

Geometric and Physical Constraints Synergistically Enhance Neural PDE Surrogates

Yunfei Huang^{1,2}, David S. Greenberg^{1,2}

¹Helmholtz Centre Hereon, Geesthacht, Germany; ²Helmholtz Al

Yunfei Huang<yunfei.huang5@gmail.com>, David S. Greenberg<david.greenberg@hereon.de>

Project Website

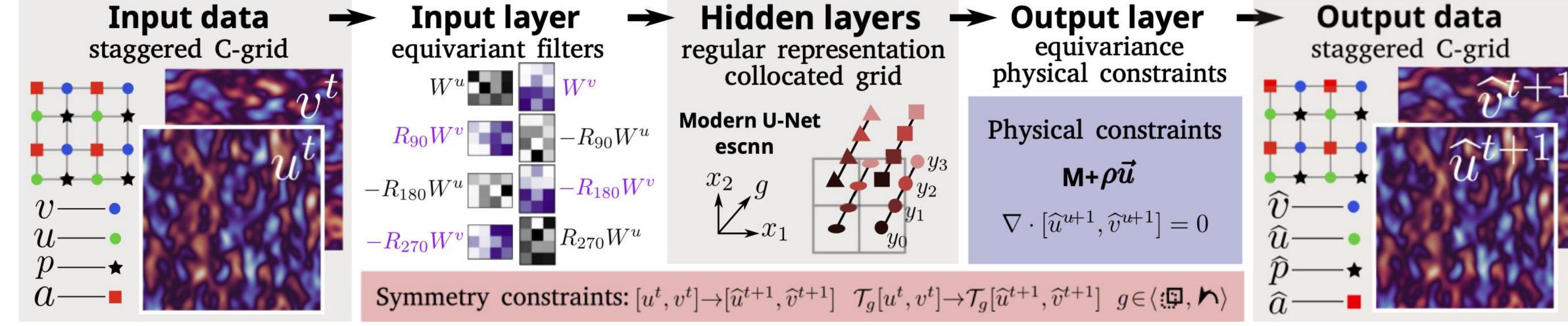


Introduction & Motivation

- Challenges for ML-based PDE prediction: long-term rollout accuracy, stability, generalization.
- Previous ML Models: can be improved by both physical and geometric constraints.
- Staggered C-grids: often used in weather, climate and fluid dynamics, but unsupported by standard equivariant convolution layers.
- Our aim: impose these constraints on C-grids, and evaluate whether their benefits can be usefully combined.

Symmetry- and Physics-Constrained Neural Surrogates

Network Architecture



The input- and output data are on C-grids. Starting from a strong modern U-net base architecture (Gupta et al., 2023), we imposed physical and symmetry constraints, individually and in combination.

Experiments

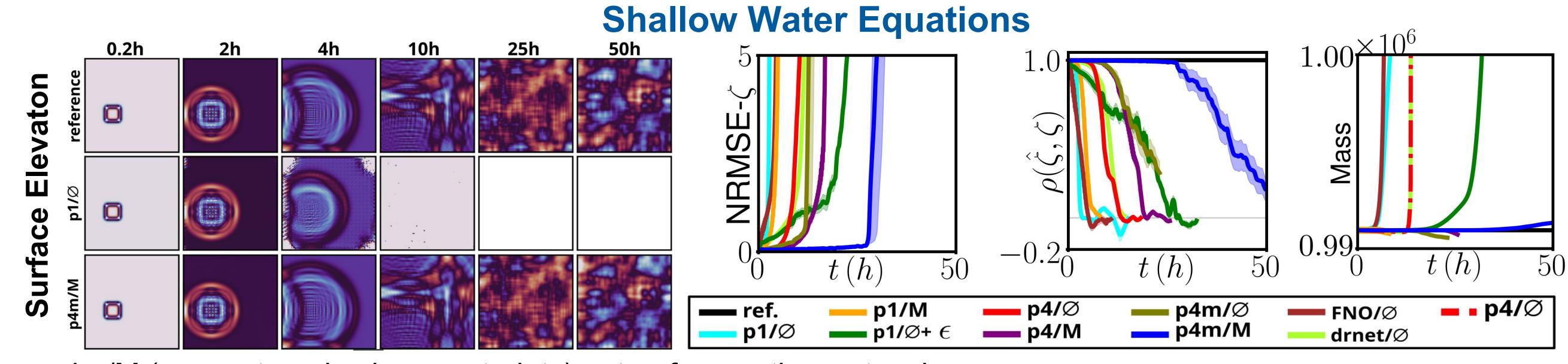
Shallow Water Equations (SWEs)

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

Incompressible Navier-Stokes (INS) & Decaying Turbulence

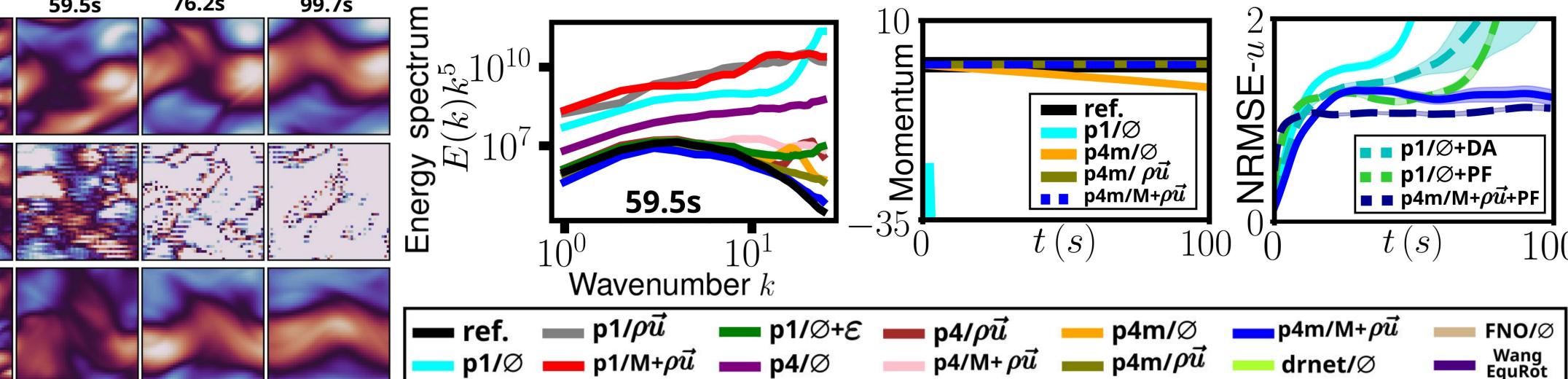
	Symmetries		
Conservation laws			
None Ø	p1/Ø	p4 /Ø	p4m/Ø
Momentum $\rho \vec{u}$	р1/ $ hoec{u}$	p4/ $ ho ec{u}$	p4m/ $ ho ec{u}$
Mass/momentum $\mathbf{M} + \rho \vec{u}$	p1/M+ $ hoec{u}$	p4/M+ $ ho ec{u}$	p4m/M+ $ ho ec{u}$

Double-Constrained Models Outperform Other Networks on SWEs & INS



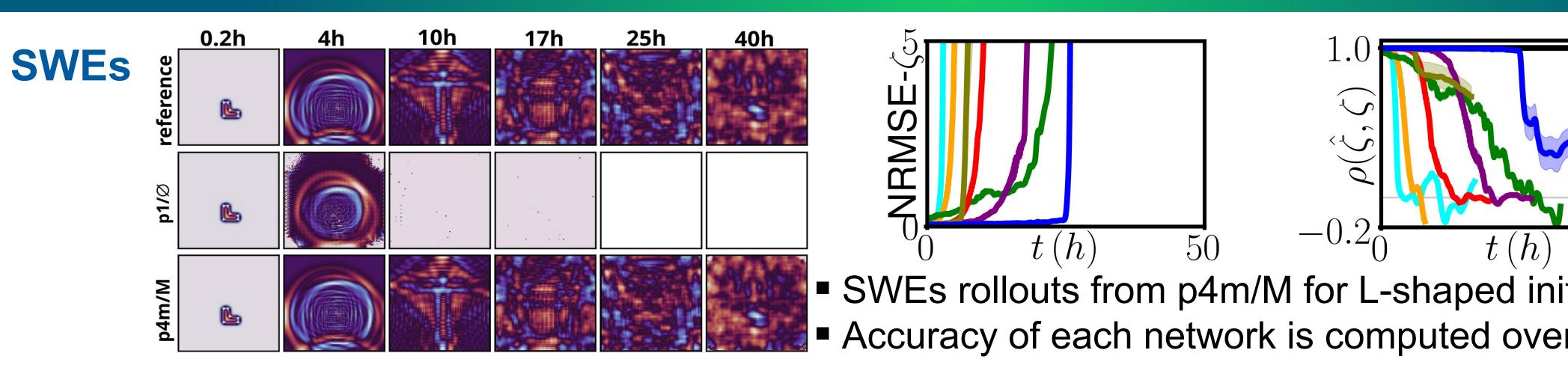
- p4m/M (symmetry+physics constraints) outperforms other networks.
- Normalized RMSE and correlation are shown for 50h rollouts, with standard error of the mean over 20 ICs.

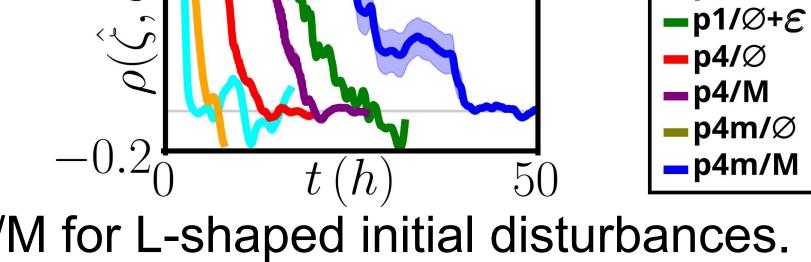
Decaying Turbulence



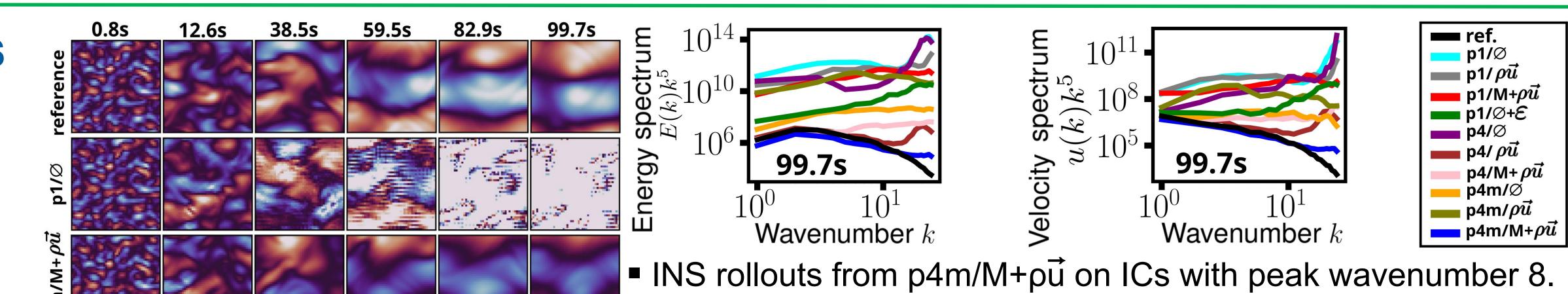
- p4m/M+ρū (symmetry+physics constraints) outperforms other networks with similar parameter counts on INS.
- Accuracy of energy spectrum and momentum with standard error of the mean over 30 ICs.

Generalization Beyond Training Data & Real Ocean Currents





- SWEs rollouts from p4m/M for L-shaped initial disturbances.
- Accuracy of each network is computed over 6 ICs.



Energy- and velocity spectrum at t=99.7s, averaged over 10 ICs.

Forecasts are shown over 300h (average over 30 ICs).

ocean ■ p4m/M+pu predicts ocean currents most accurately.

Conclusion

- We implemented the first physics+symmetry-constrained model on C-grids.
- Symmetries are more effective than physical constraints, but combining both is best.
- Our model improves generalisation to new ICs, and accurately predicts real ocean currents.