HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

ICML International Conference On Machine Learning

Helmholtz-Zentrum hereon

Geometric and Physical Constraints Synergistically Enhance Neural PDE Surrogates

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Project website

Scientific question?

Approaches to solving PDEs: Numerical methods (traditional);
Machine Learning (ML) Models (recent)

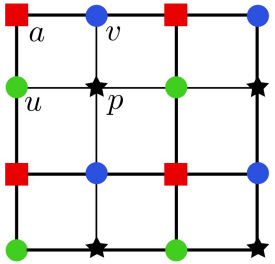
Challenges of ML model: Accurate long-term rollout; Generalization

PDEs fundamental assumptions: Symmetry and physical constraints

Previous ML Models

Related Works	symmetry constraint	physical constraint
Wandel et al. ICLR, 2021	✗	✓
Wang et al. ICLR, 2021	✓	✗

Incompressible
Navier–Stokes equation (INS)

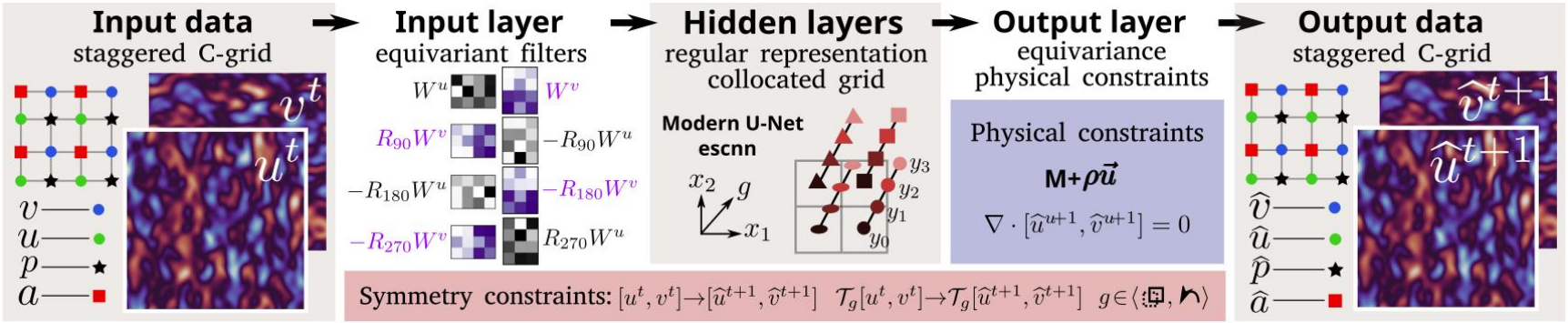


C-grid staggering
widely
Weather/
climate/
fluid dynamics

Our scientific question: **Would it be useful to combine the two constraints with the C-grid for the ML model, or would that be redundant?**

Symmetry- and physics-constrained neural surrogate

Symmetry- and physics-constrained neural surrogate



Experiments

Shallow Water Equations (SWEs)

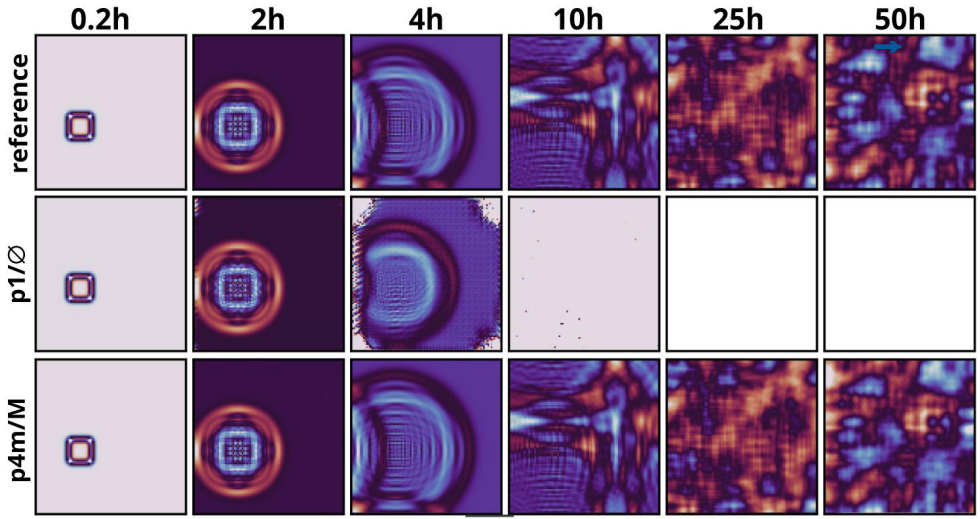
Conservation laws	Symmetries		
None ∅	p1/∅	p4/∅	p4m/∅
Mass M	p1/M	p4/M	p4m/M

Incompressible Navier–Stokes (INS) Decaying Turbulence

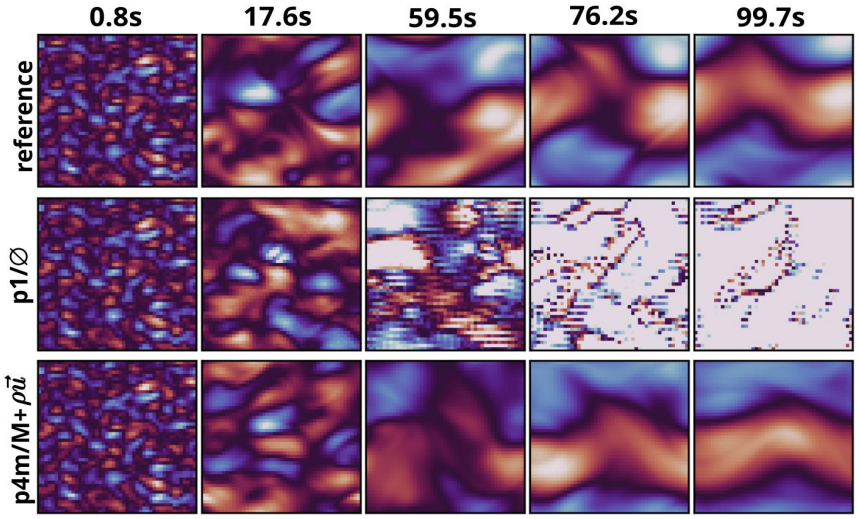
Conservation laws	Symmetries		
None ∅	p1/∅	p4/∅	p4m/∅
Momentum $\rho\vec{u}$	p1/ $\rho\vec{u}$	p4/ $\rho\vec{u}$	p4m/ $\rho\vec{u}$
Mass/momentum M+ $\rho\vec{u}$	p1/M+ $\rho\vec{u}$	p4/M+ $\rho\vec{u}$	p4m/M+ $\rho\vec{u}$

Our model outperforms other networks on SWEs and INS

Prediction of p4m/M for SWEs

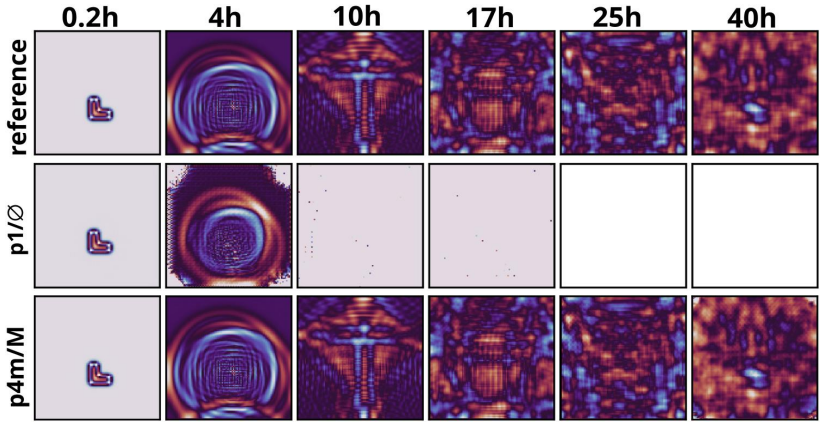


Prediction of p4m/M+ρu⃗ for INS

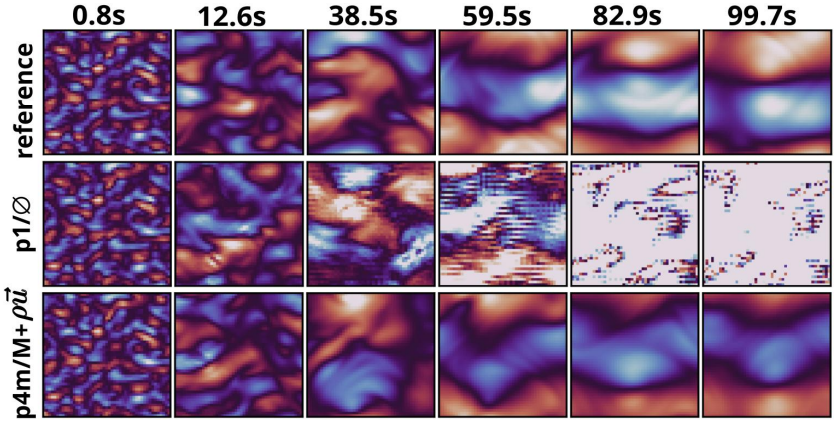


Generalization beyond training data

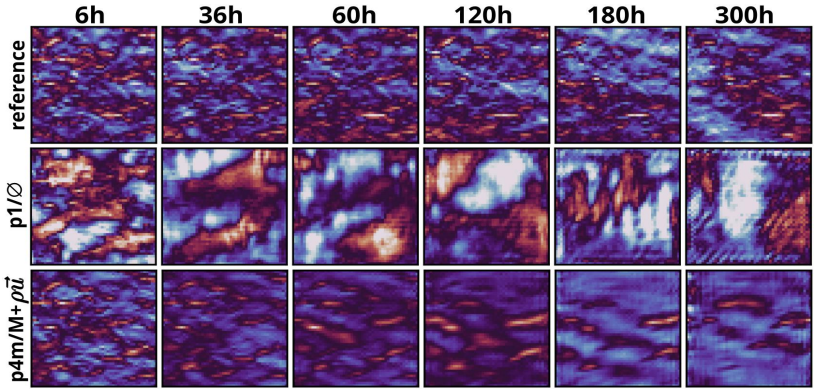
SWEs on L-shaped ICs



INS with peak wavenumber of 8



Real-world ocean currents



Conclusion

We developed a double-constrained model with input and output layers on C-grids.

We found that symmetries are more effective than physical constraints, but combining both is best.

We found our model can improve predictions in terms of generalisation and the real ocean data.

Project website