol{U}_0), \quad \forall \boldsymbol{U}_0 \in \mathbb{R}^3.$$

$\implies$ $\boldsymbol{U}$ may not be used in $f()$, only $\nabla \boldsymbol{U}$.

Recovery of tensor-invariants

Consider $y = f(A)$ with scalar $y \in \mathbb{R}$, matrix $A \in \mathbb{R}^{3\times 3}$.

Problem: Matrix invariants

$$A(\theta) = Q(\theta)\begin{pmatrix} a & b & 0 \\ c & d & 0 \\ 0 & 0 & e \end{pmatrix} Q^T(\theta), \quad Q = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$a \sim \mathcal{N}(2\mu, \beta), \;\; b \sim \mathcal{N}(\mu, \beta), \;\; c \sim \mathcal{N}(-\mu, \beta), \;\; d \sim \mathcal{N}(2\mu, \beta)$$

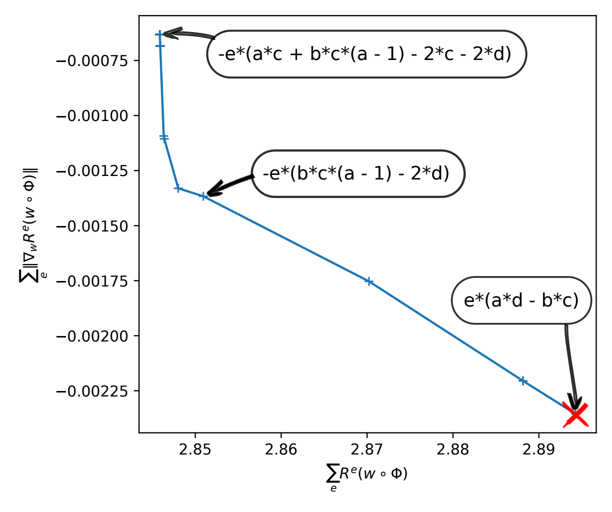
$$Y = g(\det A, \operatorname{tr} A) + \mathcal{N}(0, 1)$$

Training: $\mathcal{E}_{\text{train}} = \left\{(\theta = 0°, \mu = 1, \beta = \frac{1}{10}), (45°, 1.2, \frac{1}{10}), \ldots\right\}$

Test: $\mathcal{E}_{\text{train}} = \{(\theta = 30°, \mu = 2, \beta = 10)\}$

Pareto-optimal expressions for matrix invariant

Symbolic regression for $y = f(a, b, c, d, e)\,[= \det A]$



Turbulence model invariant detection

Predict corrective field $\mathcal{R}_k$ (error in k-equation)

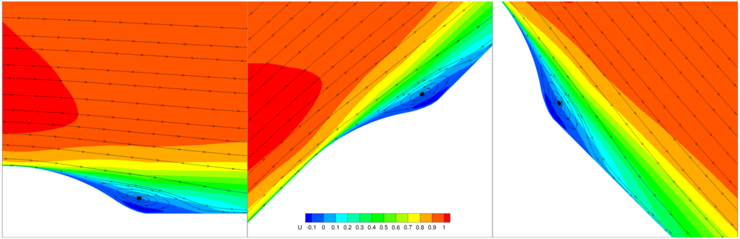
$$\frac{\mathrm{D}k}{\mathrm{D}t} = P_k - \varepsilon + \frac{\nu_T}{\sigma_k}\nabla^2 k + \mathcal{R}_k$$

In terms of features:

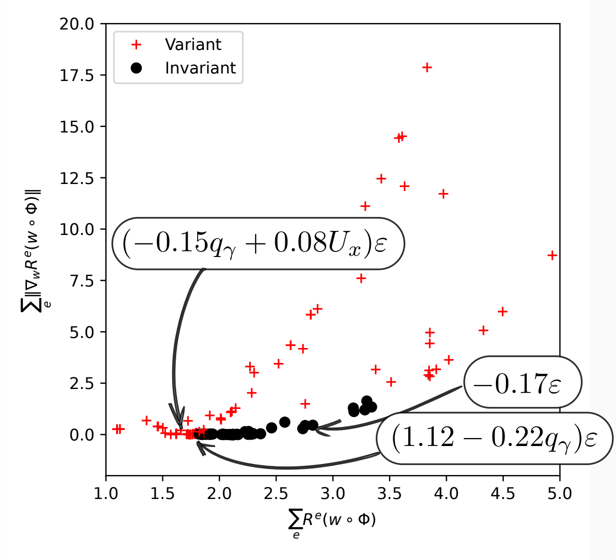
$\{\varepsilon, q_{\mathrm{Re}}, q_\gamma, q_\tau, \boldsymbol{U}, q_{\mathrm{TI}}\}$ black = invariant, red = variant

Environments:

- Various coordinate systems $Q(\theta)$
- Various Galilean frames ($\boldsymbol{U} \leftarrow \boldsymbol{U} + \boldsymbol{U}_0$)

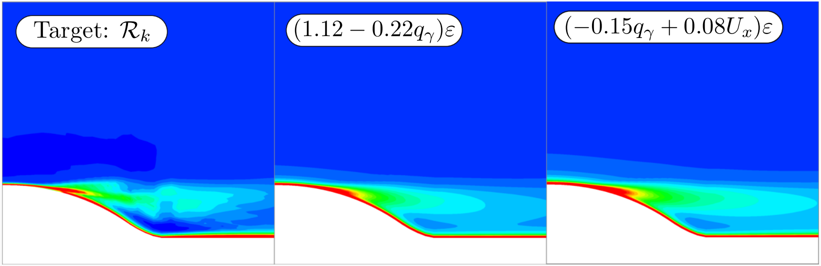


Turbulence model invariant detection



- Non-invariant models can *beat* invariant models on ERM loss.
- IRM penalty gives (imperfect) *hint* of invariance.

Turbulence model invariant detection



- Corrective fields are almost indistinguishable.
- Continue with cases where invariances is unknown...

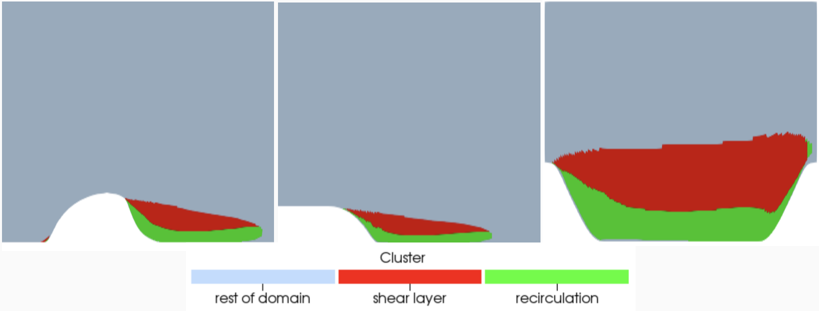
Clustering of flow domains

Goal: Isolate regions with common physics.

Approach: "Balance models" (Callaham et al. 2021)

$$\frac{\mathrm{D}k}{\mathrm{D}t} = P_k - \varepsilon + \frac{\nu_T}{\sigma_k}\nabla^2 k$$

$$\xi_{\text{cluster}} = \begin{cases} \text{shear} - \text{layer} & P_k < 0.55 \cdot \varepsilon \;\text{ and }\; k \geq 0.12 U^2 \\ \text{recirculation} & P_k \geq 0.55 \cdot \varepsilon \;\text{ and }\; k \geq 0.12 U^2 \\ \text{other} & \text{otherwise} \end{cases}$$



Prediction for shear layer

Predict corrective field $\mathcal{R}_k$ (error in k-equation) again Features (rotationally and Galilean invariant only):

$$\{\varepsilon, q_{\mathrm{Re}}, q_\gamma, q_\tau, \lambda(\nabla \boldsymbol{U}), \sigma, \nabla k\}$$

Environments: Shear-layer regions of:

- Curved backwards-facing step
- Periodic-hill
- NASA Hump

Winning model (minimizing both terms):

Prediction for shear layer

Predict corrective field $\mathcal{R}_k$ (error in k-equation) again Features (rotationally and Galilean invariant only):

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Environments: Shear-layer regions of:

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Winning model (minimizing both terms):

$$\mathcal{R}_k = -0.16 \cdot \varepsilon$$

Conclusions

1. Existing model-generation approach do not guarantee case-invariance.
2. IRM penalty is imperfect
3. A large, diverse envionment set is necessary †
4. Consider other losses to characterize invariance

† Elan Rosenfeld, Pradeep Kumar Ravikumar, and Andrej Risteski (2021). "The Risks of Invariant Risk Minimization". In: *International Conference on Learning Representations*

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References iii

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