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Symmetry Constraints Enhance Long-term Stability and Accuracy in Unsupervised Learning of Geophysical Fluid Flows

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Outline

(1) Introduction

(2) Method: hybrid PDE solver using group equivariant neural networks

(3) Applications for 1D shallow water equations

(4) Conclusion

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Fluid dynamical systems

Different types of PDEs

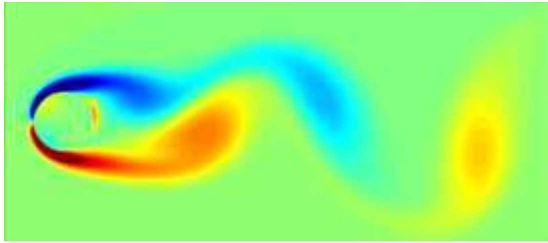
Euler equations

Cloud simulation

Harris et al. 2003

Navier–Stokes equations

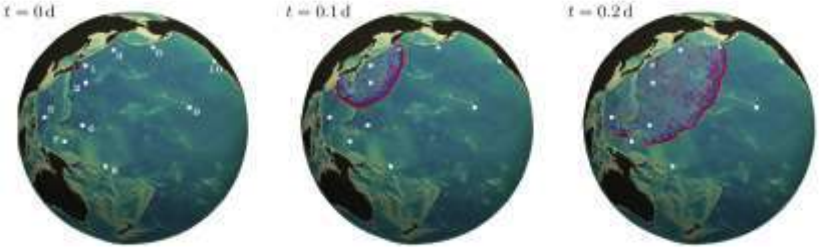
Fluid passes a cylinder



Huang. 2021

Shallow water equations

Tohoku tsunami event



Bonev et al. 2018

A general governing PDE

$$\frac{\partial q(t,x)}{\partial t} = \mathcal{F}[q] = f\left(t, x, q(t,x), \frac{dq}{dx}, \frac{d^2q}{dx^2}, \ldots\right) \quad x \in \Omega,$$

$$q(x,t) = q_\Omega(x), \quad x \in \partial\Omega,$$

$$q(x,0) = q_0(x)$$

where x and t are space and time coordinates and $q(t, x)$ is the vector of modeled variable fields at one place and time.

Solving the fluid PDE system

Traditional approaches

Finite difference method, finite element method, ...

Property: **Expensive computation cost** (e.g. small spatial and temporal resolutions and implicit scheme)

Machine learning (ML) approaches

Supervised learning, unsupervised learning

Property: **Efficient**

In this work

We construct hybrid PDE solvers using group equivariant neural networks.

This combines ML with numerical solvers.

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Unsupervised training of PDE solvers

Numerical approach

$$q_j^{n+1} = q_j^n + \Delta t \widetilde{\mathcal{F}}(q^n, q^{n+1})$$

An implicit method needs to be used for iteratively solving the system. For linear systems this is:

$$A(q^n)q^{n+1} = b(q^n)$$

ML method

$$\mathcal{L}_{\mathrm{PDE}} = \|A f_{\mathrm{CNN}}(q^n) - b^n\|_2^2$$

Here is a physical constraint for loss (unsupervised learning). We don't need simulation data for training.

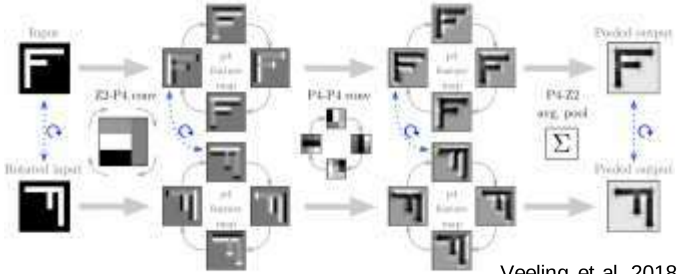
Physics-derived, unsupervised approach

ML for calculating q^{n+1}

Numerical solver for calculating A and b^n

Group equivariant convolutional networks

P4 equivariant convolutional networks



Veeling et al. 2018

$$f\,(g(.)) = g(\,f\,(.))$$

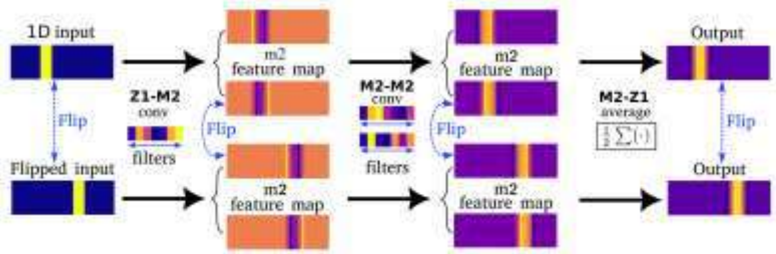
In the original paper, it has p4 and p4m. (T. Cohen & Welling, 2016)

The symmetry constraint networks show powerful capabilities for image classification and segmentation.

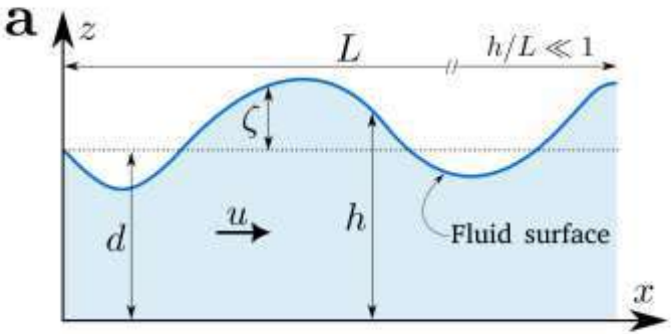
These networks for fluid dynamics remains mostly unclear.

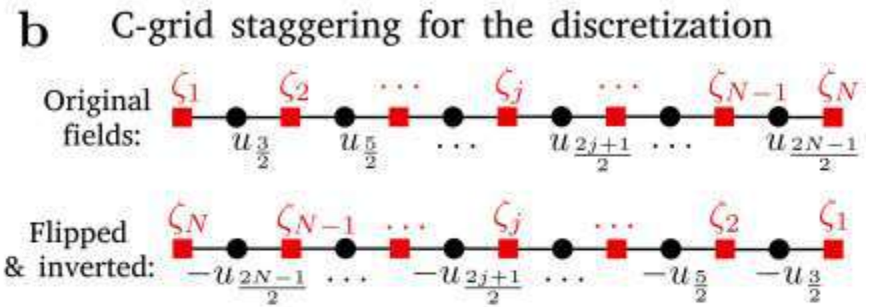
We hope this symmetry constraint can help to learn the complex fluid dynamical patten in long-term.

Group reflection-equivariant 1D convolutions neural networks (GR-CNN)



One-dimensional shallow water equations





The velocity: $$\frac{\partial u}{\partial t} = -C_D \frac{1}{h} u|u| - g \frac{\partial \zeta}{\partial x},$$

The surface elevation: $$\frac{\partial \zeta}{\partial t} = -\frac{\partial (hu)}{\partial x},$$

Random initial conditions for training and testing

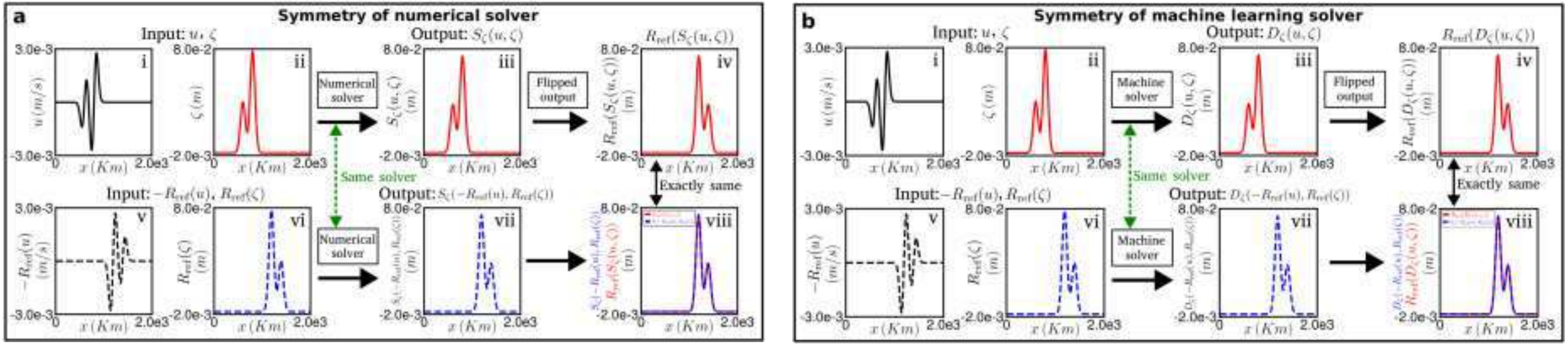
"Gaussian Bell"

$$u(x, 0) = 0,$$
$$\zeta(x, 0) = \frac{\beta}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/\sigma^2},$$

Boundary conditions

$$u(x = 0) = u(x = L) = 0,$$
$$\zeta(x = 0) = \zeta(x = L) = 0.$$

Group equivariance for mixed scalar-vector inputs



$$R_{\text{ref}}(S(\zeta^n, u^n)) = S(R_{\text{ref}}(\zeta^n), -R_{\text{ref}}(u^n))$$

$$R_{\text{ref}}(D_\zeta(u,\zeta)) = D_\zeta(-R_{\text{ref}}(u), R_{\text{ref}}(\zeta))$$

$$y^1_{j,0,\cdot} = \sum_{i=0}^{c_0-1} \left(W_{j,i,\cdot} \star x_{i,\cdot}\right) + b_j,$$

$$y^1_{j,1,\cdot} = \sum_{i=0}^{c_0-1} \left(R_{\text{ref}}(W_{j,i,\cdot}) \star x_{i,\cdot}\right) + b_j,$$

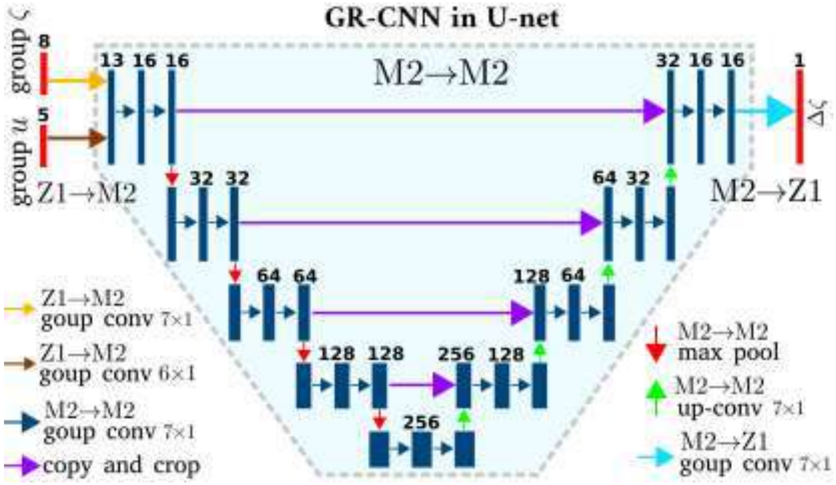
Change GR-CNN

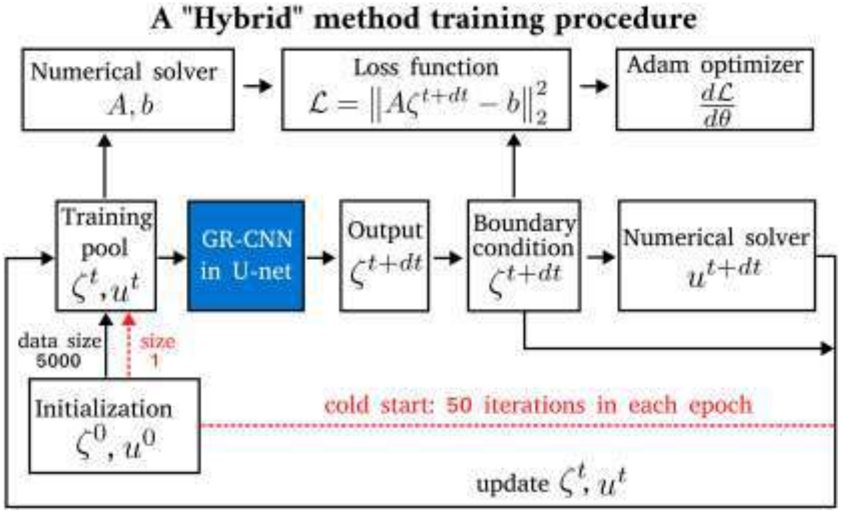
$$y^1_{j,0,\cdot} = \sum_{i=0}^{c^\zeta_{in}-1} \left(W^\zeta_{j,i,\cdot} \star \zeta_{i,\cdot}\right) + \sum_{i=0}^{c^u_{in}-1} \left(W^u_{j,i,\cdot} \star u_{i,\cdot}\right) + b_j,$$

$$y^1_{j,1,\cdot} = \sum_{i=0}^{c^\zeta_{in}-1} \left(R_{\text{ref}}(W^\zeta_{j,i,\cdot}) \star \zeta_{i,\cdot}\right) + \sum_{i=0}^{c^u_{in}-1} \left(-R_{\text{ref}}(W^u_{j,i,\cdot}) \star u_{i,\cdot}\right) + b_j.$$

Hybrid methods

Hybrid PDE solvers using group equivariant neural networks





Wandel et al., 2020

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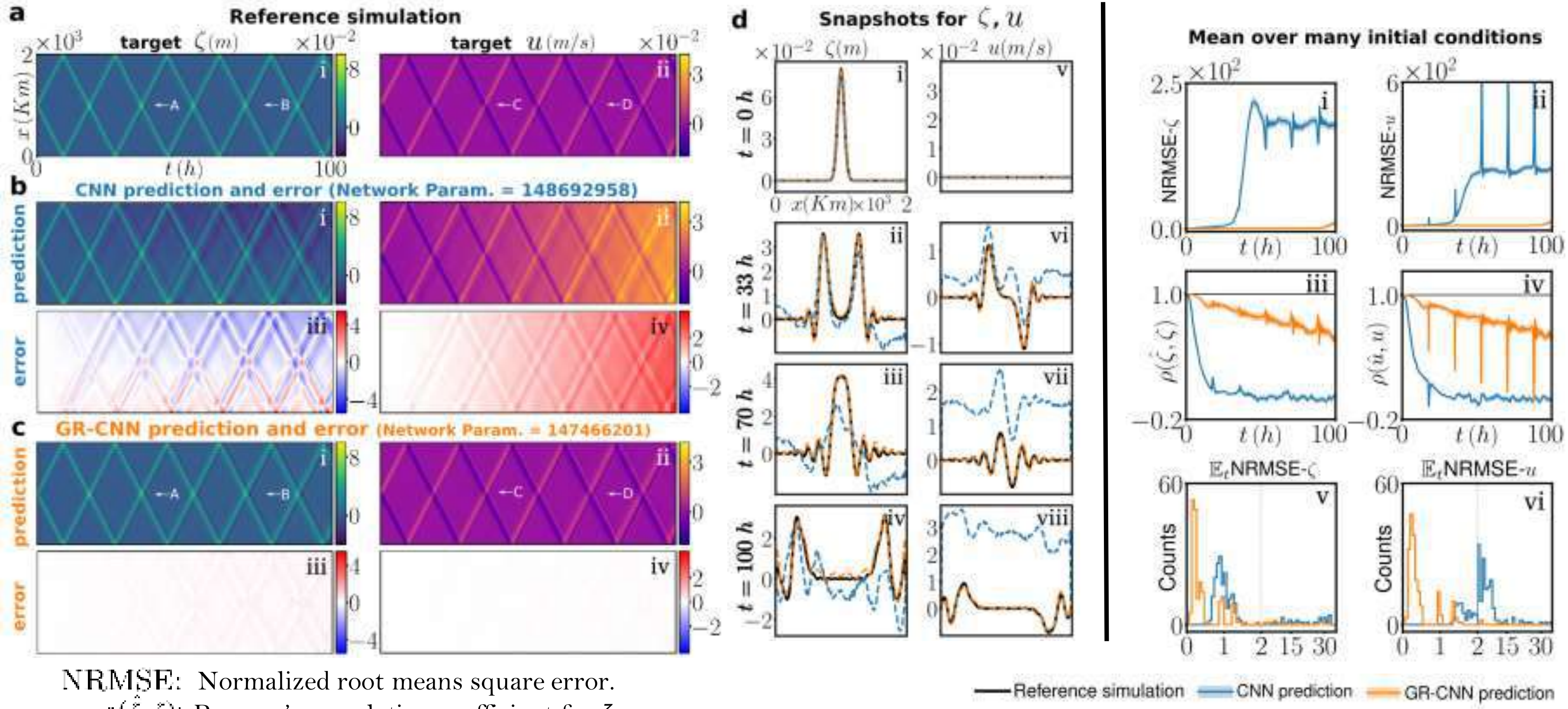
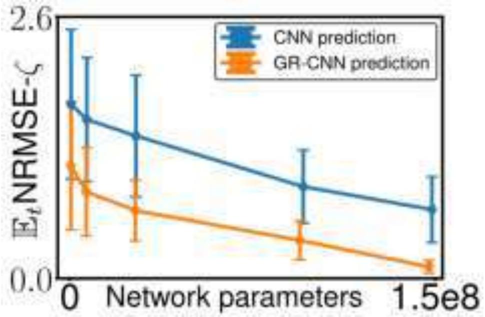
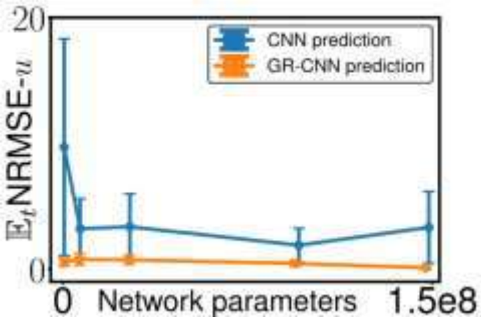
GR-CNN accurately solves the SWE



NRMSE: Normalized root means square error.
$\rho(\hat{\zeta}, \zeta)$: Pearson's correlation coefficient for ζ.
$\mathbb{E}_t$NRMSE: Time-averaged normalized root mean square error.

Different network size





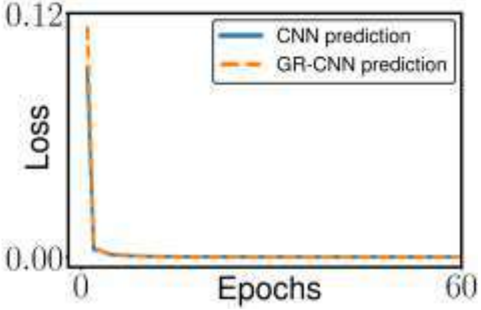
GR-CNN achieves accurate solution in different network size.

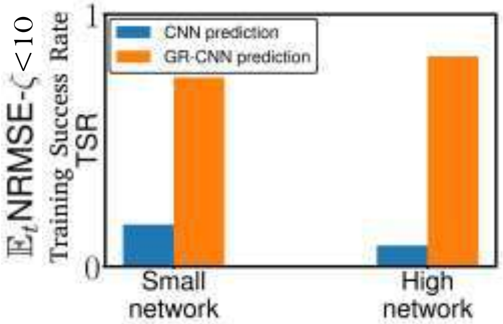
Loss values for both GR-CNN and CNN are similar during the training.

Reason: unsupervised learning trains on single time steps

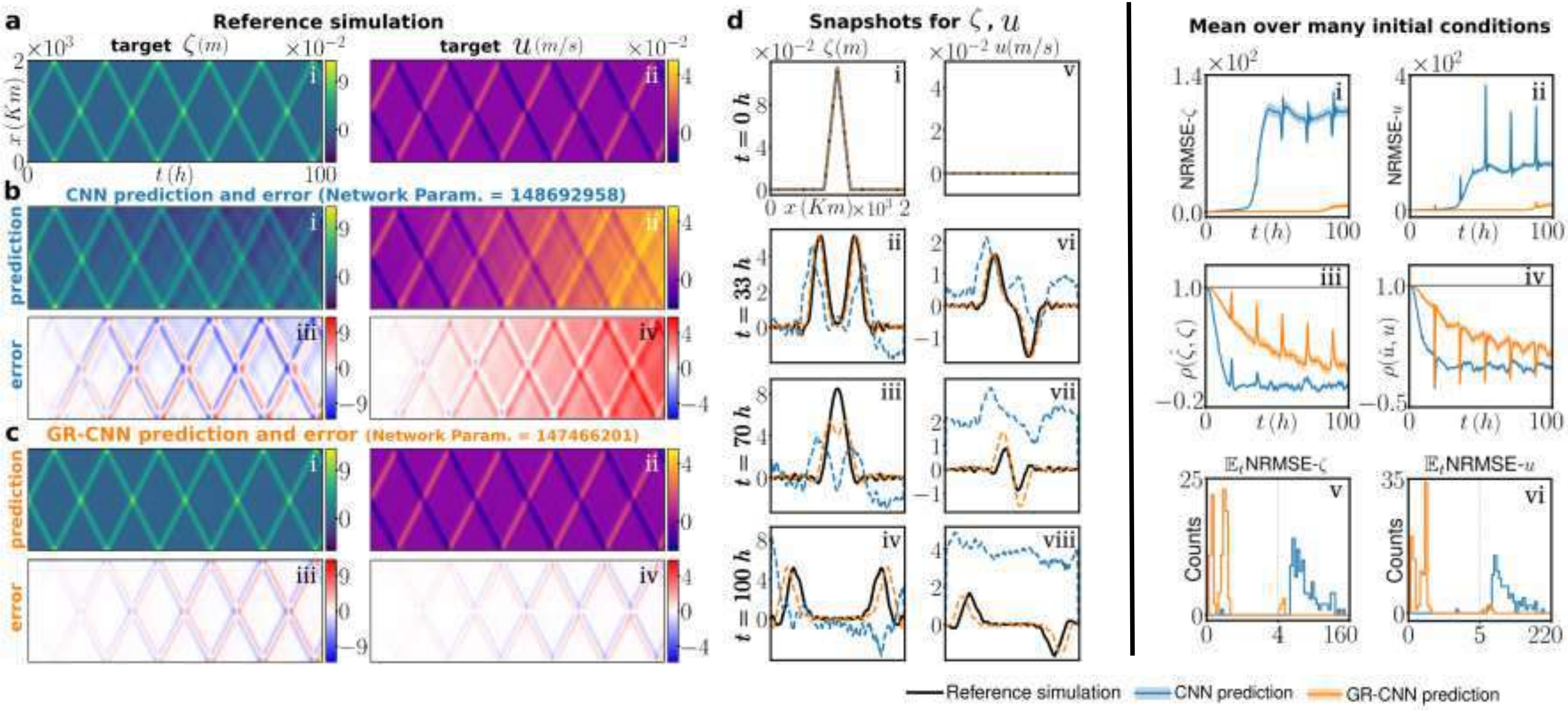
Similar loss value, but GR-CNN can improve the prediction.

GR-CNN solver is more likely to converge to the right answer

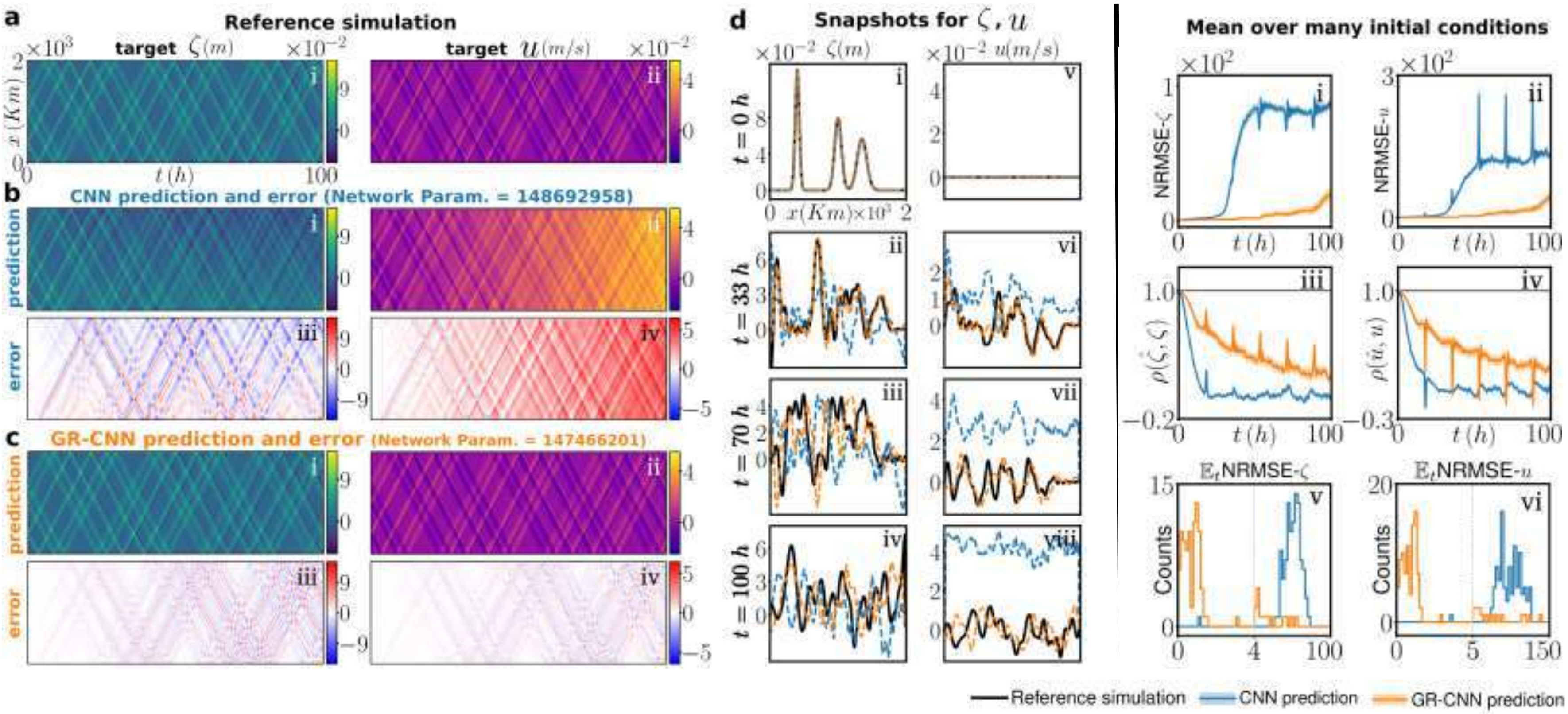




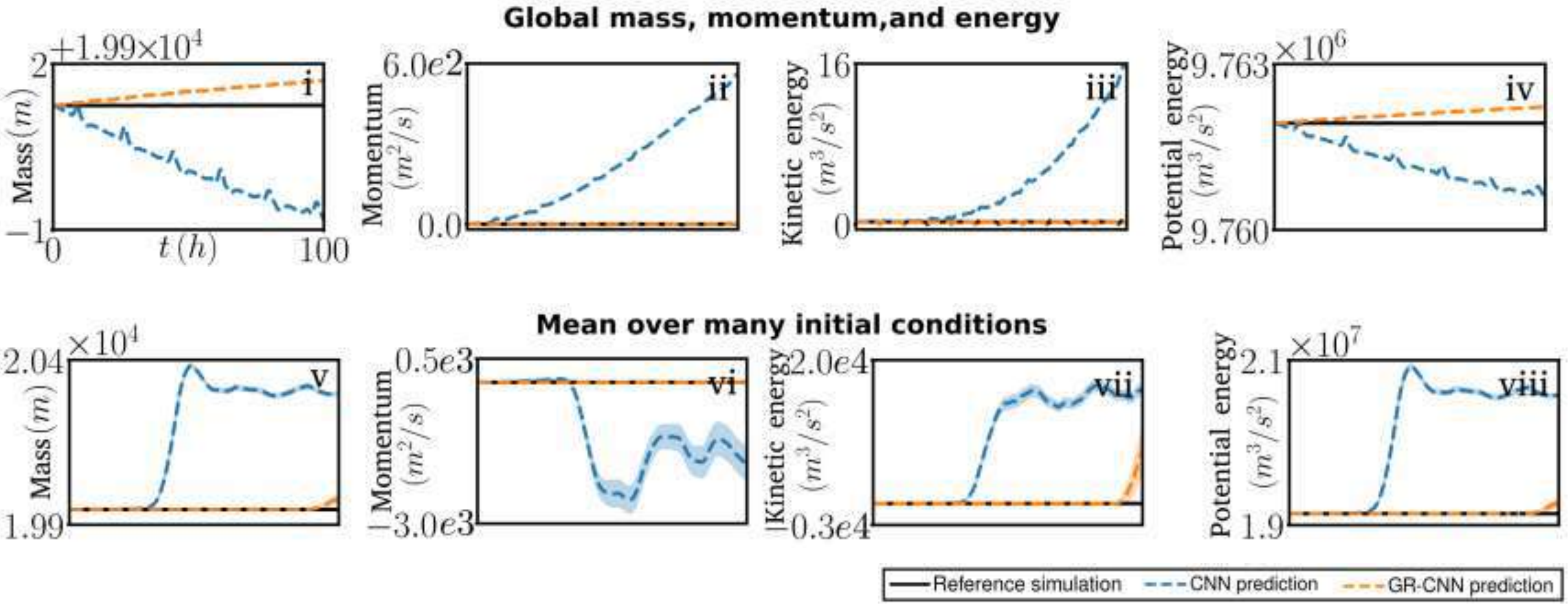
Generalization Capabilities after Training: a triangular initial condition



Generalization Capabilities after Training: multi-Gaussian initial condition



Global mass, momentum, and energy



GR-CNN solver has high accurate global mass, momentum, and energy distributions.

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Conclusion

We construct equivariant convolutional networks with mixed scalar-vector inputs for solving PDEs.

Equivariant networks strongly improve the long-term accuracy and stability in unsupervised learning tasks.

Equivariant networks improve generalization to new initial conditions, and suppress error accumulation in global momentum and energy.

Thank you for your attention