On rotational equivariance as an inductive bias in machine learning for fluids

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2nd ERCOFTAC Workshop on Machine Learning for Fluid Dynamics
2 April 2025

Outline

1. Equivariance - overview and motivation
2. Early results
    - Superresolution
    - Subgrid-scale closure modelling
    - RANS anisotropy mapping
3. Is your model currently equivariant?
4. Conclusion

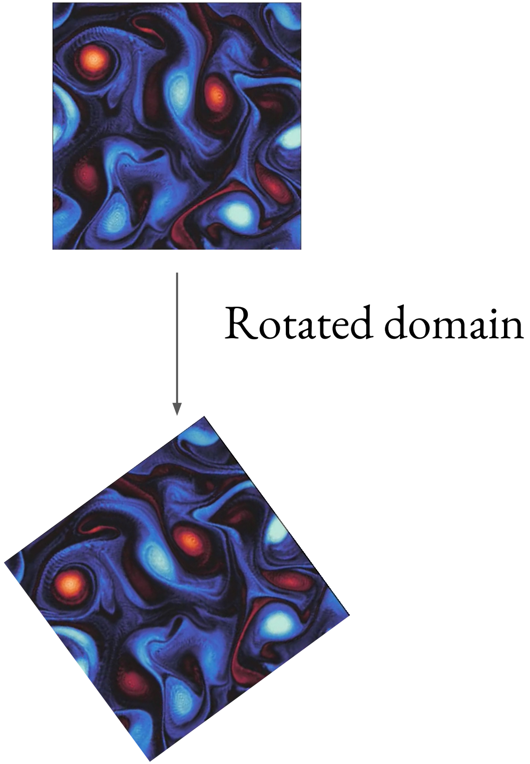
Equivariance

Navier-Stokes equations automatically transform their outputs when the inputs transform (*covariance*)

Should our ML model also generalize to new input orientations/frames?

Equivariance is cared a lot about in ML for:

- Computational chemistry
- Materials design
- Protein modelling
- Geometry



Equivariance

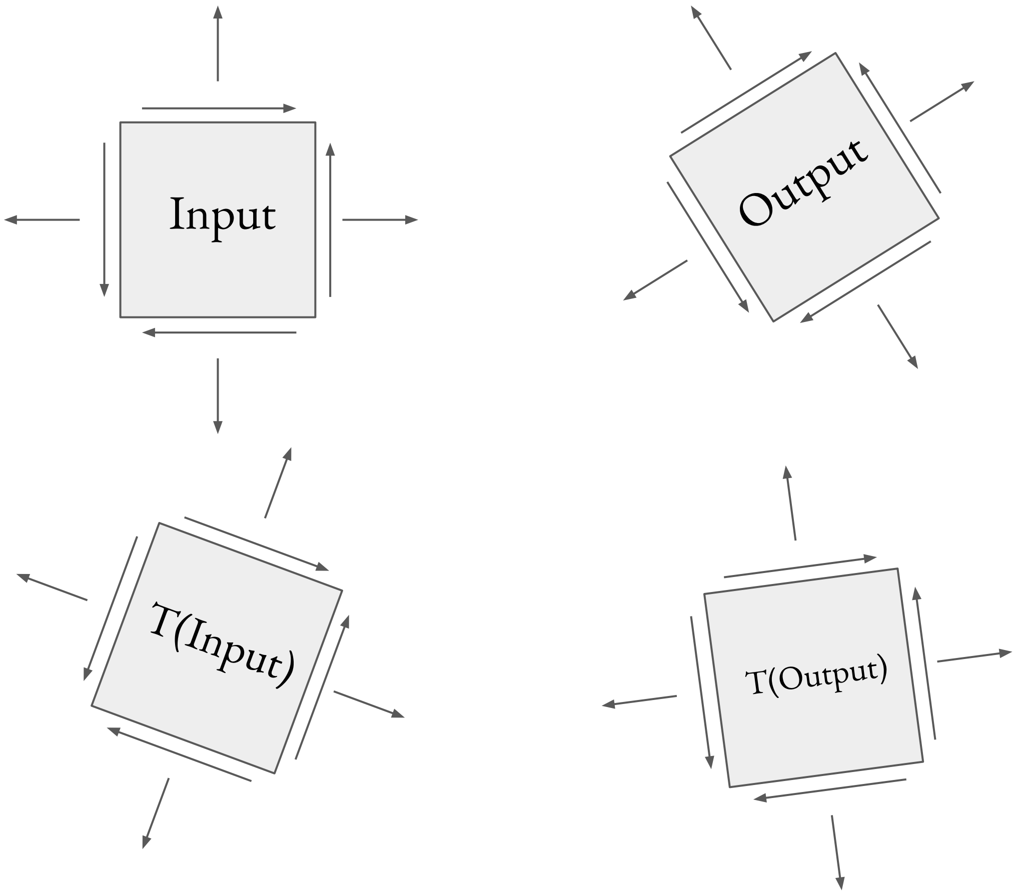
An *equivariant* model automatically transforms its output when the input is transformed.

Relevant transformations (E(3) group):

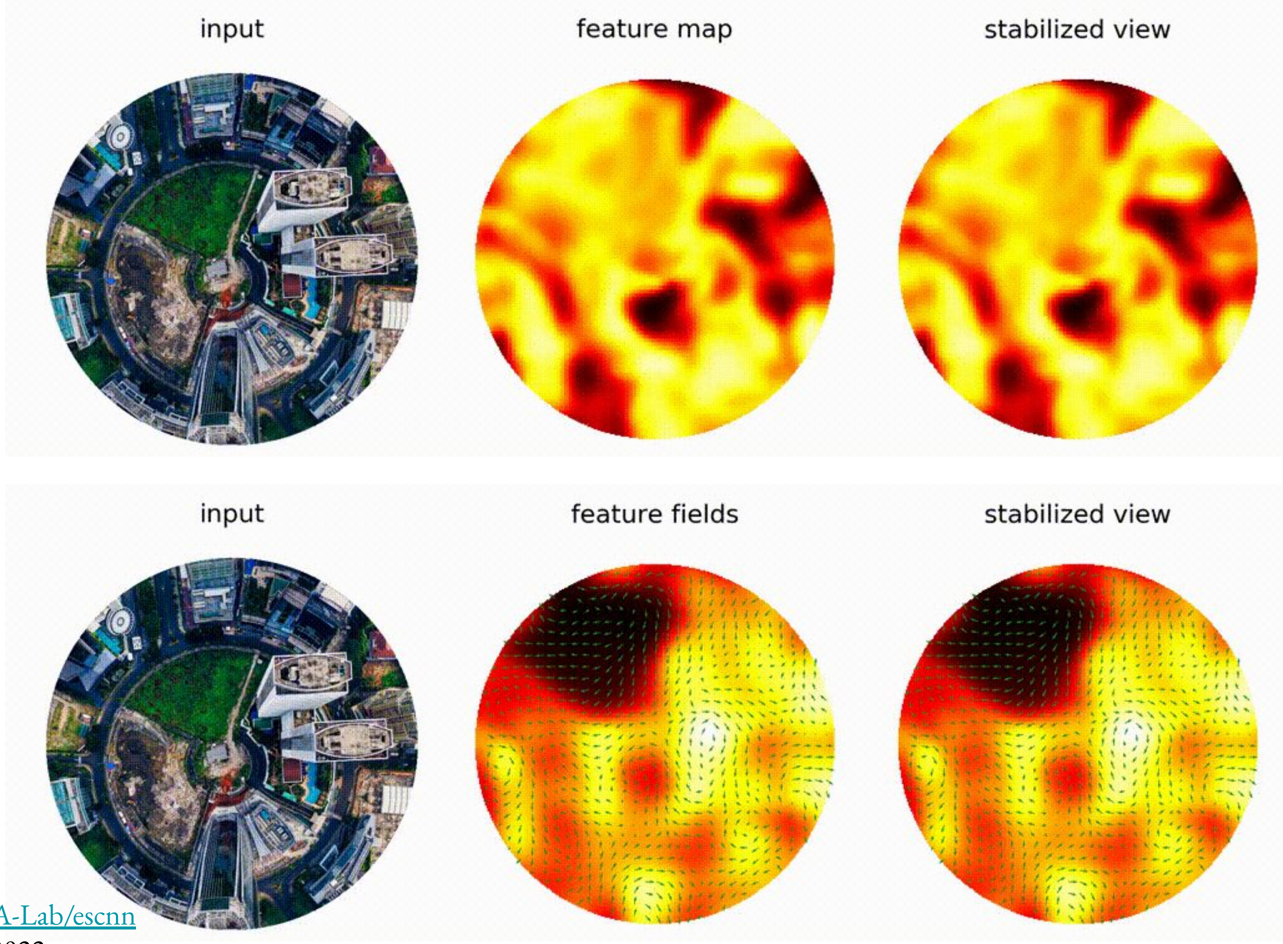
- Translations (automatic with CNNs)
- Rotations
- Reflections
- Inversions

Without equivariance:

- If the input is transformed, the output will not be.

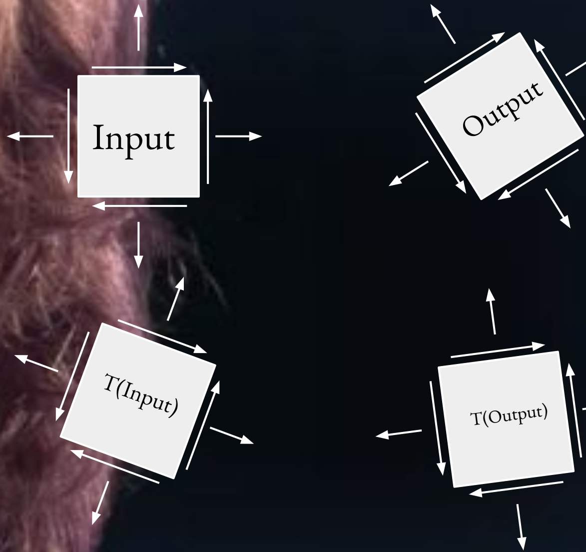


Equivariance



https://github.com/QUVA-Lab/escnn
Cesa, Lang, Weiler ICLR 2022

1. Data augmentation
   a. During training, randomly transform input/output pairs
   b. For fluids - does this happen automatically?
2. Automatically equivariant model (inductive bias)
   a. E.g. e3nn, ESCNN



In fluids, we often don't worry about teaching our models equivariance at all!

Is it possible to learn this power?

Why equivariance?

Active debate between equivariant/non-equivariant models in other domains is ongoing.

Advantages of equivariant models:

- Data efficiency
  - No data augmentation needed
- Automatic encoding/imposition of symmetry
- Model can learn local symmetries

Disadvantages:

- More complicated than your average architecture
- Symmetry is strictly imposed

Selected Tasks

1. **Superresolution of a vorticity field**
2. **Subgrid scale closure modelling**
3. Anisotropy mappings for turbulence closure modelling
    a. Results by others point towards equivariance being beneficial

RESEARCH ARTICLE | FEBRUARY 07 2025

Implicit modeling of equivariant tensor basis with Euclidean turbulence closure neural network

Grzegorz Kaszuba; Tomasz Krakowski; Bartosz Ziegler; Andrzej Jaszkiewicz; Piotr Sankowski

Check for updates

+ Author & Article Information

Physics of Fluids 37, 025137 (2025)

https://doi.org/10.1063/5.0249490 Article history

Goal:

Is equivariance a useful inductive bias in ML for fluids?

Superresolution - example output

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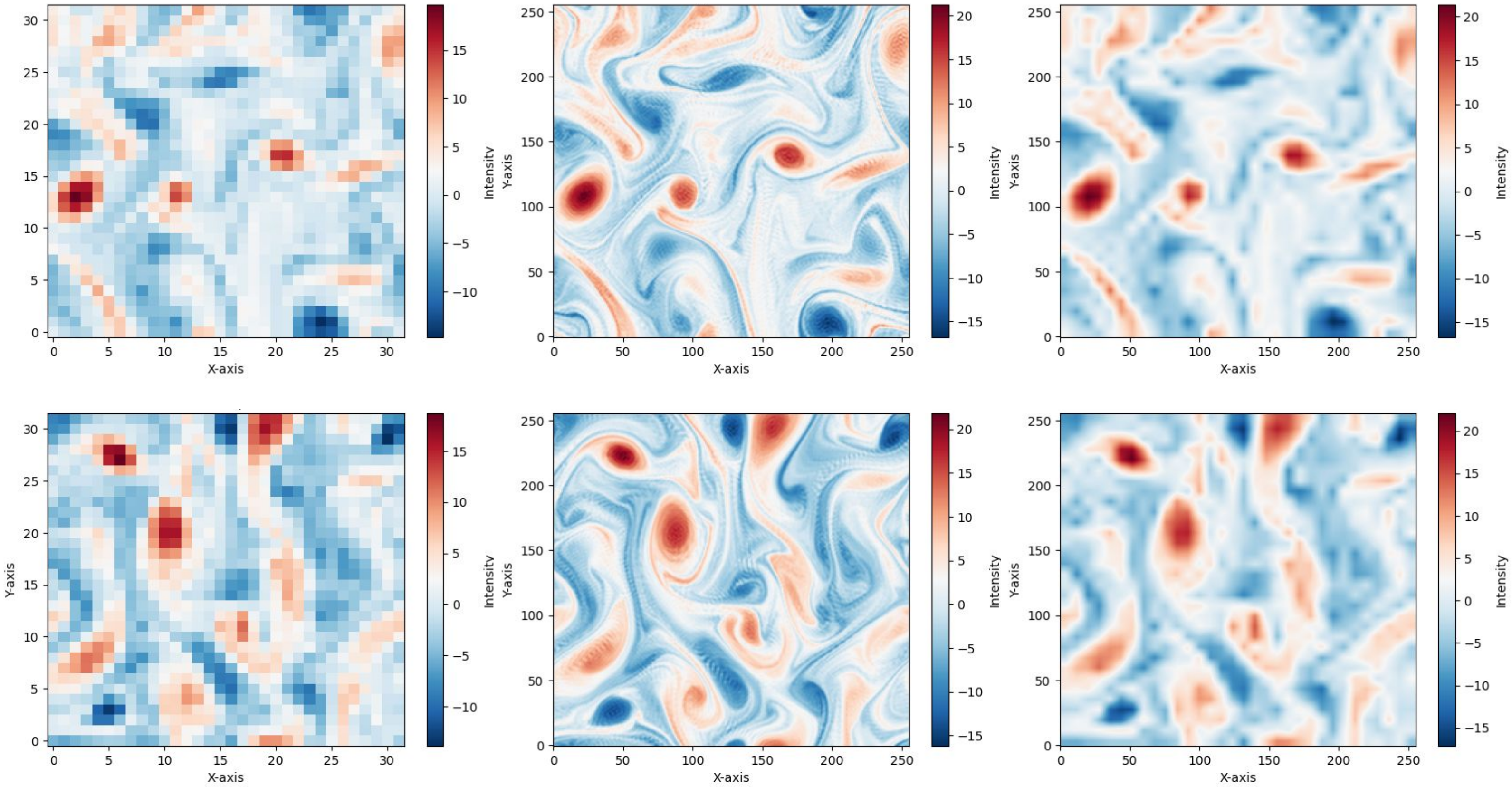
J. Balla



Superresolution - results

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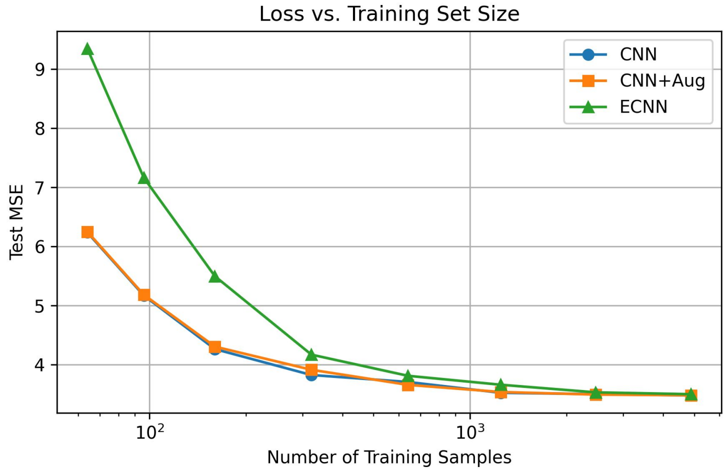
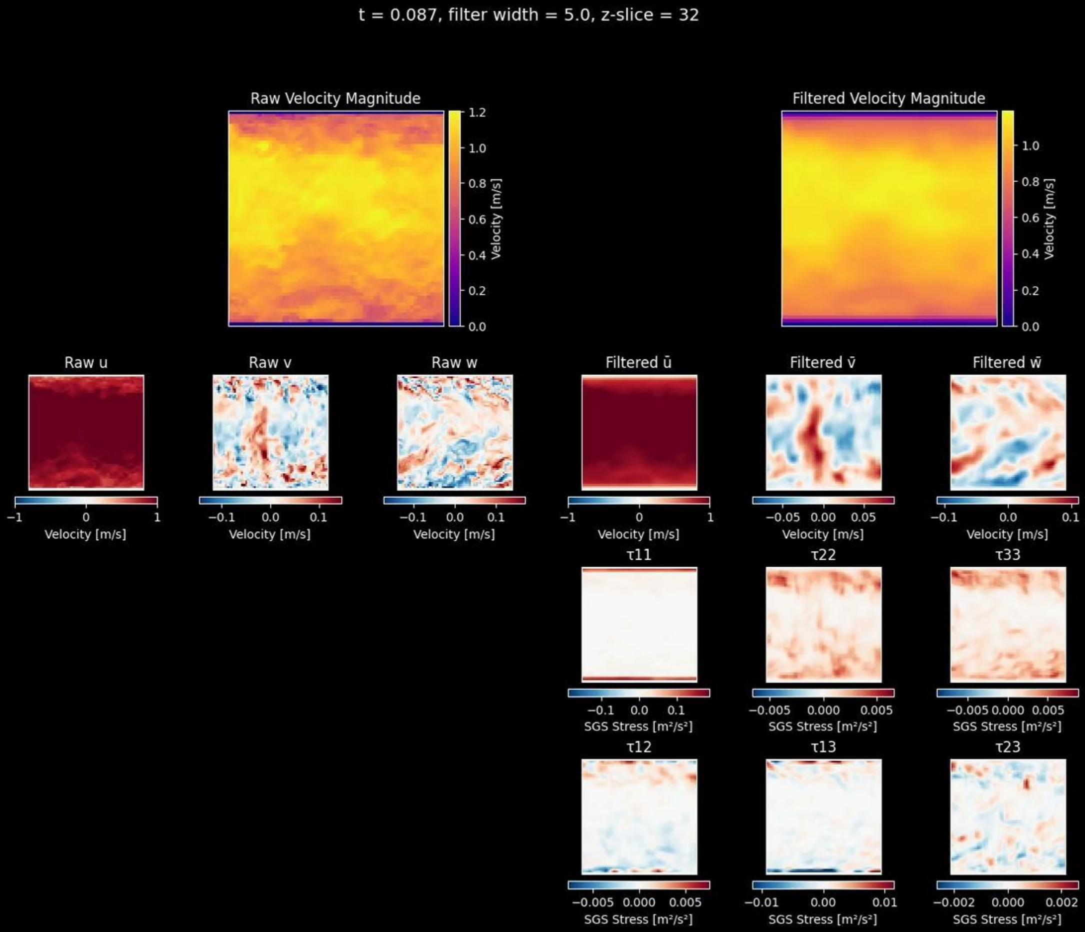
Model	Train MSE	Test MSE	Equivariance Error	Parameters
CNN	3.0760	**3.4738**	0.0447	38624
CNN + Aug	**3.0744**	3.4745	0.0486	38624
ECNN	3.0823	3.4783	$\mathbf{2.113 \cdot 10^{-6}}$	37328



- All models perform similarly on the training and test sets
- "Equivariance error" is not reduced by data augmentation for this task
- We can perform well without completely learning equivariance

Subgrid scale turbulence modelling



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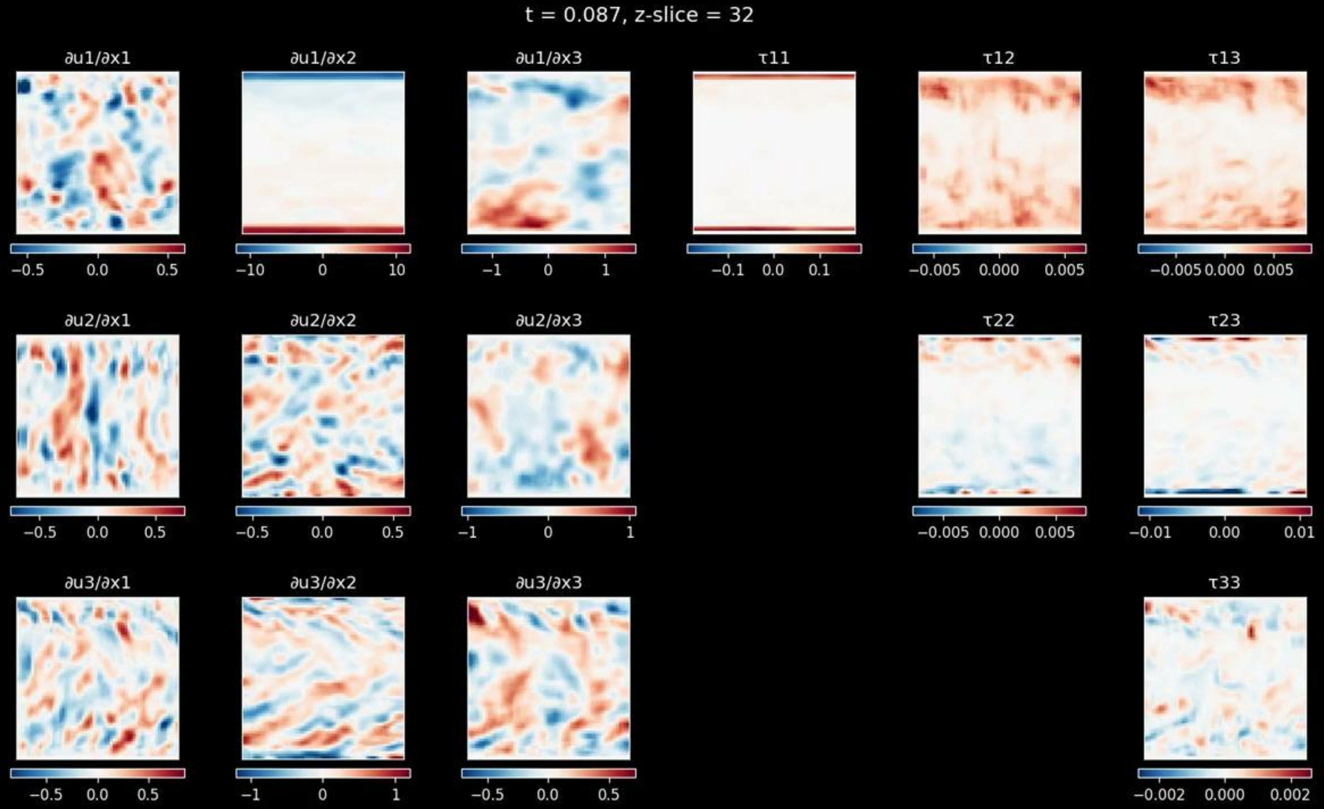
Subgrid scale turbulence modelling



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Input tensor

Output tensor

Preliminary Results: subgrid scale turbulence modelling

- Equivariance is not needed to capture large-scale patterns

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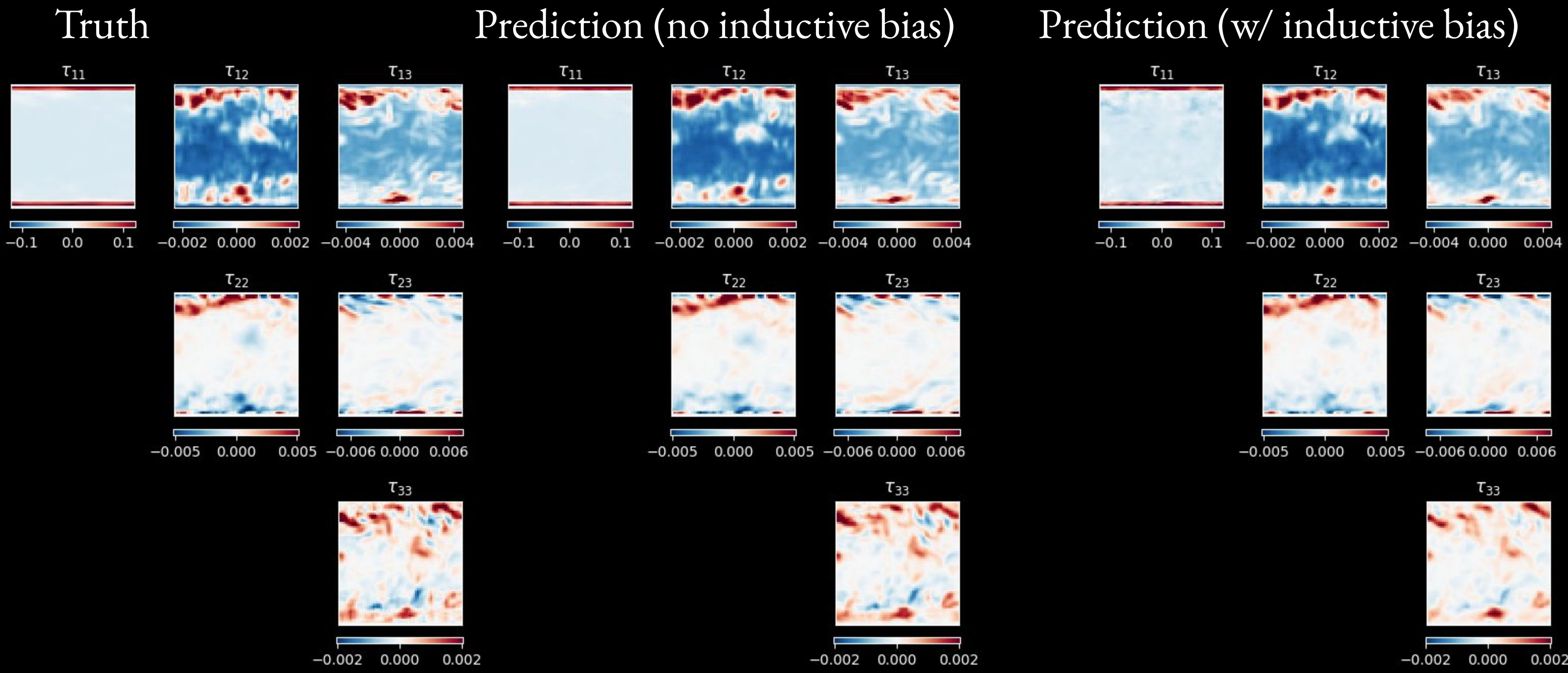
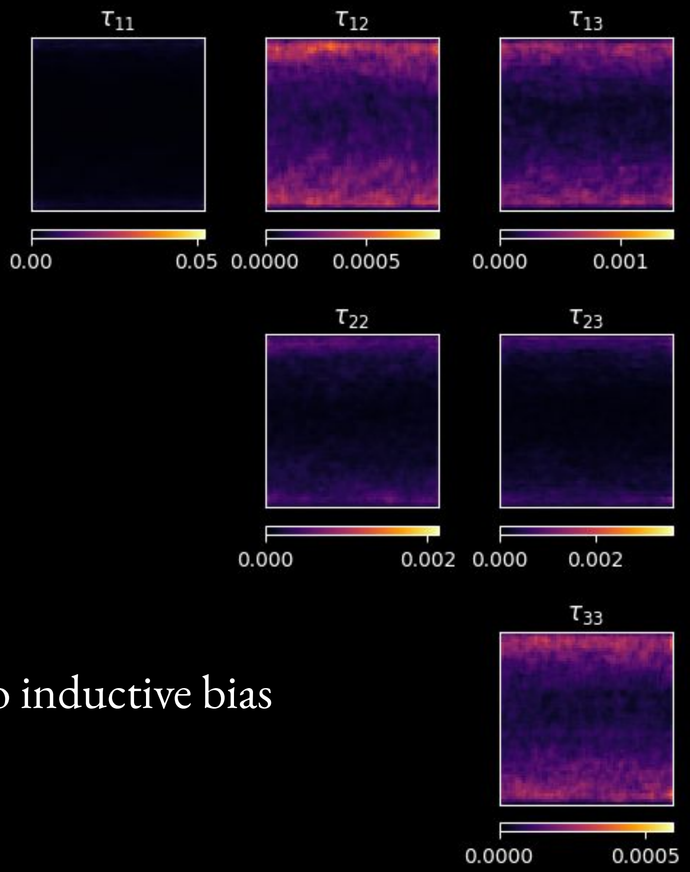
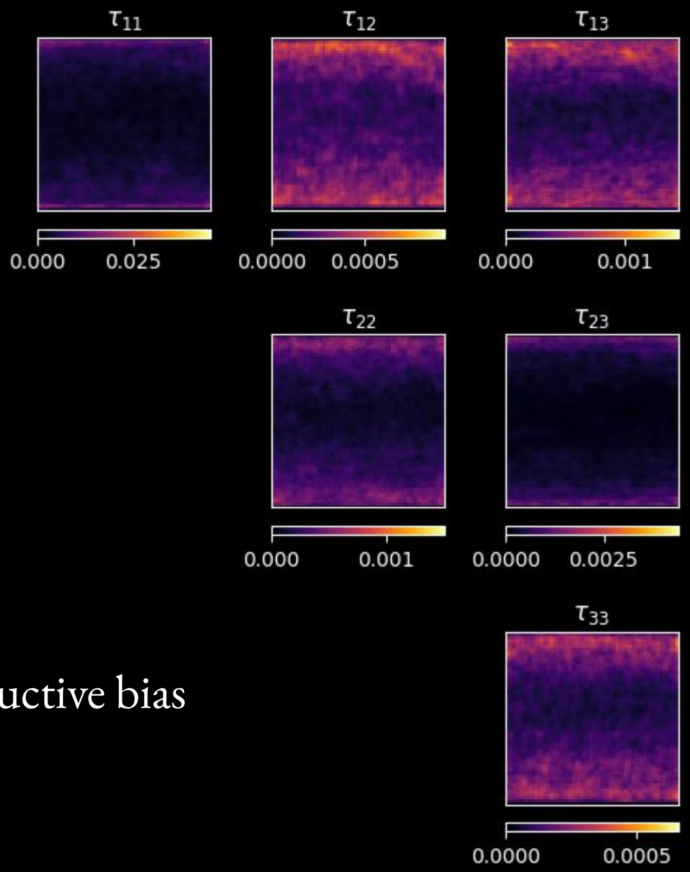


Preliminary Results: subgrid scale turbulence modelling

(Test set MAE per pixel, horizontal slice through centre of domain)



No inductive bias



Inductive bias

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Preliminary Results: subgrid scale turbulence modelling

- Generalization (covariance) test after rotation of the input tensor

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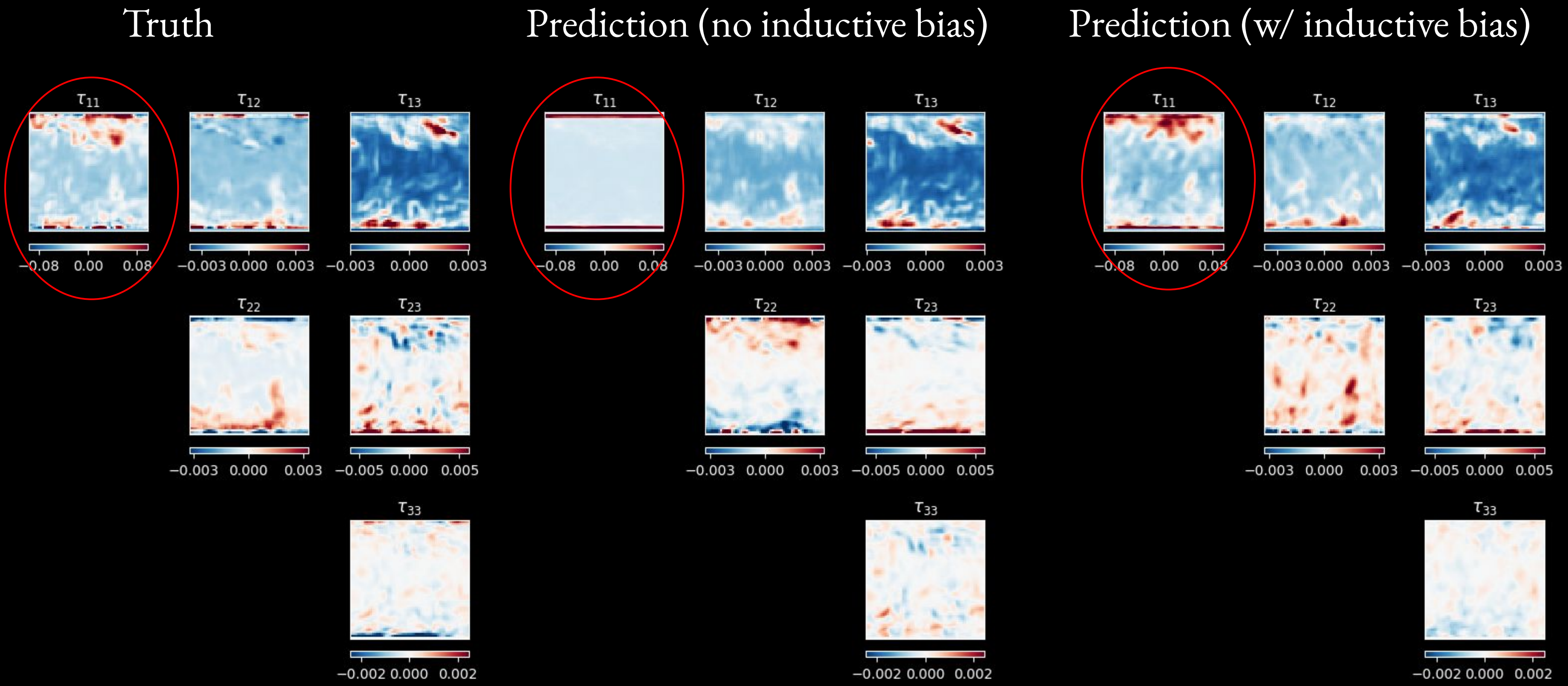

Is your model currently equivariant?

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Distributional symmetry

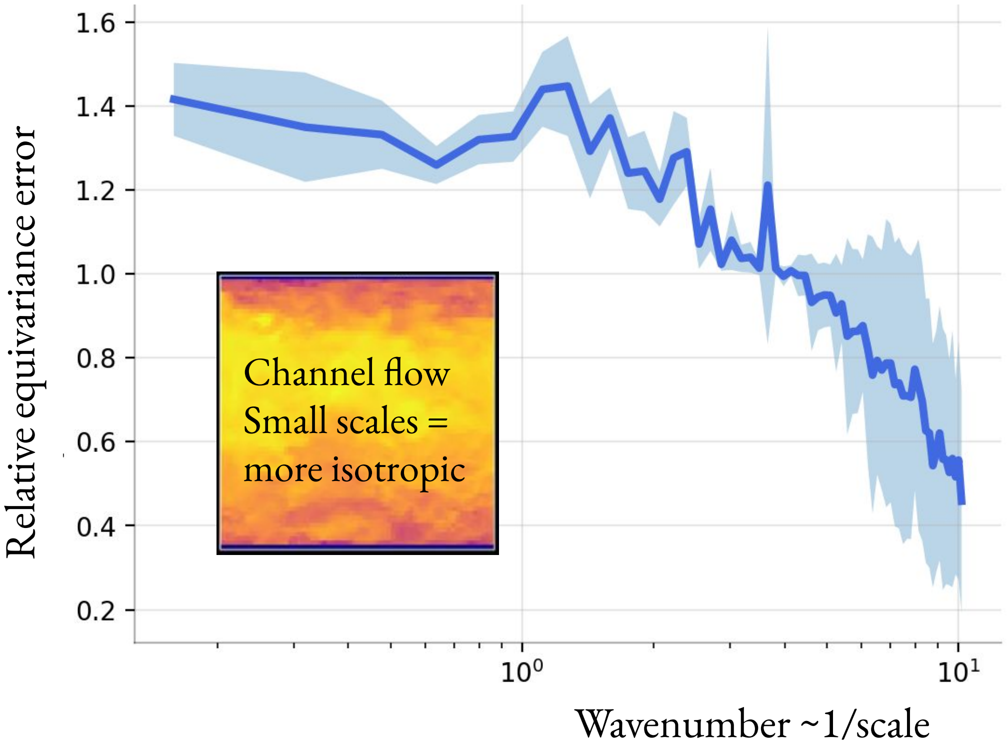
Statistical homogeneity/isotropy of the dataset

- In certain directions
- At smaller scales (Kolmogorov hypothesis)

(individual frames are inhomogeneous/anisotropic)

Result: *scale-dependent rotational data augmentation*

- Our models might be learning equivariance, but *only at the small scales* due to this Kolmogorov hypothesis-based data augmentation.



Summary

Equivariance: widely used in other scientific ML domains - has pros and cons, but the debate is ongoing

Goal: determine whether equivariance is a useful inductive bias for fluids

Limitations:

- Simple (easy) tasks considered
- Turbulent flows with a limited range of scales

Preliminary conclusions

- We *don't* need equivariance to predict large-scale flow structures
- We *do* need it to generalize to new coordinate frames
- The more anisotropic the flow, the more equivariance will help
    - For more isotropic flows - implicit data augmentation (less dependent on the coordinate frame)

Future work

- Investigate local symmetries and patterns in anisotropic flows
- Harder generalization tests - can equivariance help turbulence models generalize better?

Why not try an equivariant model for your problem? Many open source implementations exist.

Acknowledgements

NSERC CRSNG

DOE CSGF

NSF

NDSEG

MIT UROP
Undergraduate Research Opportunities Program

Appendix

Subgrid scale turbulence modelling

Task (Regression): Predict the subgrid scale stress tensor in terms of resolved tensors

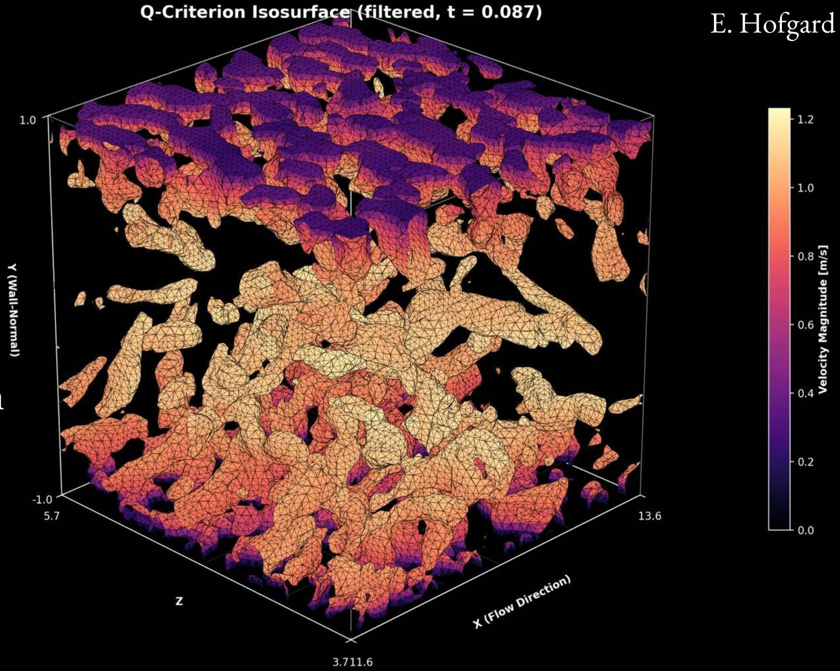
Flow: Turbulent channel flow

Dataset: Johns Hopkins Turbulence Database, Re_τ ~ 1000

Models: 3D CNN, 3D equivariant CNN using e3nn

- ~200,000 parameters for each model with 3 convolution blocks

Training/Val/Test: 70/20/10 training/validation/testing split with randomly selected timesteps

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Superresolution of vorticity field

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Task: Given a coarse resolution image of a flow field, predict a finer resolution

Flow: 2D Kolmogorov Forced Turbulence

Numerics: jax-cfd solver, 256x256 mesh, pseudo spectral solver, Crank Nicholson RK4, first order in time, second order in space, CFL < 0.5

Models: CNN, C_4-Equivariant CNN using escnn

~ 40,000 parameters for each model with 3 convolution blocks + bilinear upsampling

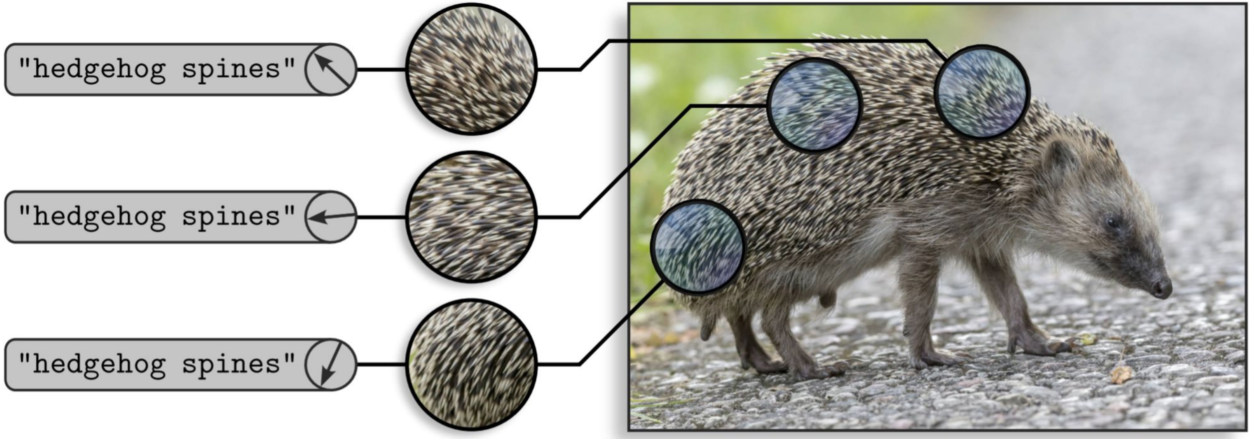
Dataset: Re = [1000, 1500, 2000,... 10000]

Training: Re = [1000, ..., 3500, 7000, ..., 10000]

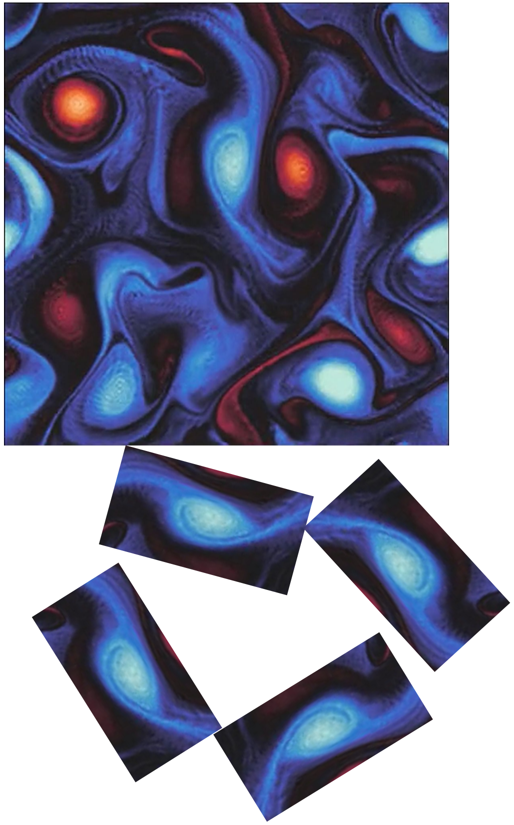
Test: Re = [5000, 5500]

Local Symmetry

Weiler, M., Forré, P., Verlinde, E., & Welling, M. (2024). Equivariant and Coordinate Independent Convolutional Networks. WORLD SCIENTIFIC. https://doi.org/10.1142/14143



(Hedgehog adapted under the free license by courtesy of Freepik.)



Anisotropy test - results

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Model	**Anisotropic MSE**	**Equivariance Error**
CNN	5.300	0.0654
CNN + Aug	5.325	0.0657
ECNN	45.625	$4.0128 \cdot 10^{-13}$