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AI-2-AI

Adding Insight to Artificial Intelligence

Prof Gabriel D Weymouth
Ship Hydrodynamics, TU Delft

GPT-4 aced the SAT Reading & Writing section with a score of 710 out of 800, which puts it in the 93rd percentile of test-takers.

GPT-4 scored in the 90th percentile of the bar exam with a score of 298 out of 400.

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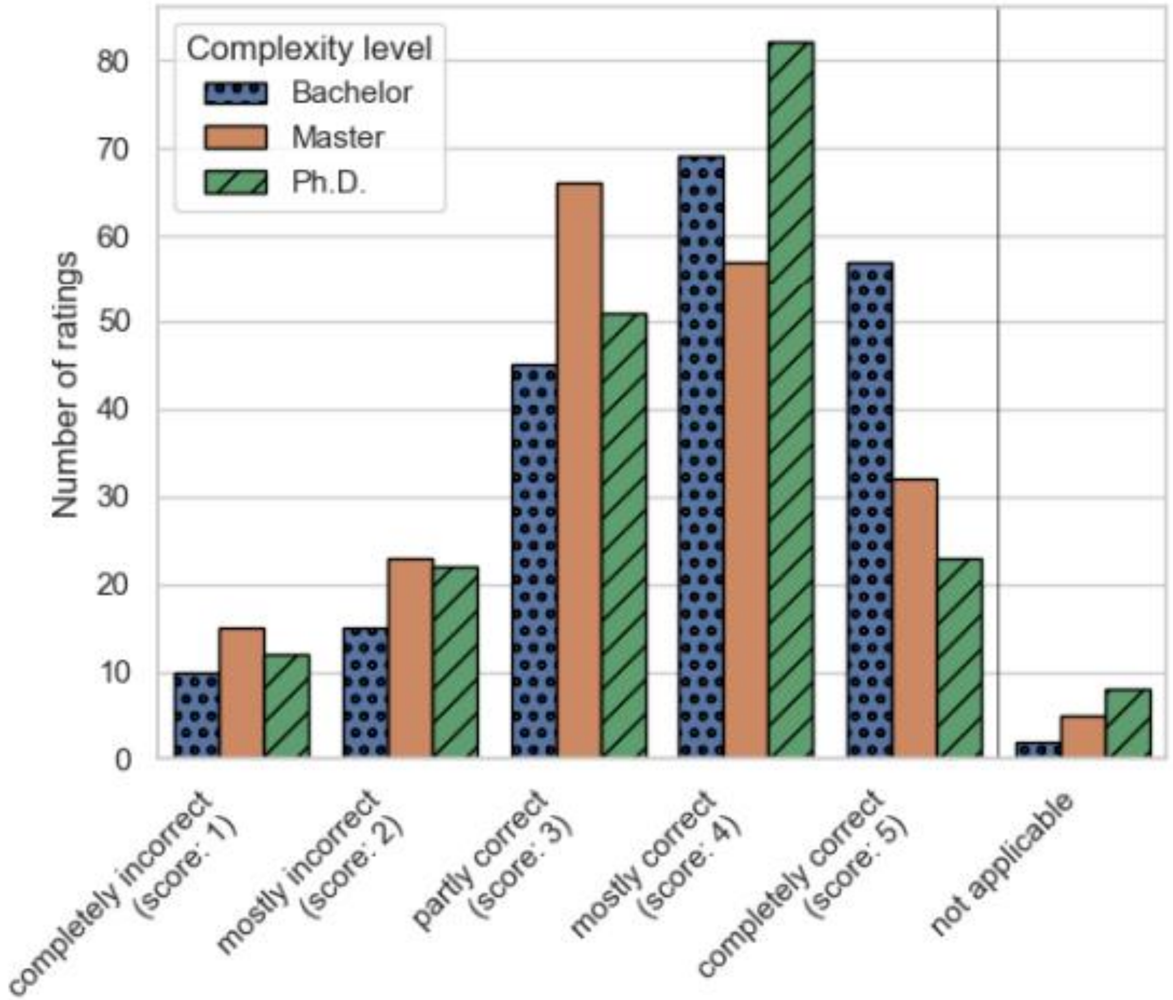
“What does ChatGPT know about natural science and engineering?”

Balhorn et al, arXiv:2309.10048, 2023

- ChatGPT answered scientific questions “mostly correct”

- Responds 10^3 times faster than students!



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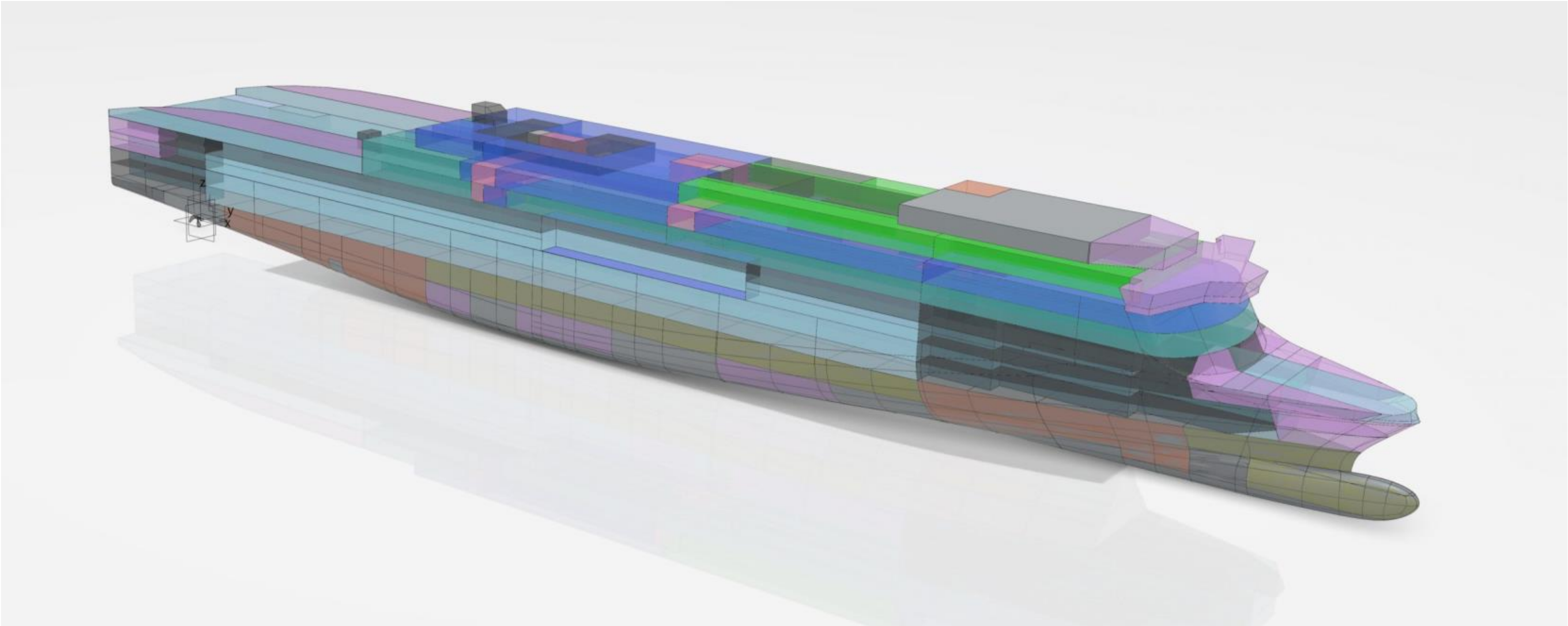
How long before AI replaces ship designers?

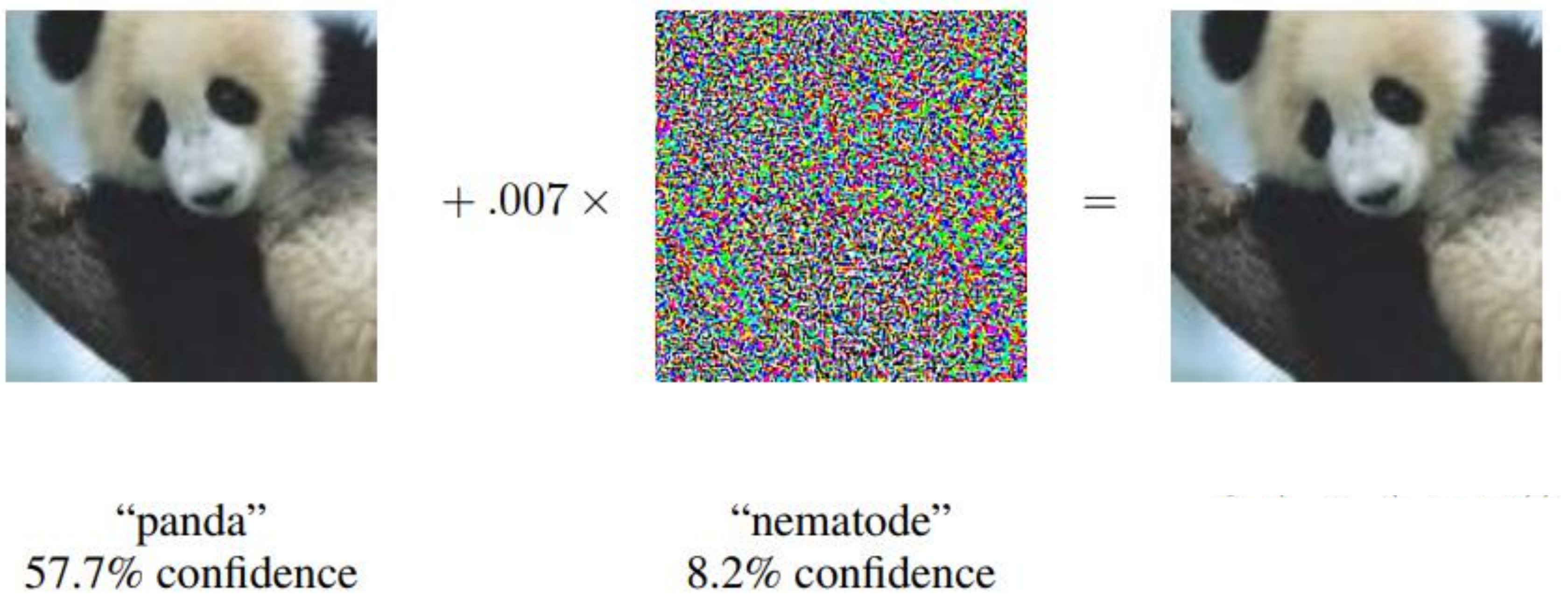


Deltamarin Ltd

Data-driven models have no contextual understanding

"Create an image of Mother Terresa fighting against poverty"

Data-driven models are interpolating, not reasoning



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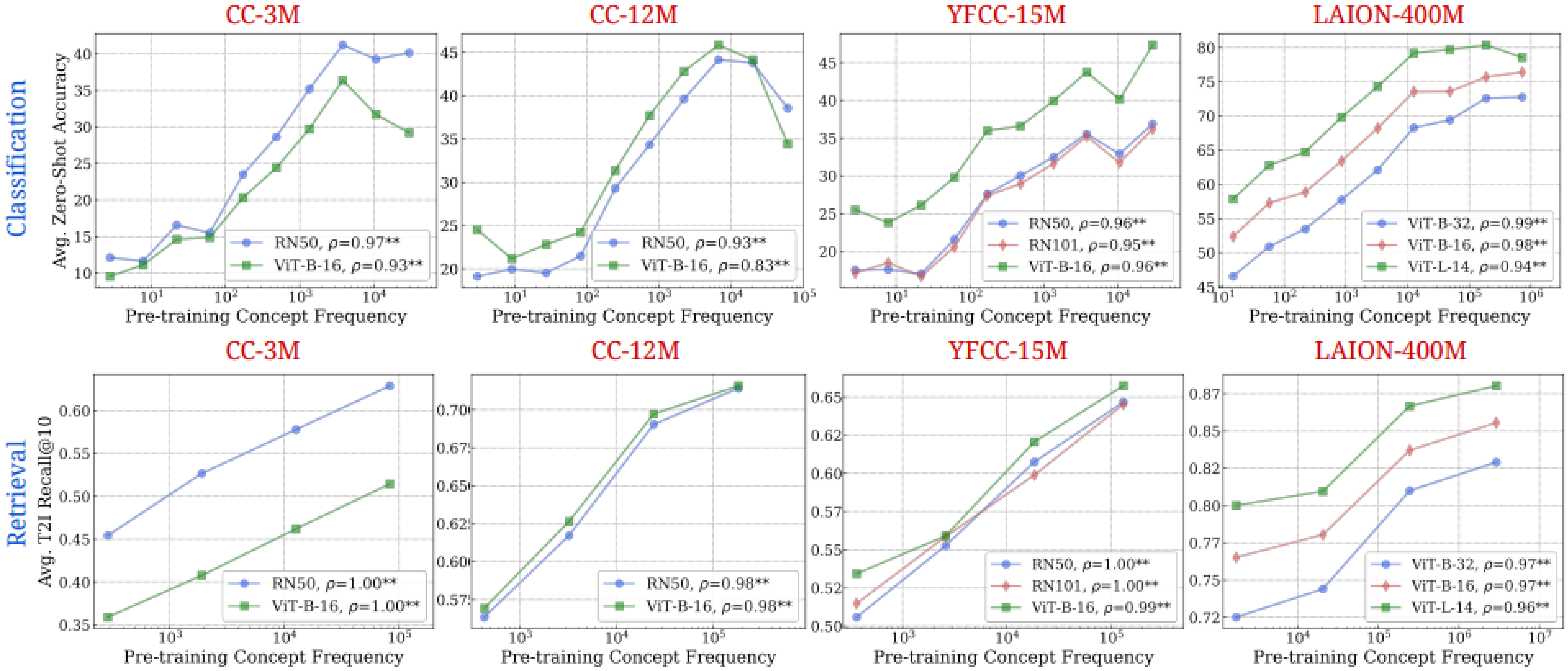
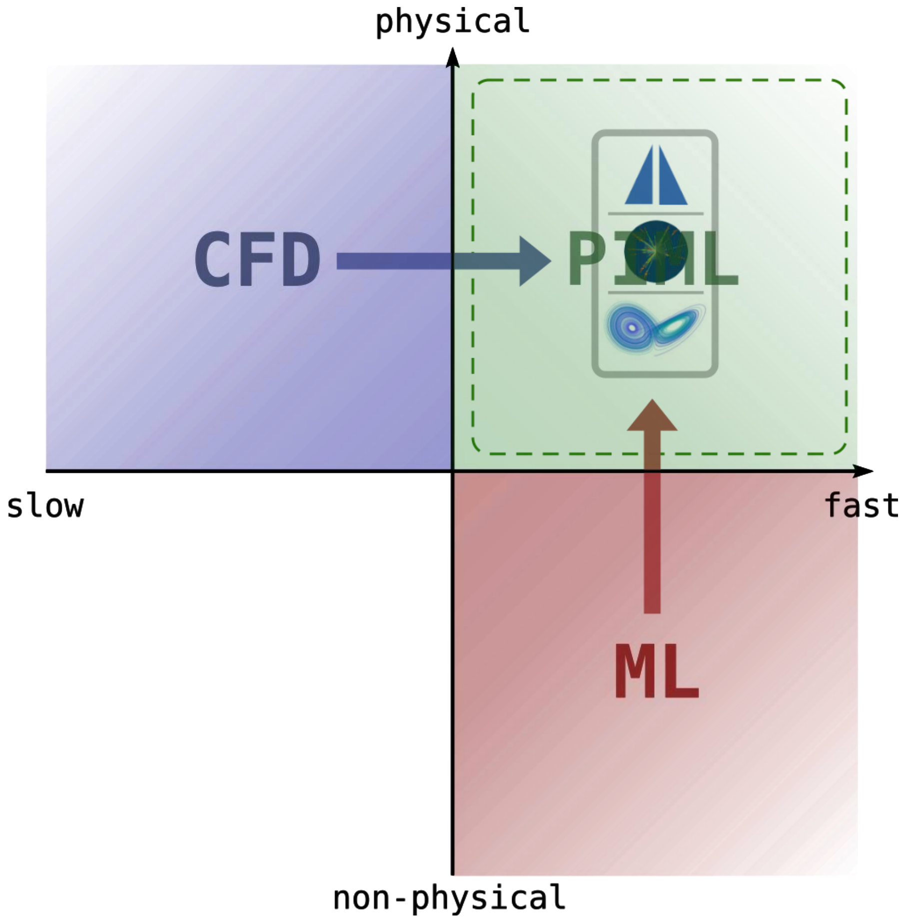
Explaining and Harnessing Adversarial Examples
Goodfellow et al, [arXiv: 1412.6572](https://arxiv.org/abs/1412.6572), 2015

Data-driven models need exponential data to improve



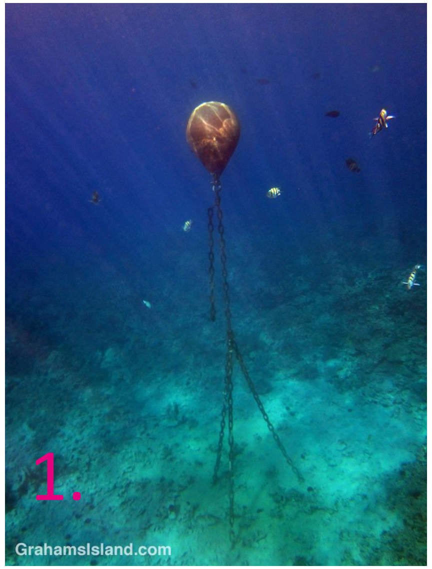
No "Zero-Shot" Learning Without Exponential Data,
Udandarao et al, arXiv: 2404.04125, 2024

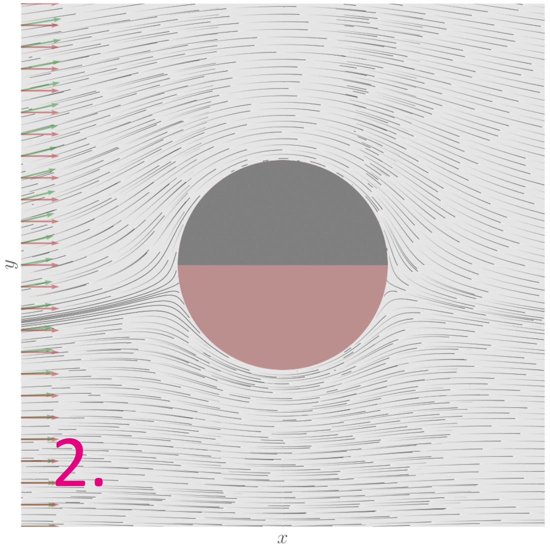
Goal: Supply physical insight to data-driven models

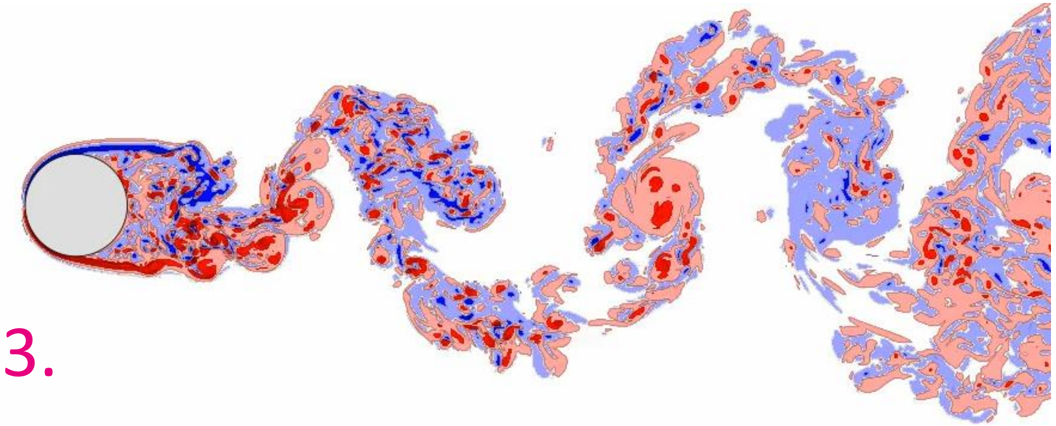


Adding Insight to Artificial Intelligence

1. Nonlinear groups for nonlinear pendulum
2. Field constraints for flow field predictions
3. 2D momentum for slender geometries

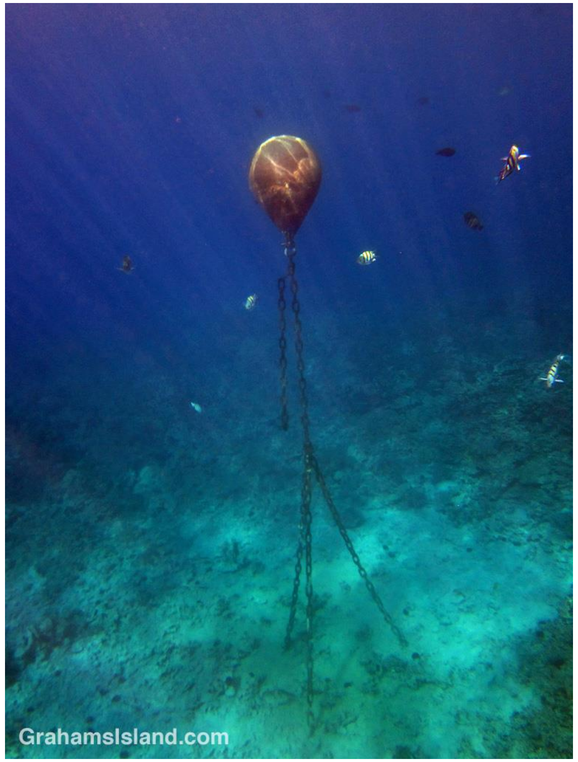






3.

Submerged nonlinear pendulum:
Model problem for *nonlinear* fluid-structure interactions



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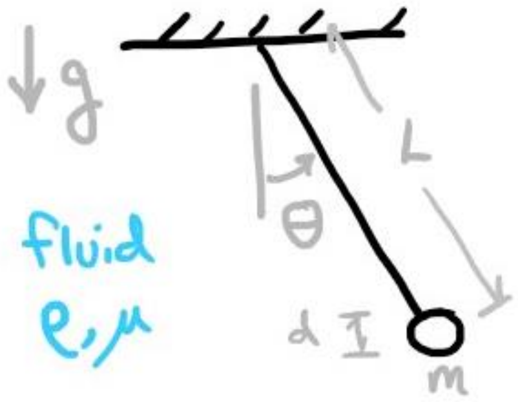
Submerged nonlinear pendulum:
Model problem for *nonlinear* fluid-structure interactions



$$\omega_n = f(\theta_0, m, L, d, \rho, \mu, g)$$

- Goal: Predict natural frequency
- Database: 1000 simulations
  - Length: 50 – 150cm,
  - Diameter: 15 – 50 mm
  - Bob material: aluminum – gold
  - Liquid: water – glycerol
  - Starting angle: -$\pi/2$ – $\pi/2$
  - Gravity: Mercury, Venus, Earth, … , Neptune

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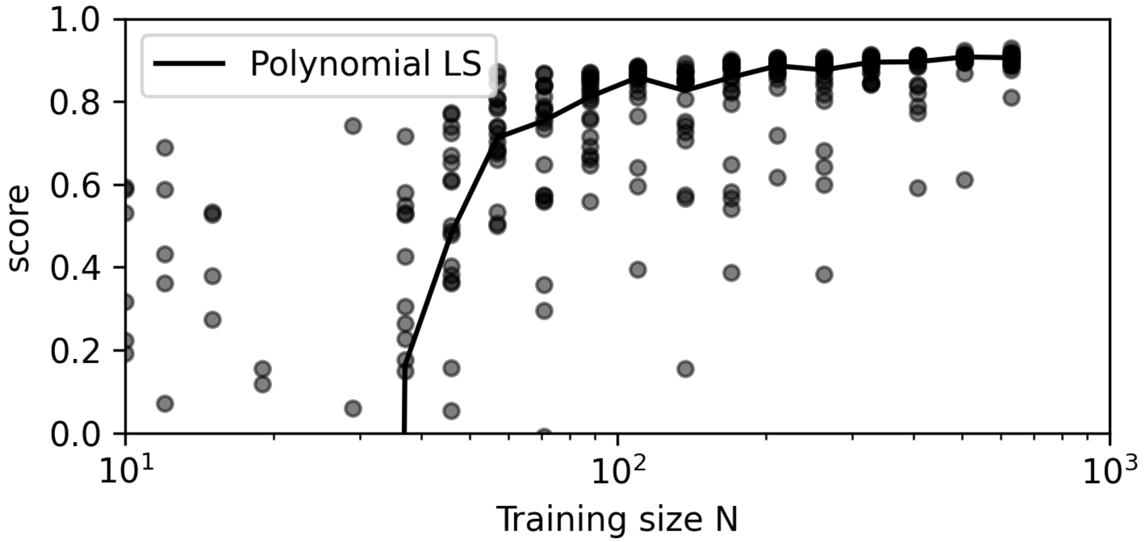
Data-driven models need exponential data



- Randomly sample N cases for training
- Dots: R^2 score on remaining 1000-N cases
- Lines: median R^2 at each training size

Data: $\vec{x}_i, y_i$

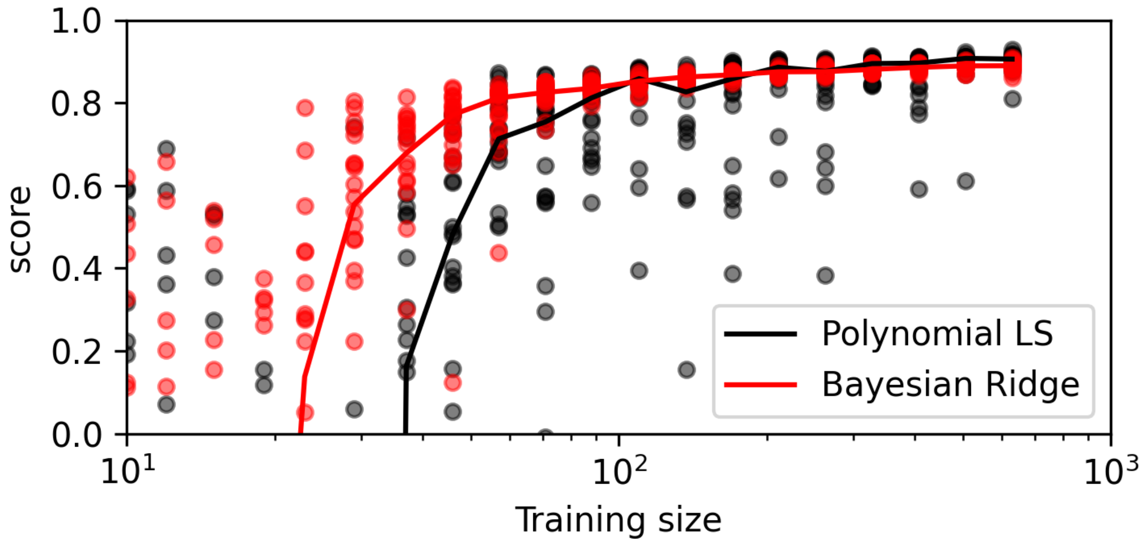
Model: $f(\vec{x}|\theta)$

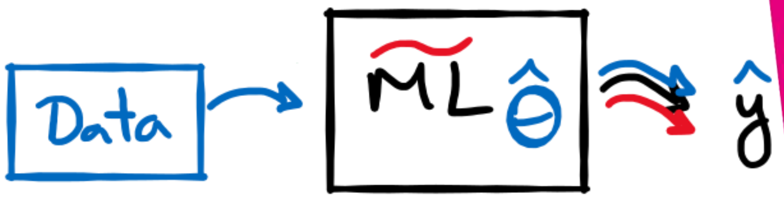
$loss(\theta|\vec{x}_i, y_i) = \sum_i \mathcal{L}(y_i - f(\vec{x}_i|\theta))$

Optimize: $\hat{\theta} = \mathrm{argmin}\ loss(\theta|\vec{x}_i, y_i)$

Predict : $\hat{y} = f(\vec{x}|\hat{\theta})$

Statistical regularization helps limit data-dependance, a bit…





$$\text{loss}(\theta \mid \vec{x}_i, y_i) = \sum_i \ell(y_i - f(\vec{x}_i \mid \theta)) + g(\theta)$$

$$\text{Optimize: } \hat{\theta} = \widetilde{\text{argmin}}\ \text{loss}(\theta \mid \vec{x}_i, y_i)$$

$$\text{Predict : } \hat{y} = \frac{1}{n} \sum_j f(\vec{x} \mid \hat{\theta}_j)$$

↳ Regularization increases loss on $\vec{x}_i, y_i$ with the goal of reduced loss "outside" $\vec{x}_i$

How can we add physical insight?

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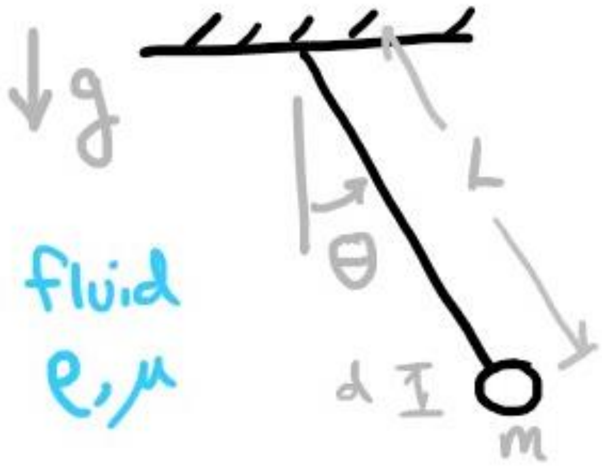
Physical knowledge constrains & simplifies ML problem



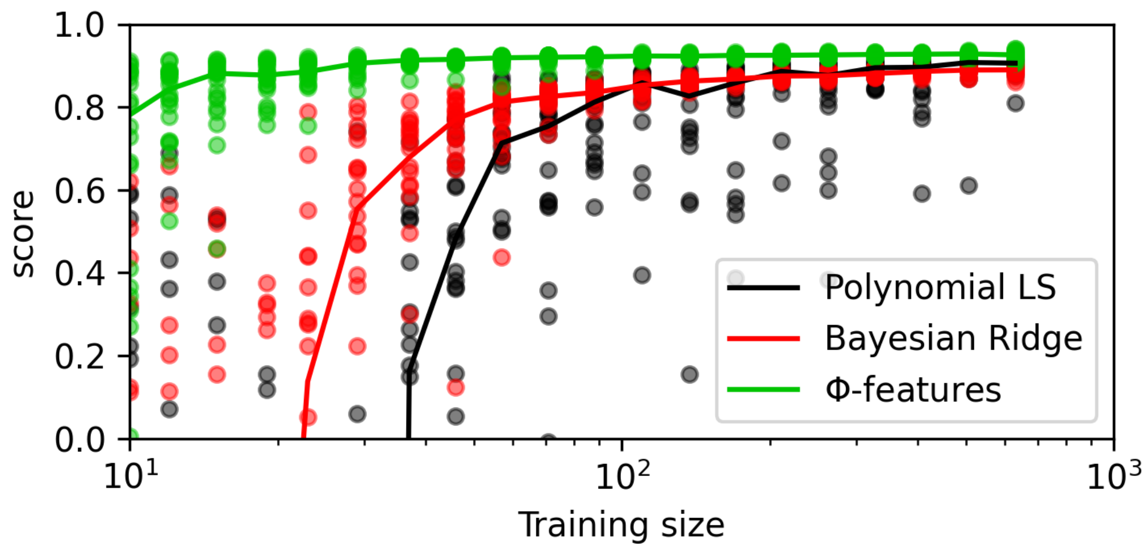
$$\omega_n = f(\theta_0, m, L, d, \rho, \mu, g)$$

$$\frac{\omega_n^2 L}{g} = f\left(\theta_0, \frac{m}{\rho d^3}, \frac{\rho}{\mu}\sqrt{\frac{d^3}{g}}, \frac{d}{L}\right)$$

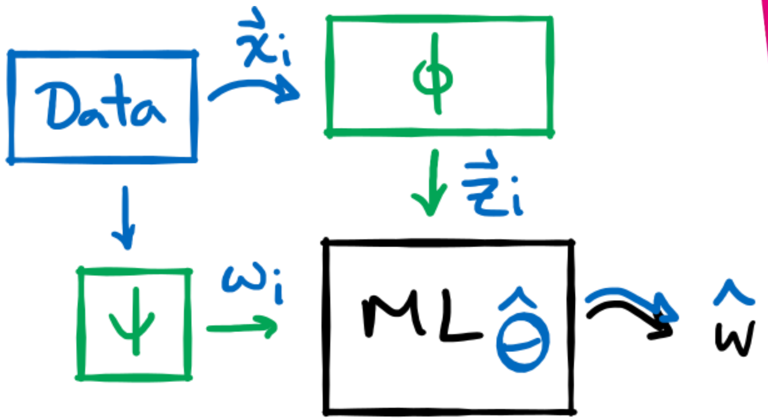
Dimensional analysis

- Reduced dimension: 7 → 4
- Nonlinear scaling of the inputs and outputs!

Physical knowledge constrains & simplifies ML problem



Almost perfect results with only 20 examples!



Features: $\vec{z}_i = \vec{\phi}(\vec{x}_i)$, $\omega_i = \psi(\vec{x}_i, y_i)$

Model: $f(\vec{z} \mid \theta) = \omega$

Predict: $\hat{y} = \psi^{-1}(f(\vec{\phi}(\vec{x}) \mid \hat{\theta}))$

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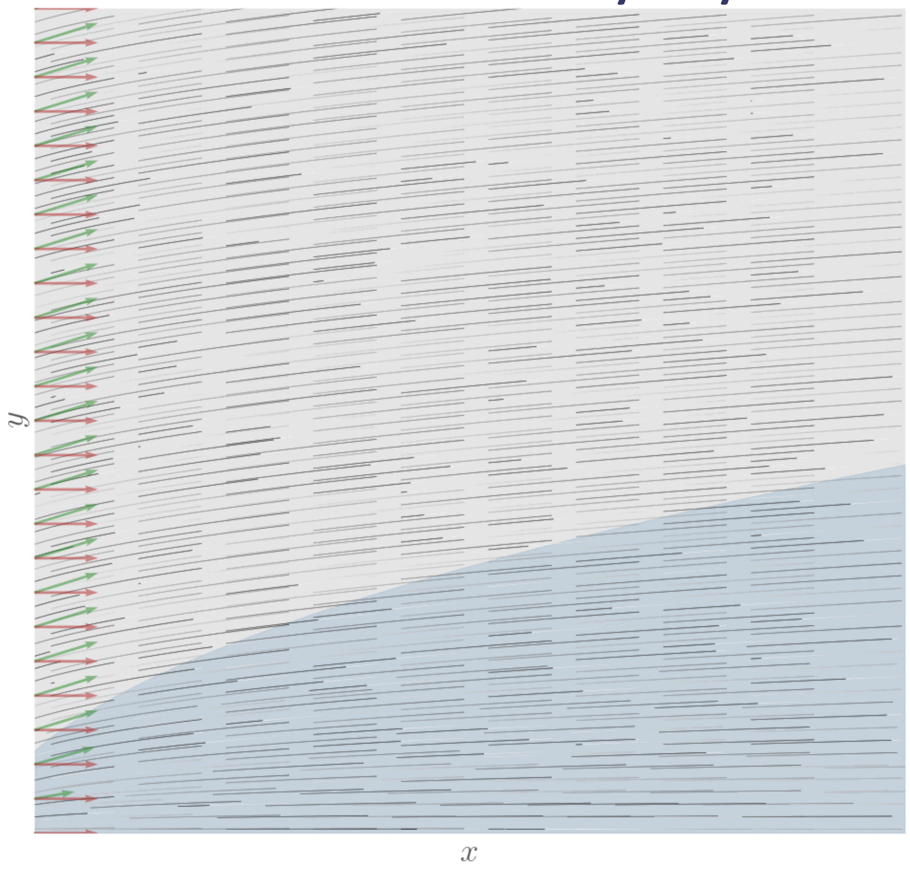
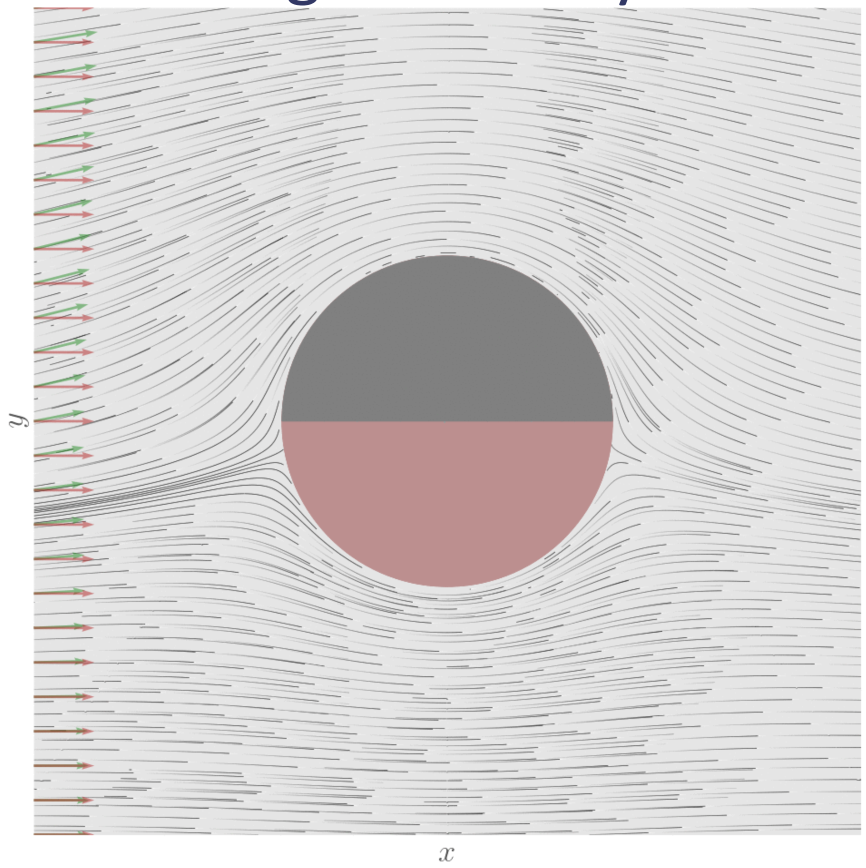
Can this be extended for quantitative field predictions?

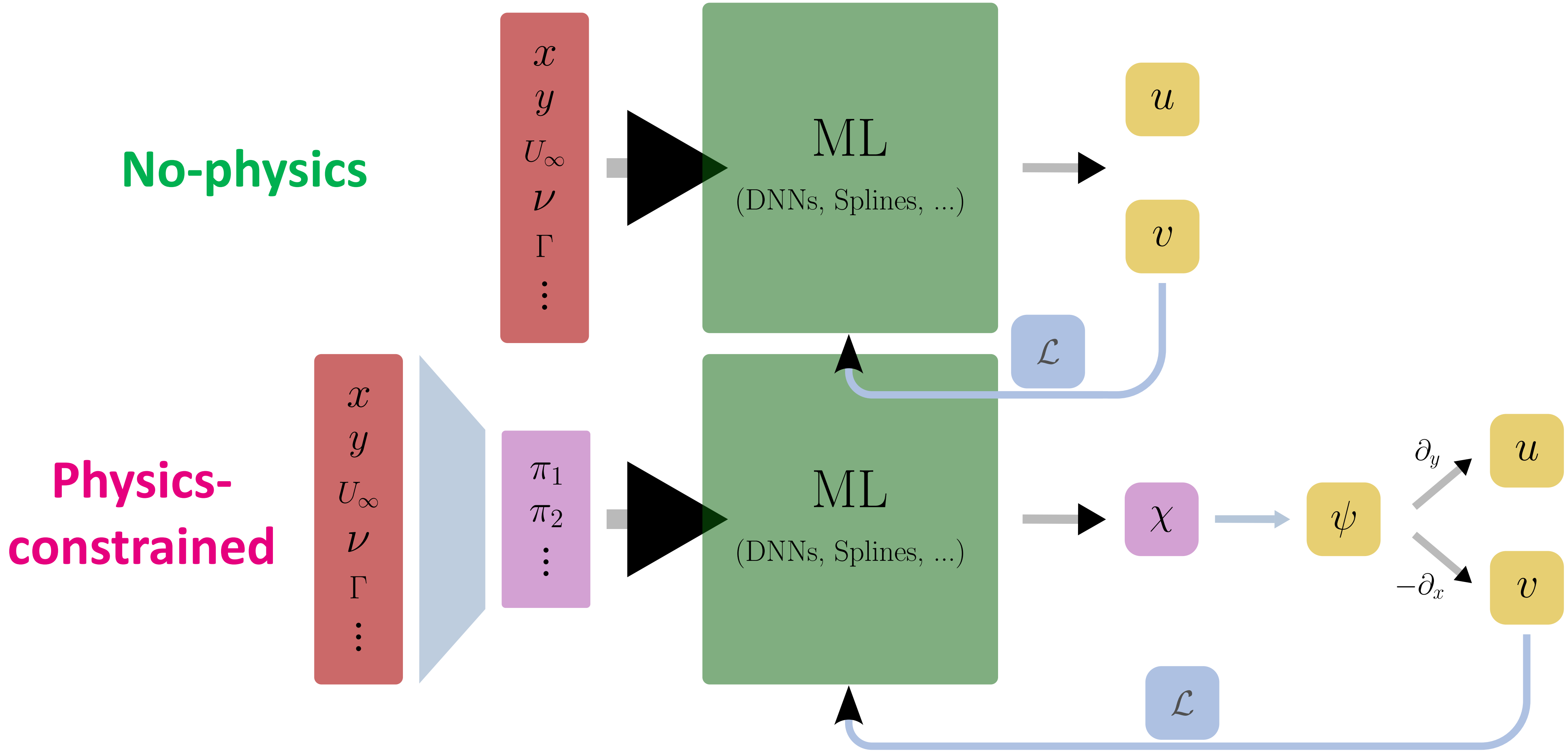
Blasius boundary layer



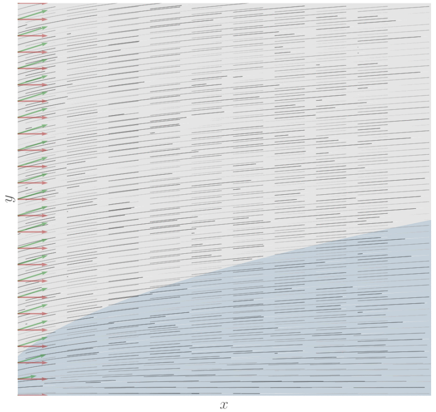
Rotating circular cylinder



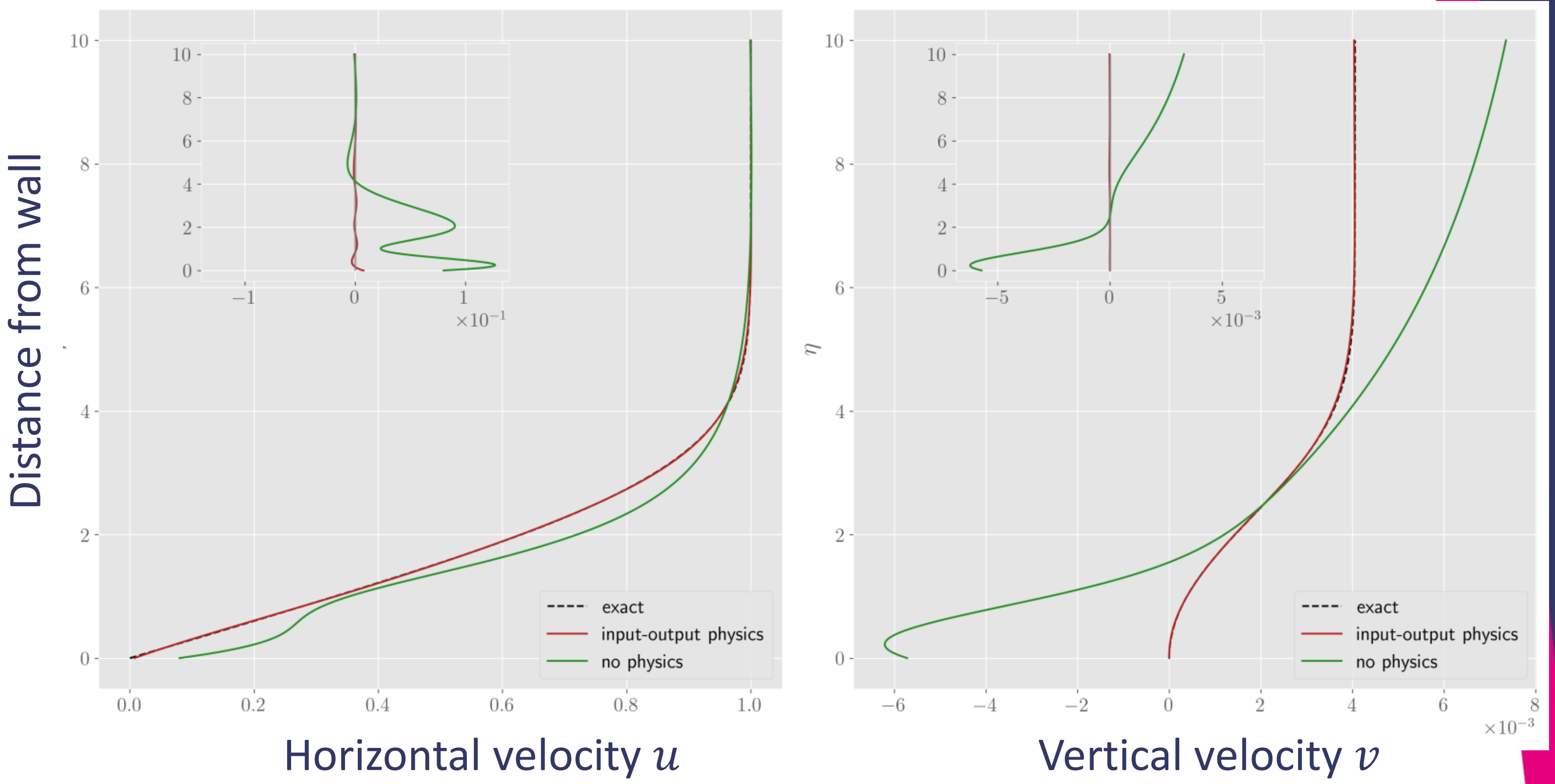
Physical knowledge constrains & simplifies ML problem



Physics-constraints massively improve predictions with small data



- Blasius Boundary Layer
  - $[x, y, U, v] \rightarrow [u, v]$
  - Tiny 6 neuron network & only 500 examples
- Pure data-driven
  - Unphysical u slip
  - Completely ignores v
- Physics-constrained
  - Essentially perfect



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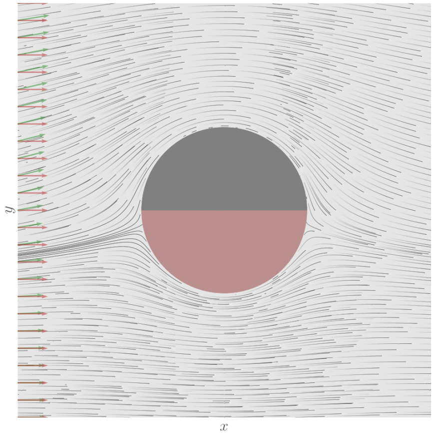
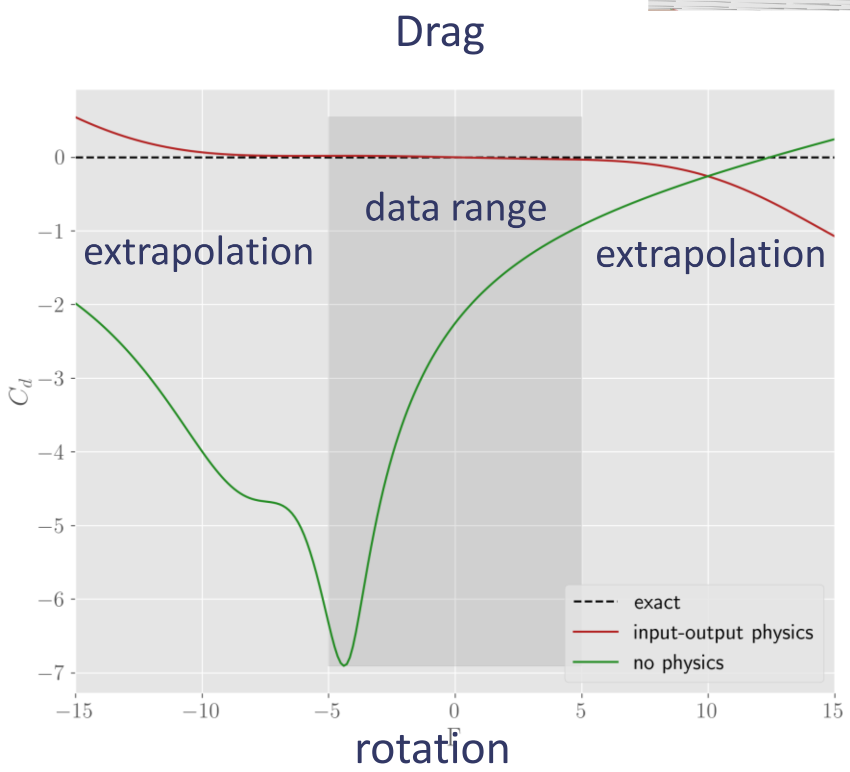
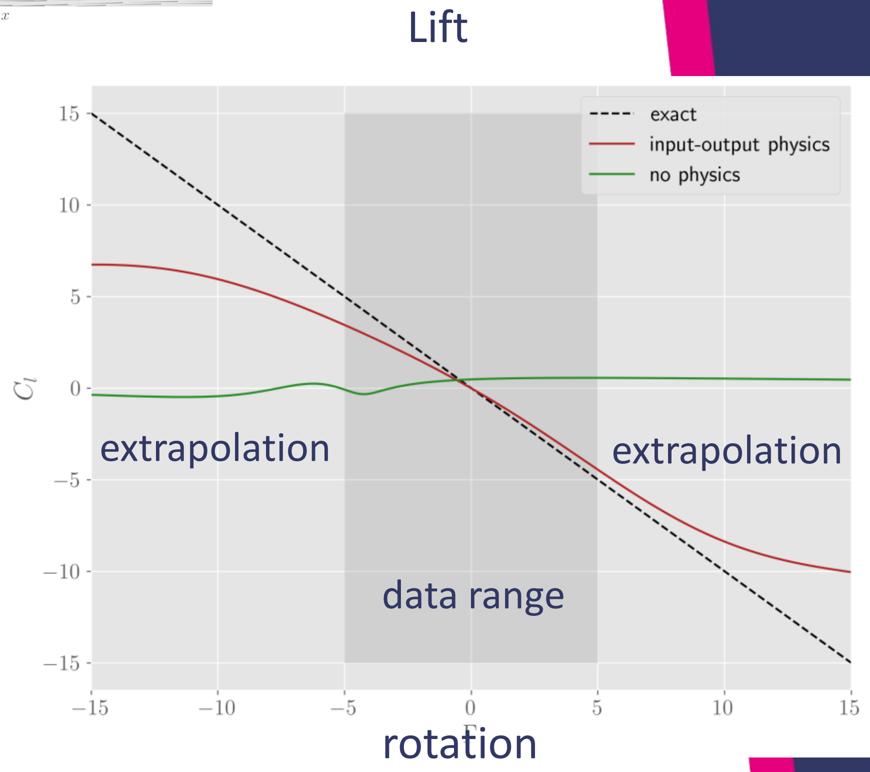
Physics-constrained is very good but still can't extrapolate

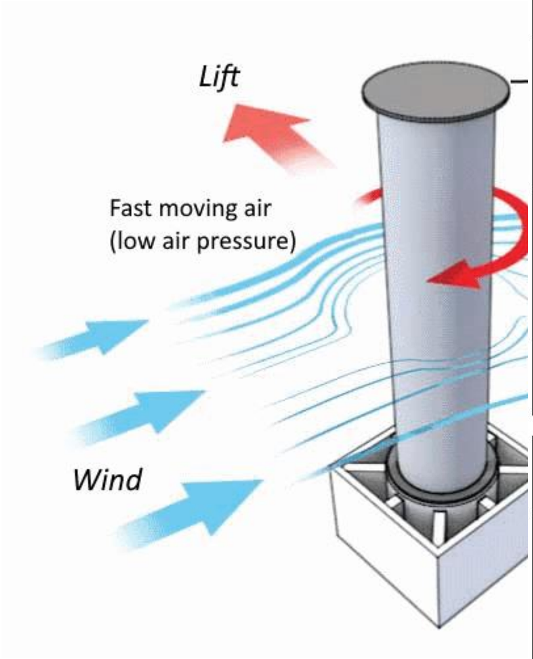
- Rotating circular cylinder
  - $[x, y, U, \Gamma, \mathrm{D}] \rightarrow [u, v]$
  - Tiny 6 neuron network & only 500 examples
- Pure data-driven
  - Fails to predict lift
  - Completely unsymmetric
- Physics-constrained
  - Good within data limits, but poor extrapolation

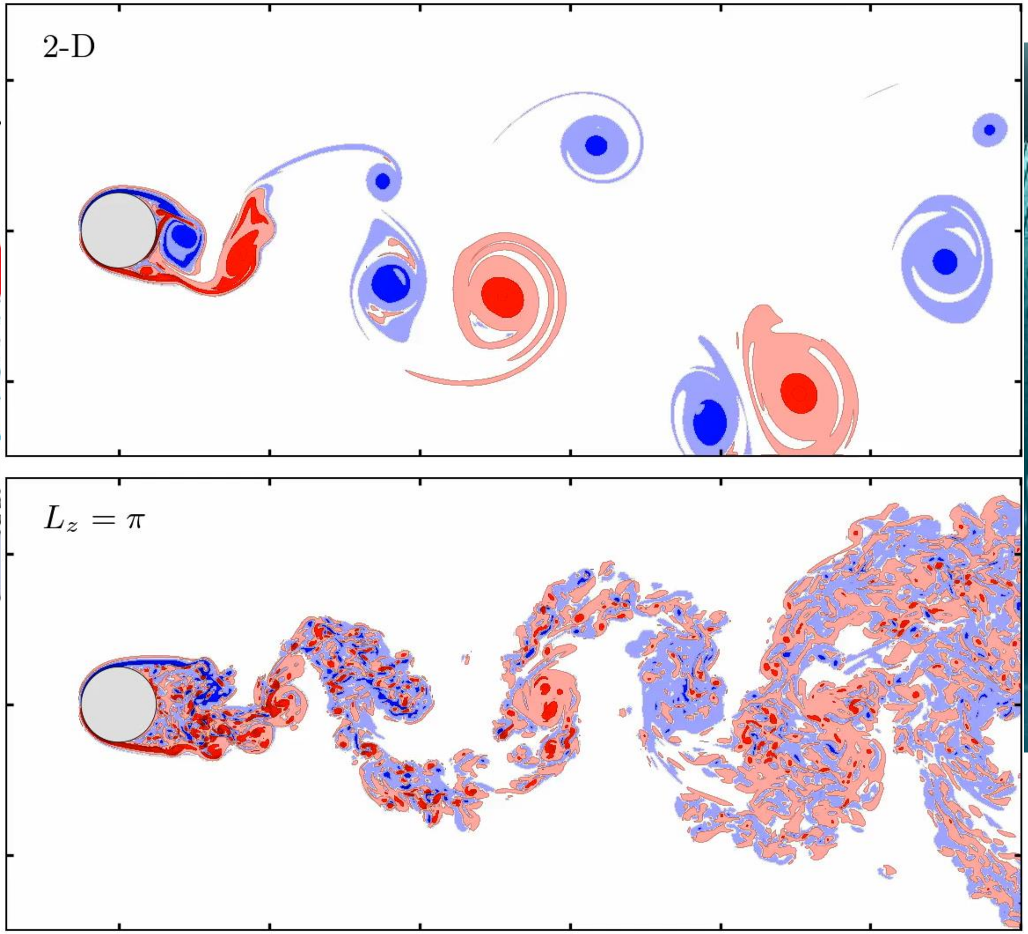




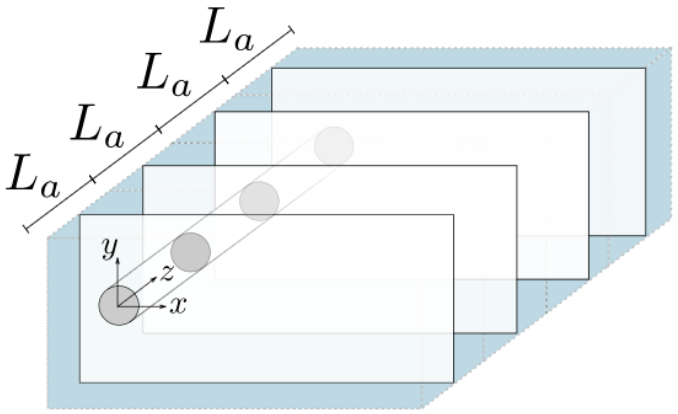


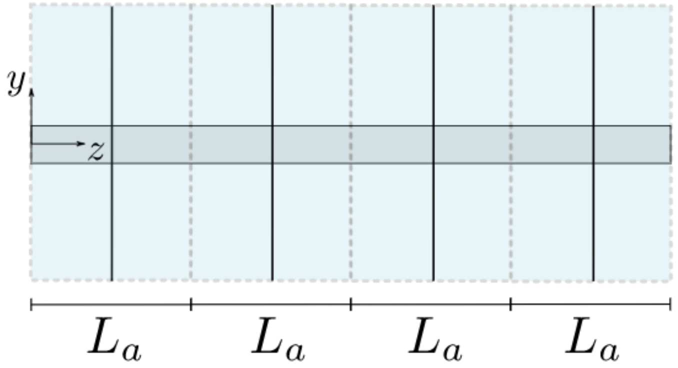
Fast 2D predictions on slender geometries don’t work because turbulence is 3D





Spanwise-averaged the momentum equation and Deep Learn the new turbulence model





From:
3D Navier-Stokes simulation

Average every L_a slice

To:
Multiple 2D Navier-Stokes simulations + extra terms

$$\langle u'u' \rangle \ \langle u'v' \rangle \ \langle v'v' \rangle$$

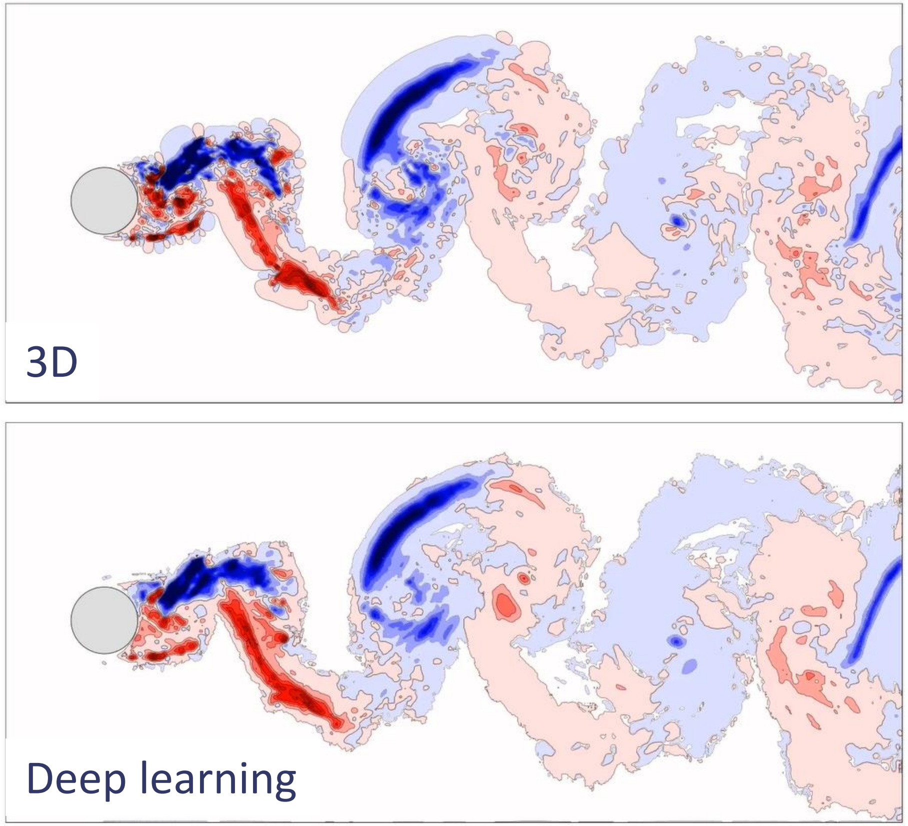
Modelled with a Convolutional Neural Network (CNN)

Recover the 3D averaged solution at every 2D plane

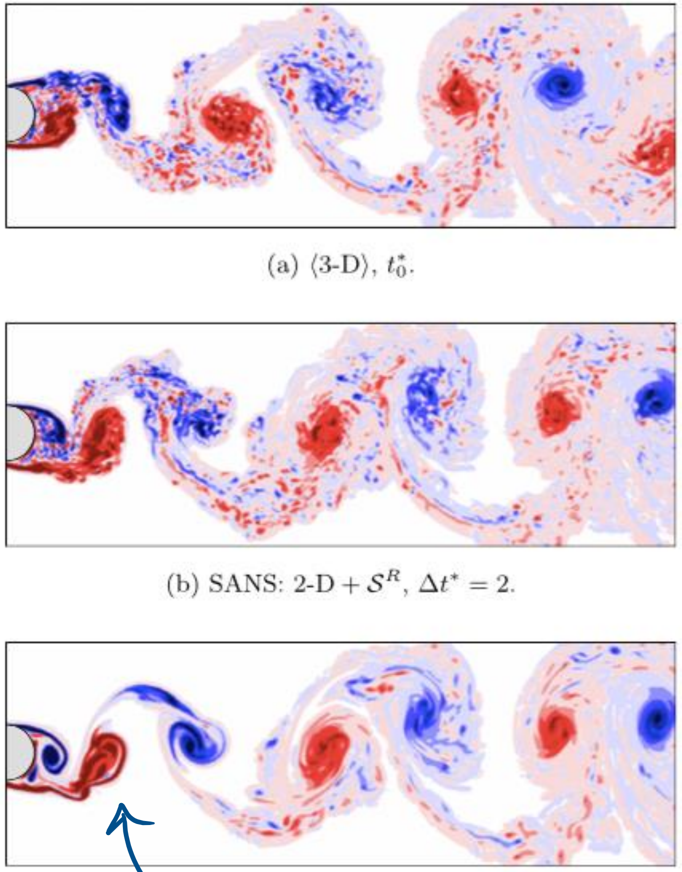
Font et al, *J Computational Physics*, 2021

Combining 2D physics + deep learning recovers 3D flow

Spanwise-stress ⟨$u'v'$⟩



Vorticity

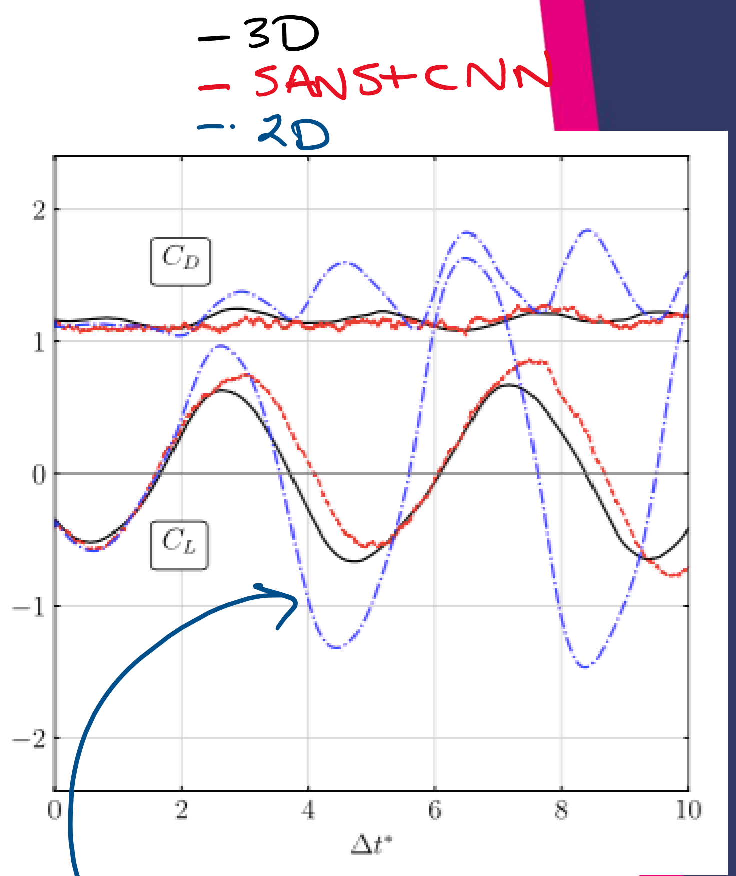


(a) ⟨3-D⟩, t_0^*.

(b) SANS: 2-D + $\mathcal{S}^R$, $\Delta t^* = 2$.

(c) 2-D, $\Delta t^* = 2$.

Lift and drag force

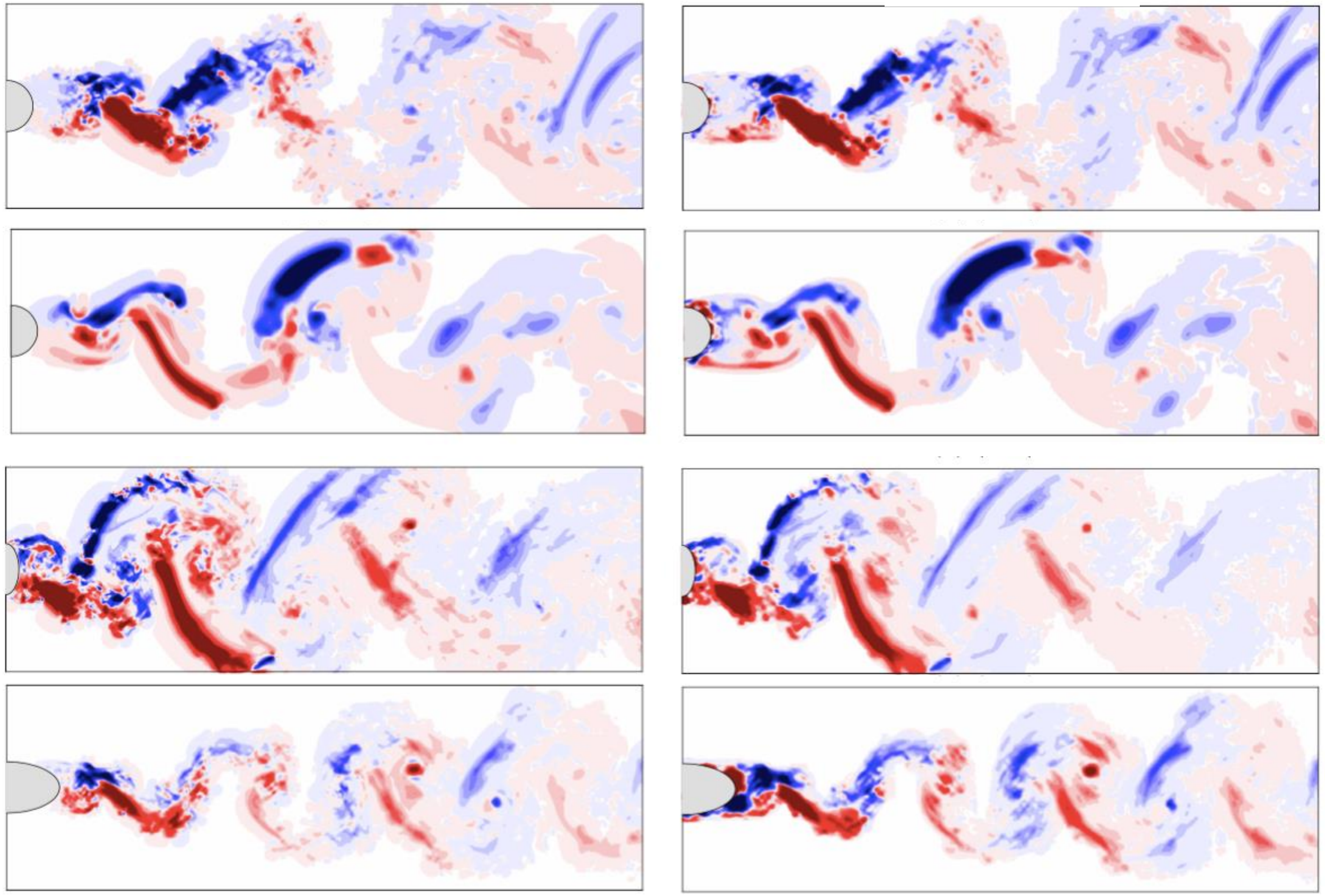


Complete deviation

Font et al, *J Computational Physics*, 2021

Generalizes well and gives 200x speed-up per span

3D simulation | 2D+DL test



Unseen Reynolds numbers

Re = 10k

Re = 3.9k

Unseen geometries

2:1 ellipse

1:2 ellipse

Font et al, *J Computational Physics*, 2021

Adding Insight to Artificial Intelligence

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Adding Insight to Artificial Intelligence

- Scaling laws and governing equations constrain ML & avoid exponential data
- Adding insight requires expertise in both ML & physics

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