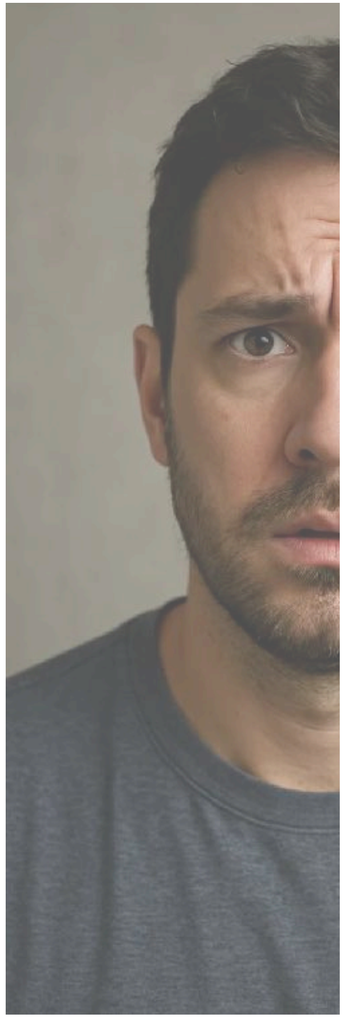
Foundation Models & Outlook

ADVANCED DEEP LEARNING FOR PHYSICS

Open Challenges

Practical Requirements:

- 1) Scaling to real-world problems
  - Training (resources & sample efficiency)
  - Inference (compute & memory)
- 2) Unstructured meshes
- 3) 3D over time
- 4) Robustness & Guarantees



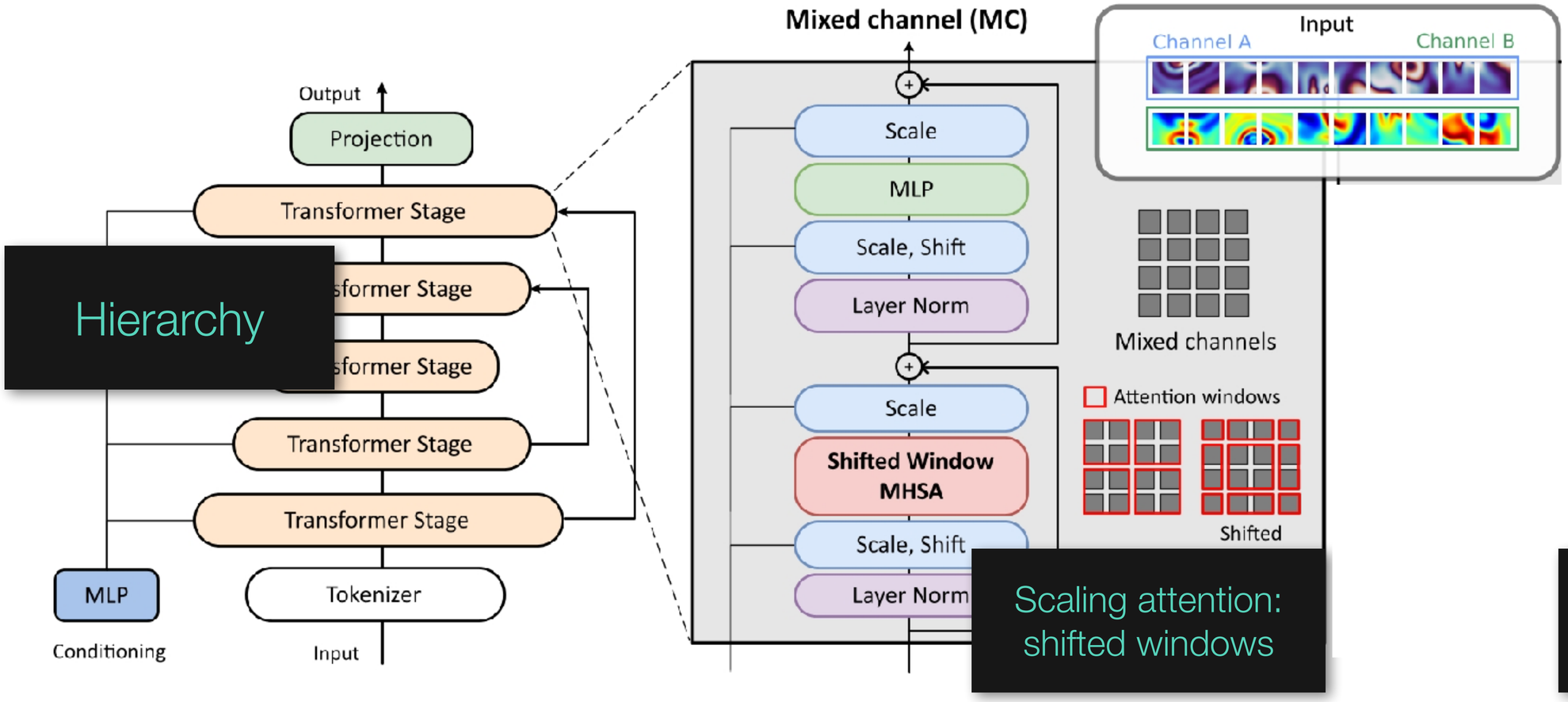
Potential Avenues: 1) Scaling

Transformer Architectures & Fine Tuning

- Transformers scale well (better than CNNs and GraphNets)
- Fine Tuning: pre-train large model, then adapt with small dataset
- Re-use infrastructure from LLMs

1) Scaling: Transformer Outlook

Scalability for PDE Problems



Hierarchy

Scaling attention: shifted windows

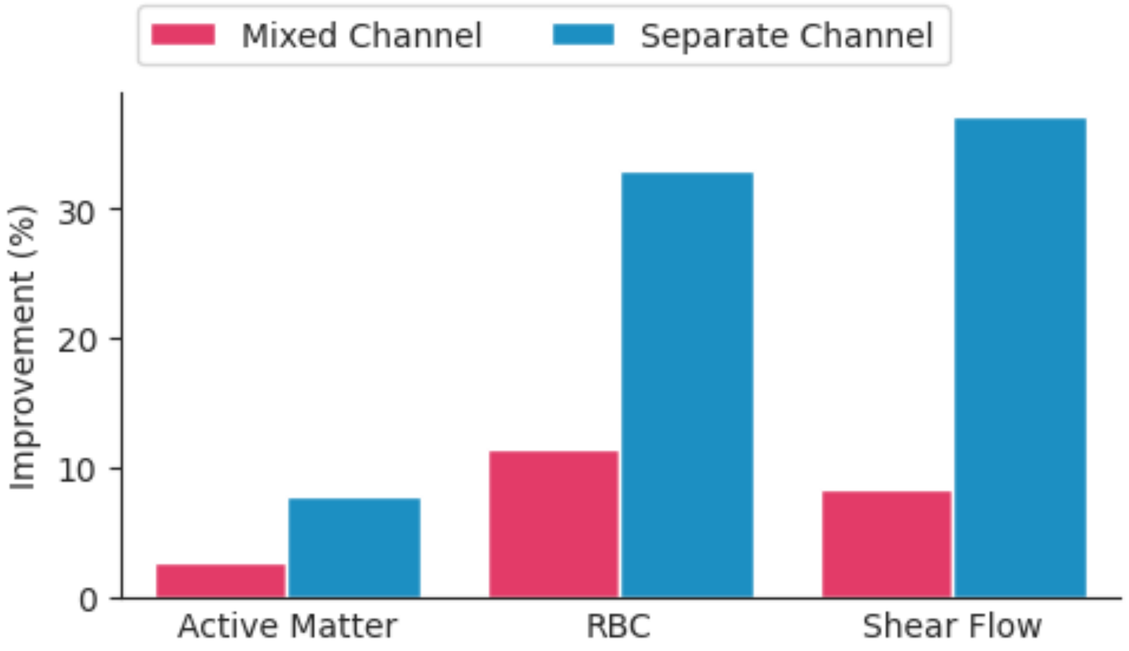
For flexibility… (SWin per channel)

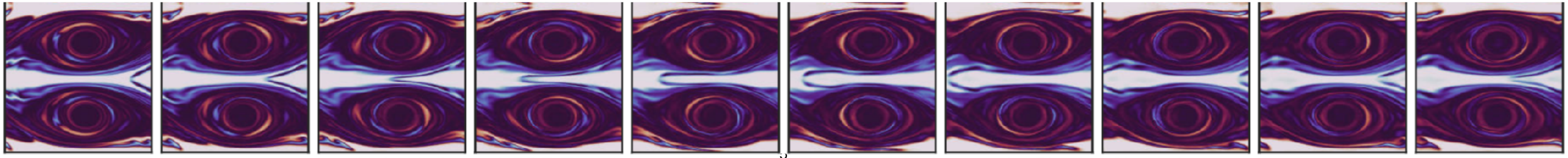
Holzschuh et. al: PDE-Transformer: Efficient and Versatile Transformers for Physics Simulations

1) Scaling: Fine-Tuning

Fine-Tuning: Targeting Small Data Regimes

- Pre-train on canonical PDEs
- Apply to new cases: load pre-trained model and continue…



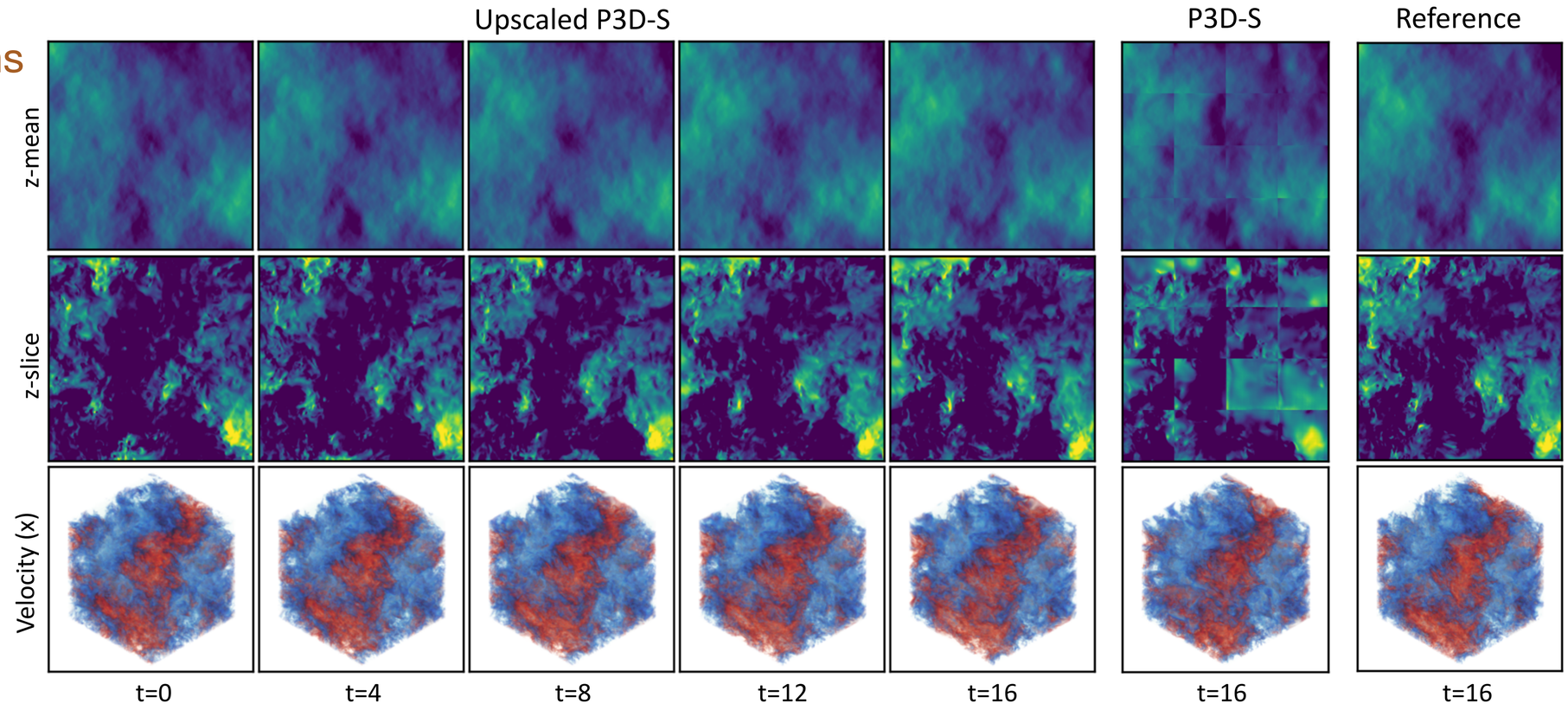


Holzschuh et. al: PDE-Transformer: Efficient and Versatile Transformers for Physics Simulations

3) 3D Problems

Extension of PDE Transformer Architecture

- Scales to large resolutions (with some tricks)
- Here: 512^3 turbulence (ca. 400M DOFs)
- Train model on 128^3 regions, then combine multiple regions via *context-network*

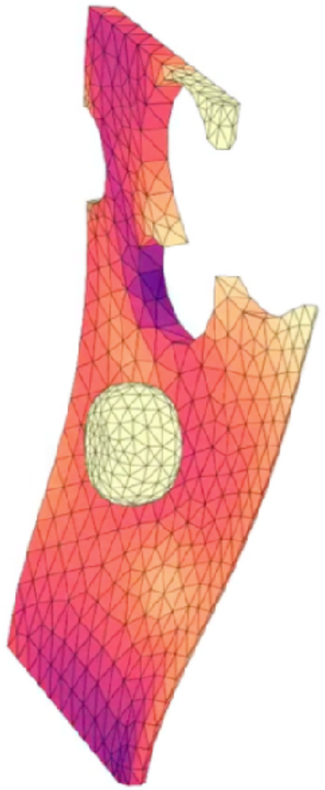


Holzschuh et. al: PDE-Transformer: Efficient and Versatile Transformers for Physics Simulations

2) Unstructured Meshes

Working with Real-world Inputs

- Real-world applications feature highly complex geometries
- Obstacles, boundary conditions, regions of interest …
- Meshing can be more expensive than physics simulation



4) Theory & Guarantees

(Beyond our Scope)

- Linear case well studied; non-linear fundamentally more challenging
- Busy area, work in progress…
- (Btw.: *classic solvers* in hybrid approaches give guarantees!)

Summary & Outlook

Wide Range of Topics

1. Supervised Learning
2. Physical Losses
3. Differentiable Physics
4. Graph Networks
5. Diffusion Models
6. Reinforcement Learning
7. (Foundation Models)

Physics-Based AI / Deep Learning

Outlook

🤨 Classic solvers will always remain better in some areas

- Example: spectral solvers for linear problems; exponential convergence ⚡

👉 Work out areas where NNs excel!

- Nitty, gritty details of real world problems ✨

- Non-linearities, complex boundaries ✨

- Noisy data and ambiguous measurements ✨

Physics-Based AI / Deep Learning

Approximate Global Summary

✅ Powerful new methodology

✅ Extremely promising outlook

❌ Quite a few open challenges…

❌ Established workflows & thresholds for classic computational tools

End