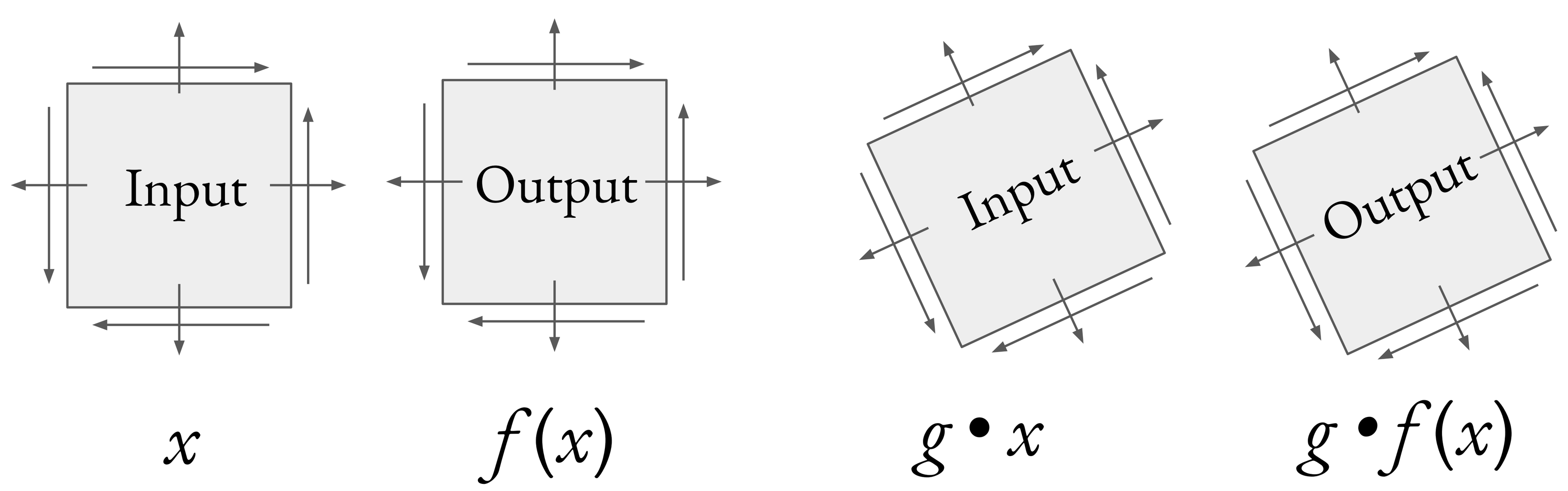
# Equivariant Machine Learning of Sub-Grid Scale Closure Models for Large Eddy Simulation

**Ryley McConkey**, Julia Balla, Elyssa Hofgard, Tess Smidt
Massachusetts Institute of Technology

MIT Center for Computational Science & Engineering · NDSEG · NSF IAIFI · NSERC CRSNG

## What is equivariance?

A model $f(x)$ is **equivariant** with respect to rotations if, for any rotation $g$, it satisfies $f(g \bullet x) = g \bullet f(x)$.
An **equivariant** model appropriately rotates it's outputs when the inputs are rotated.



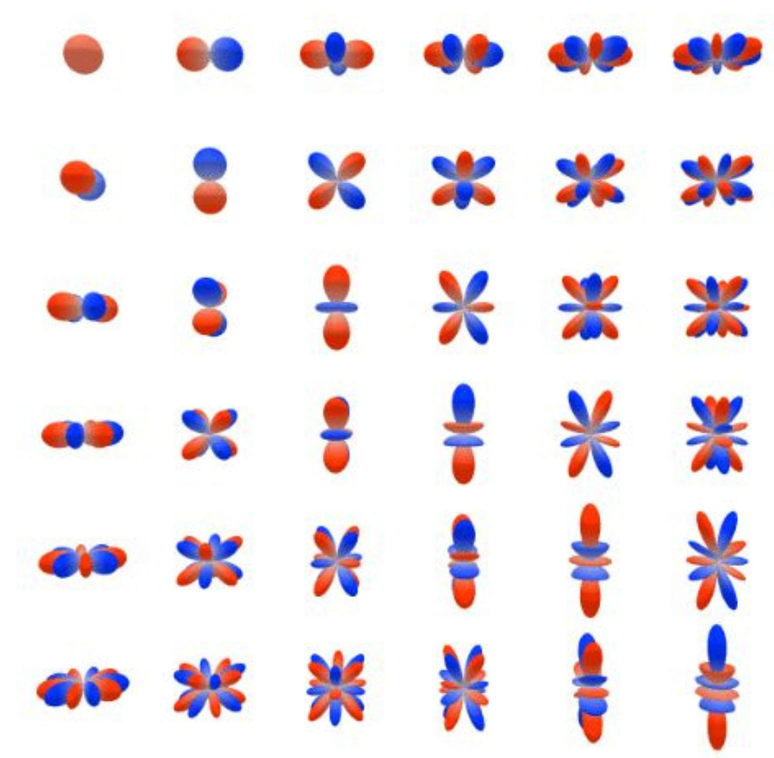

## Why equivariance?

In other scientific machine learning domains (chemistry, atomistic physics, material science), it's actually up for debate. But the debate hasn't started in turbulence yet.

**Physics-based inductive biases help generalization**
Turbulence is particularly interesting, because it's a rotational phenomenon itself.

**It respects the physics**
The Navier-Stokes Equations automatically transform their fields. Why doesn't your model?

## How can we achieve equivariance?



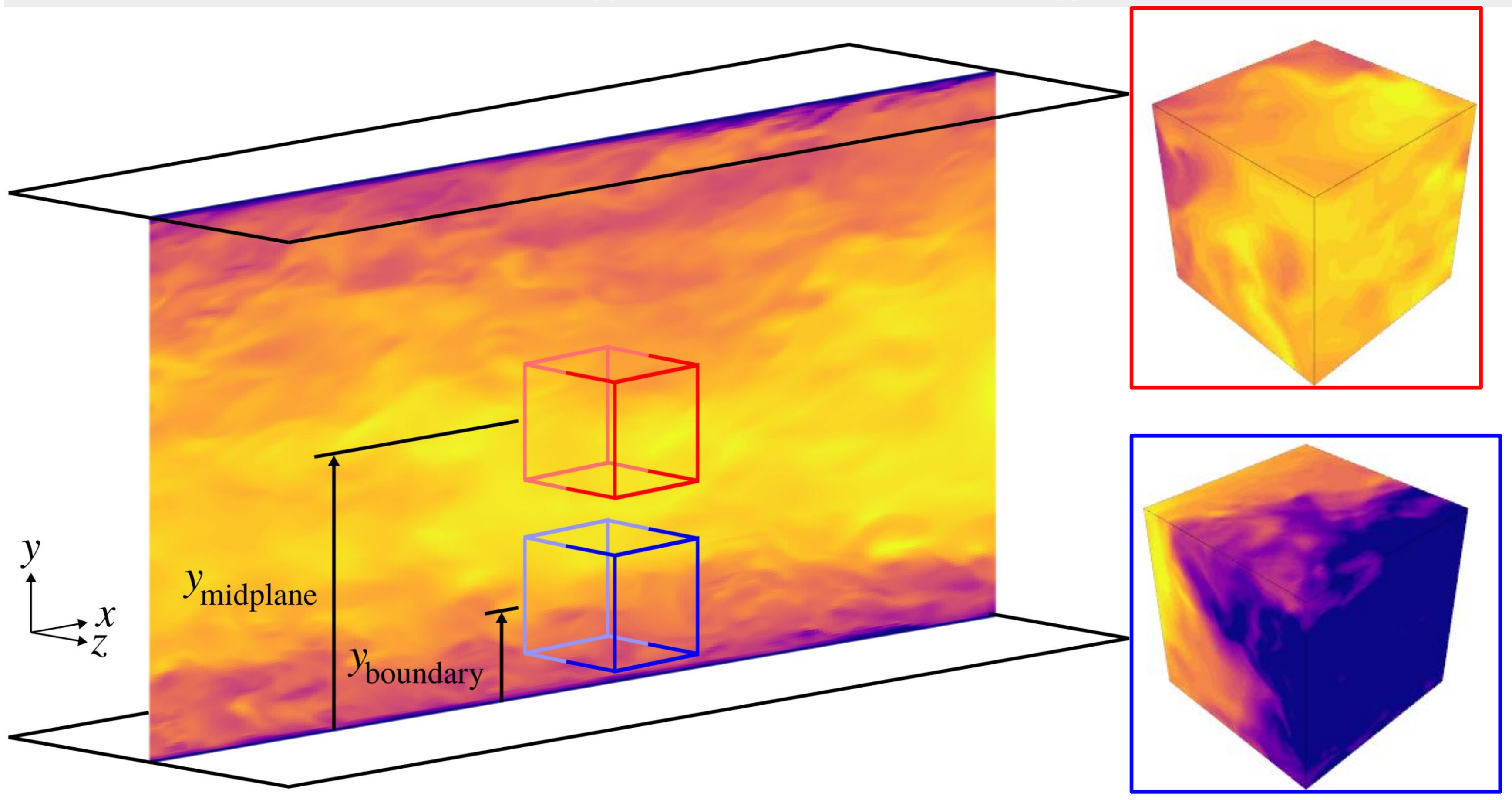
*Spherical harmonic basis for building an equivariant model.*

**Learning bias (soft constraint)**

- Randomly rotate input/output pairs together during training
- Model learns to not rely on a particular coordinate frame

**Inductive bias (hard constraint)**
e.g., using a Euclidean neural network (e3nn). The model automatically respects all desired symmetries.

## Experiment setup

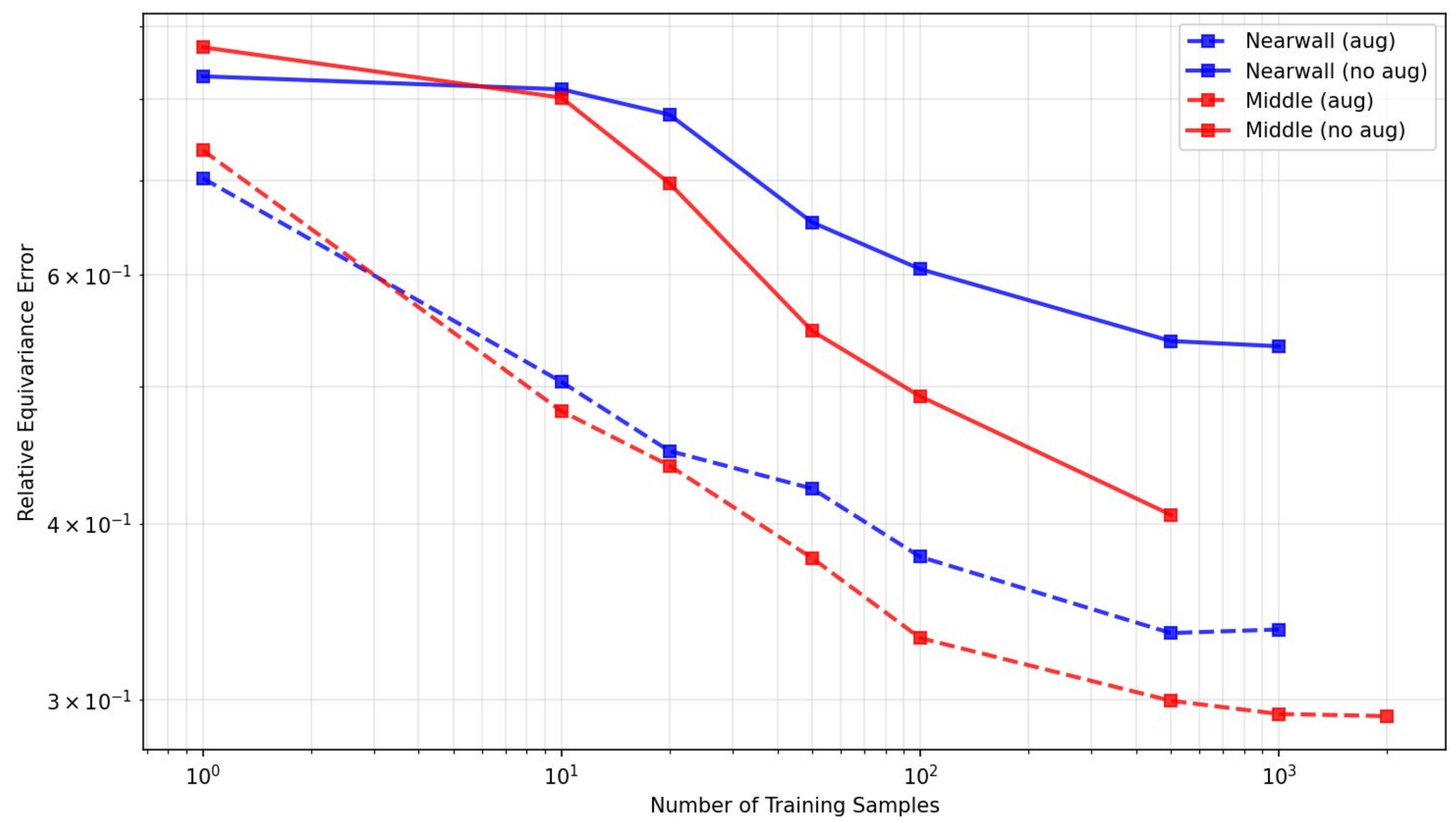



**Task:** predict the subgrid scale stress tensor from the filtered velocity gradient tensor
Between two subdomains (**midplane**, **near-wall**) compare:

1. No equivariance enforcement
2. Equivariance as a learning bias
3. Equivariance as an inductive bias

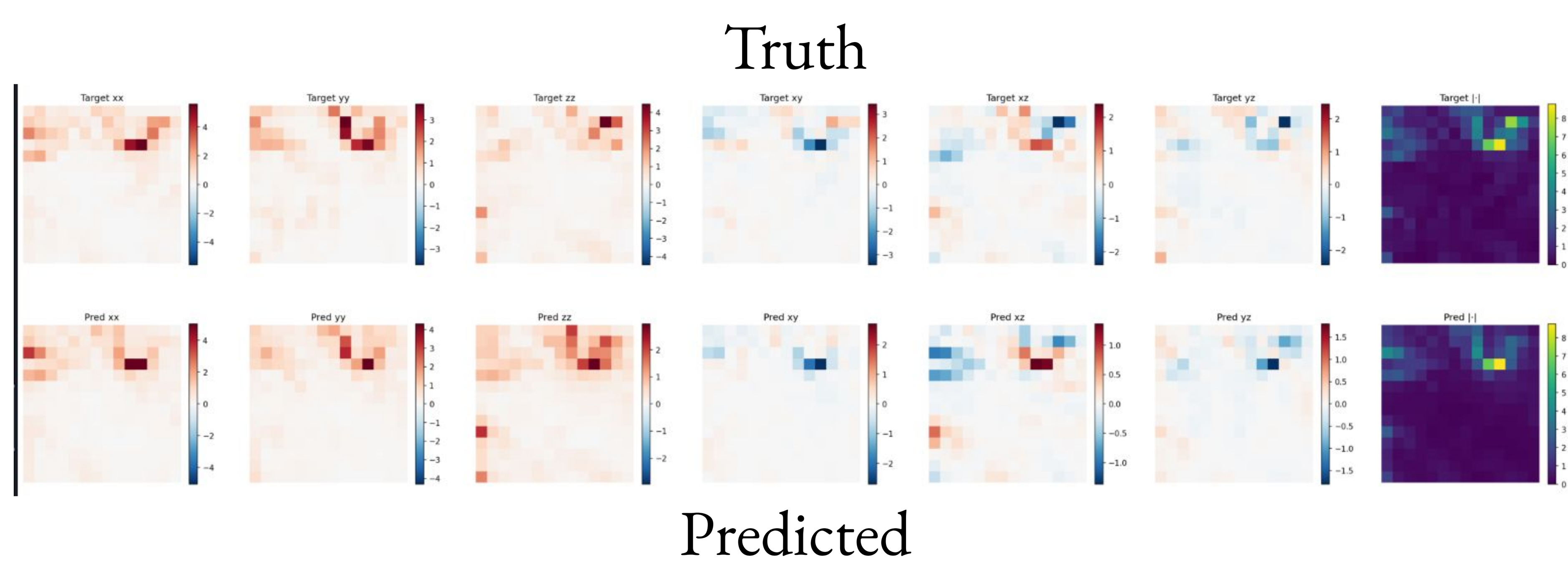
Using a CNN and ENN with similar parameters.

## Results




**Takeaway 3:** Equivariance, however achieved, helps generalization to higher Reynolds numbers.

- Both soft and hard constrained models outperform the plain CNN when generalizing from Re = 1000 to Re = 5200.




**Takeaway 1:** Turbulence data itself provides some amount of rotational augmentation.

**Takeaway 2:** Anisotropic turbulence doesn't provide as much augmentation.

Aside: with ERCOFTAC, we're putting together a **field-wide benchmark for data-driven RANS** turbulence modelling!
github.com/rmcconke/closure-challenge-benchmark