# TAEN:
# A Model-Constrained Tikhonov Autoencoder Network for Forward and Inverse Problems

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Probabilistic and High Order Inference, Computation, Estimation, and Simulation (PHO-ICES)

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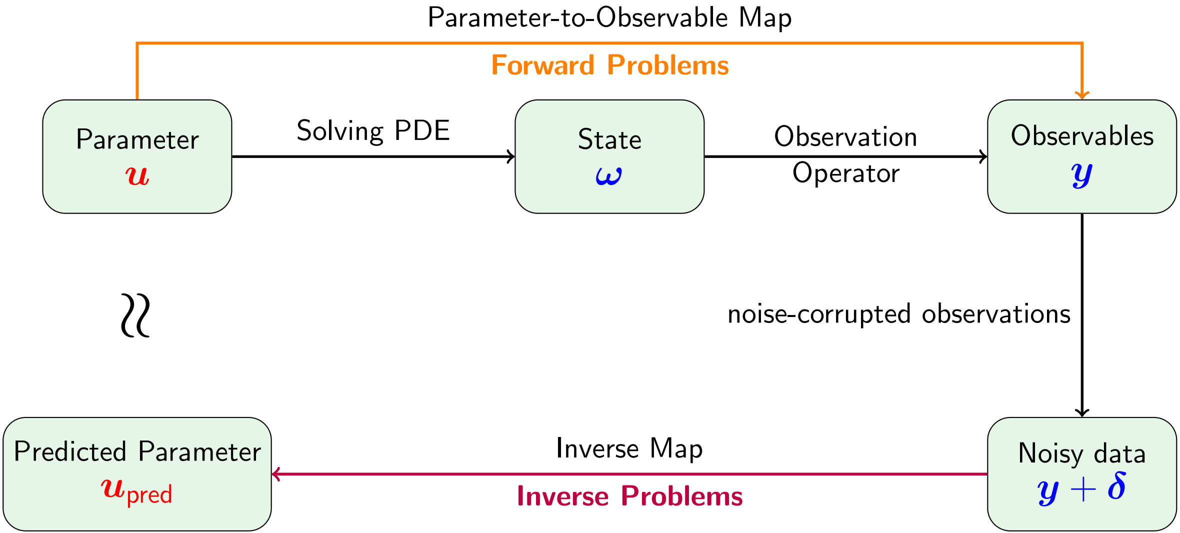
# Forward and inverse problems



# Motivation

# Overview: surrogate models for inverse and forward problems

# Problem settings

We consider

- The linear forward problem

$$\boldsymbol{y} = B \circ \underbrace{G\boldsymbol{u}}_{\omega} + \delta,$$

  where $B$ is observational operator, $G$ is linear forward map, and $\delta$ is white noise.

- The equivalent linear inverse problem

$$\boldsymbol{u} = (B \circ G)^{\dagger}\, \boldsymbol{y} = \mathrm{G}^{B\dagger} \boldsymbol{y}.$$

We want to learn linear autoencoder surrogate models

- Encoder $\Psi_{\mathrm{e}}(\boldsymbol{y}) = W_e \boldsymbol{y} + \mathbf{b}_e$ for inverse map $\mathrm{G}^{B\dagger}$.
- Decoder $\Psi_{\mathrm{d}}(\boldsymbol{u}) = W_d \boldsymbol{u} + \mathbf{b}_d$ for forward map $G$ or PtO map $G^B$.

# Autoencoder (AE) approaches

**We discuss**

1. Naive Autoencoder (`nAE`)
2. Model-constrained Autoencoder (`mcAE`)
3. Tikhonov Autoencoder Network Approach (`TAEN`)

# Naive Autoencoder (nAE) - error estimation

Given a dataset of pairs $\{U, Y\}$, we can learn forward and inverse surrogate models by

first optimizing the encoder $\Psi_{\mathrm{e}}^{*} = \min_{\Psi_{\mathrm{e}}} \frac{1}{2} \left\| \Psi_{\mathrm{e}}\left(Y\right) - U \right\|_F^2,$

then decoder with pre-trained encoder $\Psi_{\mathrm{d}}^{*} = \min_{\Psi_{\mathrm{d}}} \frac{1}{2} \left\| \Psi_{\mathrm{d}}\left(\Psi_{\mathrm{e}}^{*}\left(Y\right)\right) - Y \right\|_F^2.$

Applying 1st optimality condition for the optimal solutions $\Psi_{\mathrm{e}}^{*}$ and $\Psi_{\mathrm{d}}^{*}$, we have

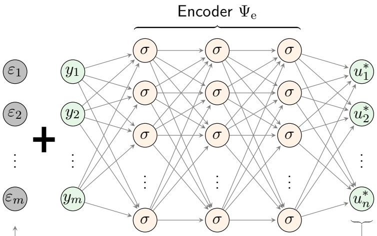
- test inverse solution error

$$\boldsymbol{\varepsilon}_{\boldsymbol{u}^{\text{test}}}^{\texttt{nAE}} = \left\| \Psi_{\mathrm{e}}^{*}(\boldsymbol{y}^{\text{test}}) - \boldsymbol{u}^{\text{test}} \right\|_2^2 = \left\| \left( \bar{U}\bar{Y}^{\dagger}\mathrm{G}^{B} - \mathbf{I} \right) \left( \boldsymbol{u}^{\text{test}} - \bar{\boldsymbol{u}} \right) \right\|_2^2.$$

- test forward solution error, with $Z = \Psi_{\mathrm{e}}^{*}(Y)$ is the encoder inverse solution,

$$\boldsymbol{\varepsilon}_{\boldsymbol{y}^{\text{test}}}^{\texttt{nAE}} = \left\| \Psi_{\mathrm{d}}^{*}(\boldsymbol{u}^{\text{test}}) - \boldsymbol{y}^{\text{test}} \right\|_2^2 = \left\| \bar{Y} \left( \bar{Z}^{\dagger} - \bar{U}^{\dagger} \right) \left( \boldsymbol{u}^{\text{test}} - \bar{\boldsymbol{u}} \right) \right\|_2^2 > 0,$$

# Model-constrained Autoencoder (mcAE) - embedding physics model

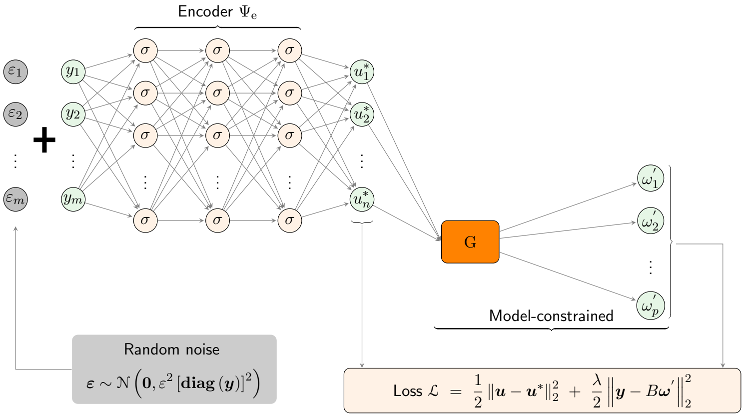



Random noise

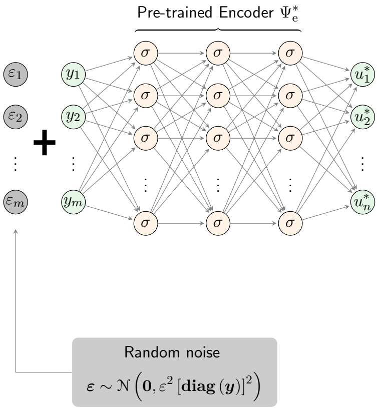
$$\boldsymbol{\varepsilon} \sim \mathcal{N}\left(\mathbf{0}, \varepsilon^2 \left[\mathbf{diag}\left(\boldsymbol{y}\right)\right]^2\right)$$

Loss $\mathcal{L} = \frac{1}{2}\left\|\boldsymbol{u} - \boldsymbol{u}^*\right\|_2^2 + \frac{\lambda}{2}\left\|\boldsymbol{y} - B\boldsymbol{\omega}'\right\|_2^2$

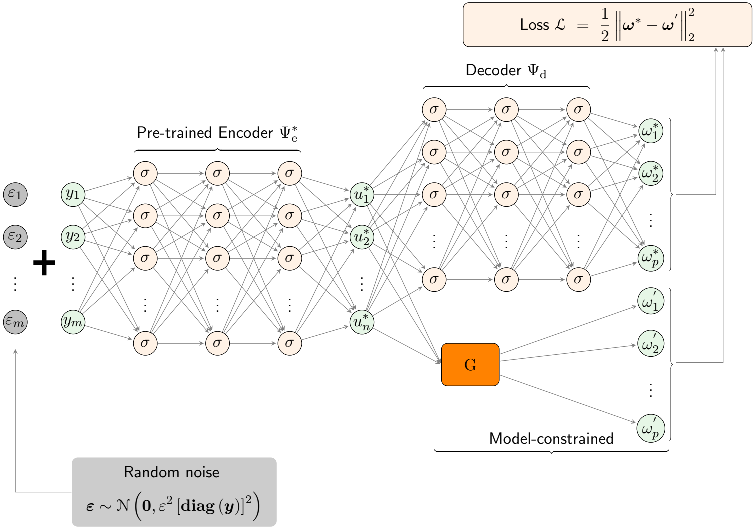
# Model-constrained Autoencoder (mcAE) - embedding physics model



# Model-constrained Autoencoder (`mcAE`) - embedding physics model



# Model-constrained Autoencoder (mcAE) - embedding physics model



# Model-constrained Autoencoder (mcAE) - error estimation

mcAE loss functions

$$\Psi_{\mathrm{e}}^{*} = \min_{\Psi_{\mathrm{e}}} \frac{1}{2} \left\| U - \Psi_{\mathrm{e}}\left(Y\right) \right\|_{F}^{2} + \frac{\lambda}{2} \left\| Y - \mathrm{G}^{B}\left(\Psi_{\mathrm{e}}\left(Y\right)\right) \right\|_{F}^{2},$$

$$\Psi_{\mathrm{d}}^{*} = \min_{\Psi_{\mathrm{d}}} \frac{1}{2} \left\| \mathrm{G}\left(\Psi_{\mathrm{e}}^{*}\left(Y\right)\right) - \Psi_{\mathrm{d}}\left(\Psi_{\mathrm{e}}^{*}\left(Y\right)\right) \right\|_{F}^{2}.$$

Applying 1st optimality condition, and **if $\bar{Y}$ is a full row rank**, we have

- test inverse solution error

$$\varepsilon_{\boldsymbol{u}^{\text{test}}}^{\mathtt{mcAE}} = \left\| \left(\mathbf{I} + \lambda {\mathrm{G}^{B}}^{T} \mathrm{G}^{B}\right)^{-1} \left(\left(\bar{U}\bar{Y}^{\dagger}\mathrm{G}^{B} - \mathbf{I}\right)\left(\boldsymbol{u}^{\text{test}} - \bar{\boldsymbol{u}}\right)\right) \right\|_{2}^{2}$$

which is smaller than

$$\varepsilon_{\boldsymbol{u}^{\text{test}}}^{\mathtt{nAE}} = \left\| \left(\bar{U}\bar{Y}^{\dagger}\mathrm{G}^{B} - \mathbf{I}\right)\left(\boldsymbol{u}^{\text{test}} - \bar{\boldsymbol{u}}\right) \right\|_{2}^{2}.$$

- test forward solution error

$$\varepsilon_{\boldsymbol{\omega}^{\text{test}}}^{\mathtt{mcAE}} = 0.$$

# Key issue of `mcAE`: Error estimation is data-dependent

Recall the test inverse solution error

$$\varepsilon^{\texttt{mcAE}}_{\boldsymbol{u}^{\text{test}}} = \left\| \left(\mathbf{I} + \lambda \mathrm{G}^{B^T} \mathrm{G}^B\right)^{-1} \left( \left( \bar{U} \bar{Y}^\dagger \mathrm{G}^B - \mathbf{I} \right) \left( \boldsymbol{u}^{\text{test}} - \bar{\boldsymbol{u}} \right) \right) \right\|_2^2$$

where

- $\bar{U}, \bar{Y}$ is centralized training data.
- $\bar{\boldsymbol{u}}$ is the average of training PoI samples.

If training data $U, Y$ is limited, surrogate models heavily bias on given training data. Hence, leading to high test inverse error.

Our TAEN approach is introduced to deal with this issue

# TAEN: Tikhonov Autoencoder Network Approach

Recall the `mcAE` loss functions

$$\Psi_{\mathrm{e}}^* = \min_{\Psi_{\mathrm{e}}} \frac{1}{2} \left\| U - \Psi_{\mathrm{e}}\left(Y\right) \right\|_F^2 + \frac{\lambda}{2} \left\| Y - \mathrm{G}^B\left(\Psi_{\mathrm{e}}\left(Y\right)\right) \right\|_F^2,$$

$$\Psi_{\mathrm{d}}^* = \min_{\Psi_{\mathrm{d}}} \frac{1}{2} \left\| \mathrm{G}\left(\Psi_{\mathrm{e}}^*\left(Y\right)\right) - \Psi_{\mathrm{d}}\left(\Psi_{\mathrm{e}}^*\left(Y\right)\right) \right\|_F^2.$$

In TAEN, we use the prior mean of PoI, $\boldsymbol{u}_0$, thus true PoI samples are no longer required.

$$\Psi_{\mathrm{e}}^* = \min_{\Psi_{\mathrm{e}}} \frac{1}{2} \left\| \boldsymbol{u}_0 \mathbb{1}^T - \Psi_{\mathrm{e}}\left(Y\right) \right\|_F^2 + \frac{\lambda}{2} \left\| Y - B \circ \mathrm{G}\left(\Psi_{\mathrm{e}}\left(Y\right)\right) \right\|_F^2,$$

$$\Psi_{\mathrm{d}}^* = \min_{\Psi_{\mathrm{d}}} \frac{1}{2} \left\| \mathrm{G}\left(\Psi_{\mathrm{e}}^*\left(Y\right)\right) - \Psi_{\mathrm{d}}\left(\Psi_{\mathrm{e}}^*\left(Y\right)\right) \right\|_F^2.$$

Applying 1st optimality condition, and **if $\bar{Y}$ is a full row rank**, we have

- test inverse solution error

$$\varepsilon_{\boldsymbol{u}^{\text{test}}}^{\texttt{mcAE}} \leq \left\| \boldsymbol{u}^{\text{test}} - \boldsymbol{u}_0 \right\|_2^2$$

- test forward solution error

$$\varepsilon_{\boldsymbol{\omega}^{\text{test}}}^{\texttt{mcAE}} = 0,$$

# Obtaining a full row rank $\bar{Y}$ from 1 observation sample $\boldsymbol{y}$

# Summary of error estimation

## Error estimation on test samples

| Approaches | forward error $\varepsilon_{\boldsymbol{y}^{\text{test}}} / \varepsilon_{\boldsymbol{\omega}^{\text{test}}}$ | Inverse error $\varepsilon_{\boldsymbol{u}^{\text{test}}}$ | Ability to learn with 1 sample $\boldsymbol{y}$ |
|---|---|---|---|
| `nAE` | inevitably $> 0$ | $\left\Vert \left(\bar{U}\bar{Y}^{\dagger}\mathrm{G}^{B} - \mathbf{I}\right)\left(\boldsymbol{u}^{\text{test}} - \bar{\boldsymbol{u}}\right)\right\Vert_2^2$ | none |
| `mcAE` | 0 | $\leq \left\Vert \left(\bar{U}\bar{Y}^{\dagger}\mathrm{G}^{B} - \mathbf{I}\right)\left(\boldsymbol{u}^{\text{test}} - \bar{\boldsymbol{u}}\right)\right\Vert_2^2$ | only forward |
| `TAEN` | 0 | $\leq \left\Vert \boldsymbol{u}^{\text{test}} - \boldsymbol{u}_0\right\Vert_2^2$ | forward and inverse |

- Please see our preprint for discussions for non-linear problems.

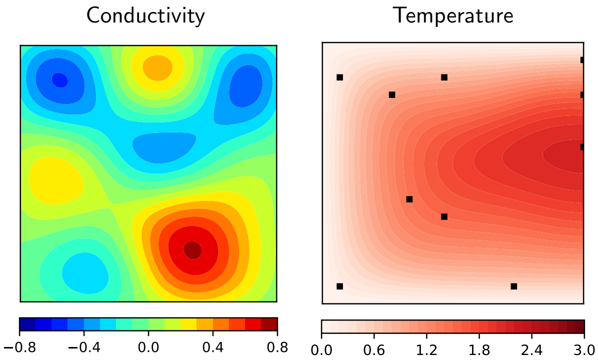
# Numerical results

## Results

- 2D Heat equation
- 2D Navier Stokes equation
- Computational cost and speedup

# 2D Heat equation

$$
\begin{aligned}
-\nabla \cdot (e^u \nabla \omega) &= 20 \quad \text{in } \Omega = (0,1)^2 \\
\omega &= 0 \quad \text{on } \Gamma^{\text{ext}} \\
\mathbf{n} \cdot (e^u \nabla \omega) &= 0 \quad \text{on } \Gamma^{\text{root}},
\end{aligned}
$$




Forward problem: Given the heat conductivity field, we aim to predict the temperature field.
Inverse problem: Given 10 observations, we aim to reconstruct the heat conductivity field.

# 2D Heat equation: relative error

## Relative error over 500 test samples ($\varepsilon = 0.1$)

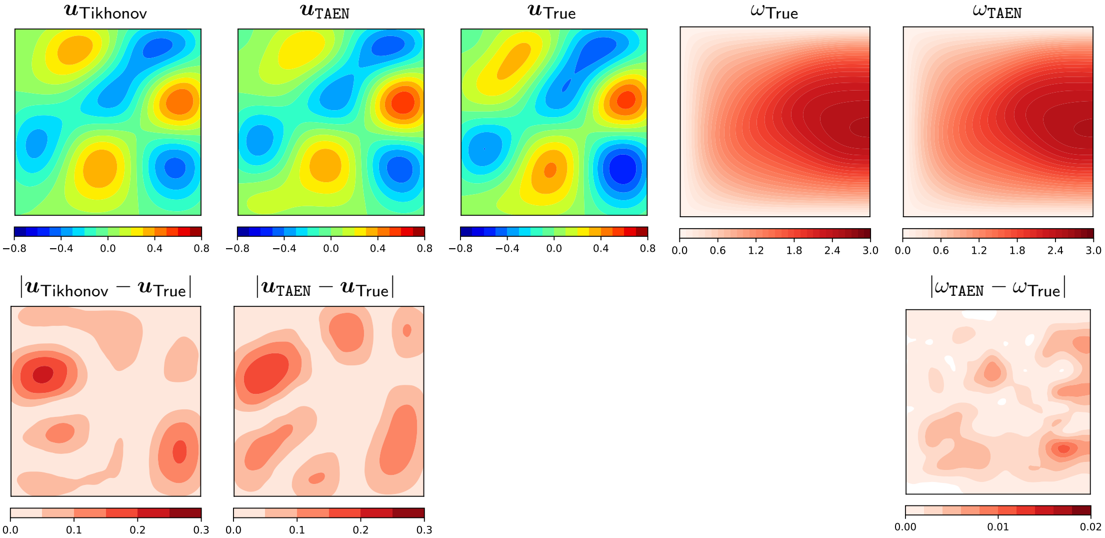
| Approach | 1 training sample | | 100 training samples | |
|---|---|---|---|---|
| | Inverse (%) | Forward | Inverse (%) | Forward |
| `nAE` | 107.55 | $2.90\times10^{-1}$ | 50.18 | $1.09\times10^{-1}$ |
| `mcAE` | 108.28 | $4.21\times10^{-2}$ | 46.32 | $4.56\times10^{-4}$ |
| `TAEN` | 45.23 | $1.57\times10^{-4}$ | 45.03 | $1.22\times10^{-4}$ |
| Tikhonov | 44.99 | | 44.99 | |

## Arbitrarily chosen samples for 1 training sample case

The statistic of inverse solution error over 10 cases

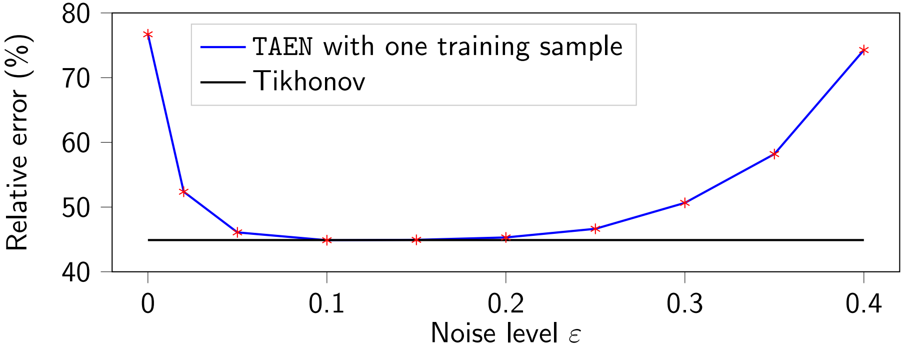
$$45.32 \pm 0.32\%$$

# 2D Heat equation: a test sample prediction



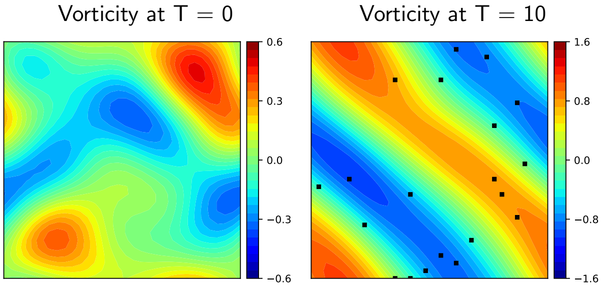
# 2D Heat equation: how much randomization noise?

Relative error of inverse solution over 500 test samples with different noise levels.



# 2D Navier–Stokes equation

$$
\begin{aligned}
\partial_t \omega(x,t) + v(x,t)\cdot\nabla\omega(x,t) &= \nu\Delta\omega(x,t) + f(x), && x\in(0,1)^2, t\in(0,T],\\
\nabla\cdot v(x,t) &= 0, && x\in(0,1)^2, t\in(0,T],\\
\omega(x,0) &= u(x), && x\in(0,1)^2,
\end{aligned}
$$




Forward problem: Given initial vorticity, we aim to predict the final vorticity.

Inverse problem: Given 20 observations at T = 10, we aim to reconstruct the initial vorticity.

# 2D Navier–Stokes equation: relative error

## Relative error over 500 test samples ($\varepsilon = 0.25$)

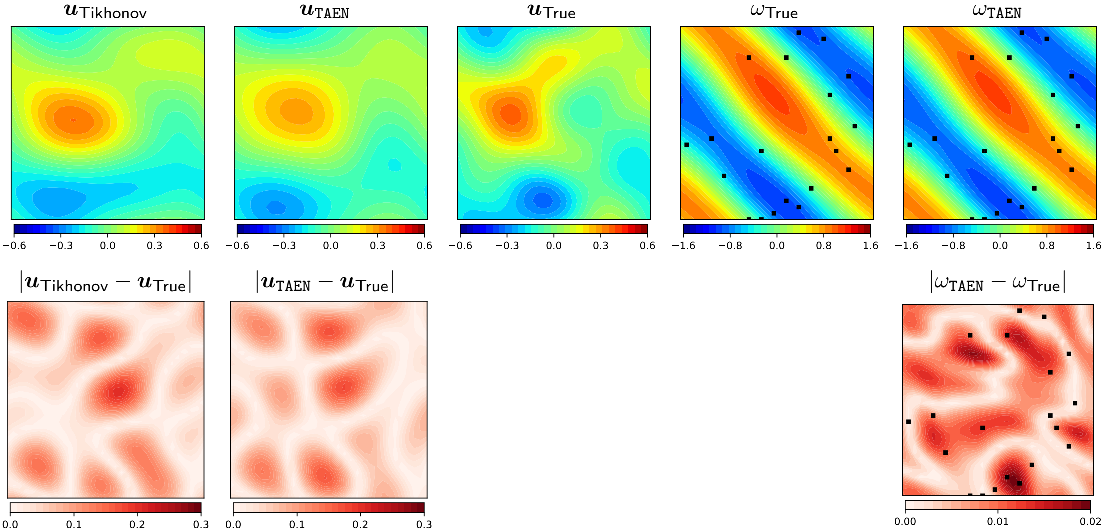
| | 1 training sample | | 100 training samples | |
|---|---|---|---|---|
| **Approach** | **Inverse (%)** | **Forward** | **Inverse (%)** | **Forward** |
| nAE | 103.94 | 5.60 | 40.20 | $5.94 \times 10^{-1}$ |
| mcAE | 46.43 | $5.15 \times 10^{-1}$ | 27.29 | $2.20 \times 10^{-3}$ |
| TAEN | 25.68 | $2.14 \times 10^{-3}$ | 24.54 | $1.49 \times 10^{-3}$ |
| Tikhonov | 22.71 | | 22.71 | |

## Arbitrarily chosen samples for 1 training sample case

The statistic of inverse solution error over 12 cases

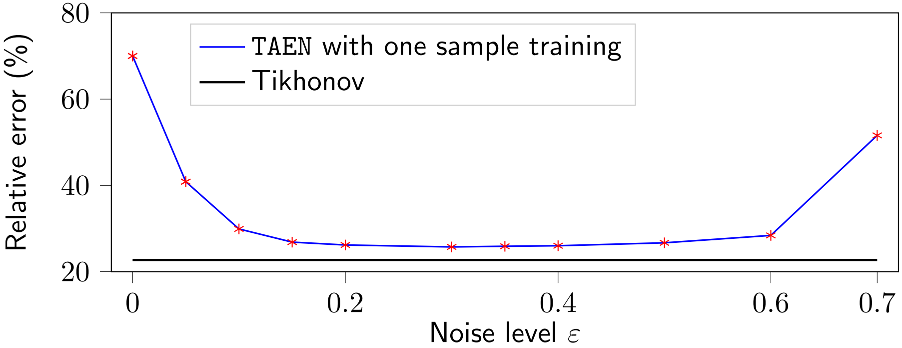
$$25.88 \pm 0.19\%$$

# 2D Navier–Stokes equation: a test sample prediction



# 2D Navier–Stokes equation: how much randomization noise?

Relative error of inverse solution over 500 test samples with different noise levels.



# Train/test computational cost & speed up for TAEN

Train/Test computation cost & Speed up for TAEN
Implemented on NVIDIA A100 GPUs (TACC)

| | | **Heat equation** | **Navier–Stokes** |
|---|---|---|---|
| Training Encoder + Training Decoder (hours) | | 2 | 16 |
| Test/Inference (second) | Inverse (Encoder) | $2.74 \times 10^{-4}$ | $2.93 \times 10^{-4}$ |
| | Forward (Decoder) | $2.86 \times 10^{-4}$ | $3.06 \times 10^{-4}$ |
| Numerical solvers (second) | Inverse (Tikhonov) | $4.36 \times 10^{-2}$ | 7.26 |
| | Forward | $3.01 \times 10^{-2}$ | 0.38 |
| Speed up | Inverse | 159 | 24,785 |
| | Forward | 105 | 1,241 |

# Conclusion

## TAEN (under review)

- is able to learn forward and inverse maps with only 1 observation sample
- is robust to a wide range of data randomization noise level
- is robust to an arbitrarily chosen observation sample
- provides real-time solvers

Drawbacks:

- has expensive training cost due to differentiable PDE solvers
- is not helpful for rich data scenarios

## Future work

- Relax the requirement for differentiable solvers
- Extend to large-scale problems
- ...