# Sensitivity-Constrained Fourier Neural Operators for Forward and Inverse Problems in Parametric Differential Equations

Abdolmehdi Behroozi, Chaopeng Shen and Daniel Kifer (Pennsylvania State University)

ICLR 2025

## Abstract

We introduce Sensitivity-Constrained Fourier Neural Operators (SC-FNO) to improve parameter inversion and sensitivity estimation in parametric differential equations (PDEs). Standard Fourier Neural Operators (FNOs) fail to capture parameter sensitivities, limiting accuracy and generalization. SC-FNO addresses this by enforcing sensitivity constraints, enhancing inversion quality, robustness, and data efficiency. **Our contributions** include introducing SC-FNO as a novel extension of FNOs, integrating sensitivity constraints for improved inversion, and demonstrating its effectiveness across benchmark problems. SC-FNO provides a scalable and robust framework for solving parametric PDEs.

## Materials & Methods

**Motivation** Accurately recovering parameters and their sensitivities is crucial for solving inverse problems in scientific computing, yet existing neural operators struggle with these tasks, leading to poor generalization and instability.

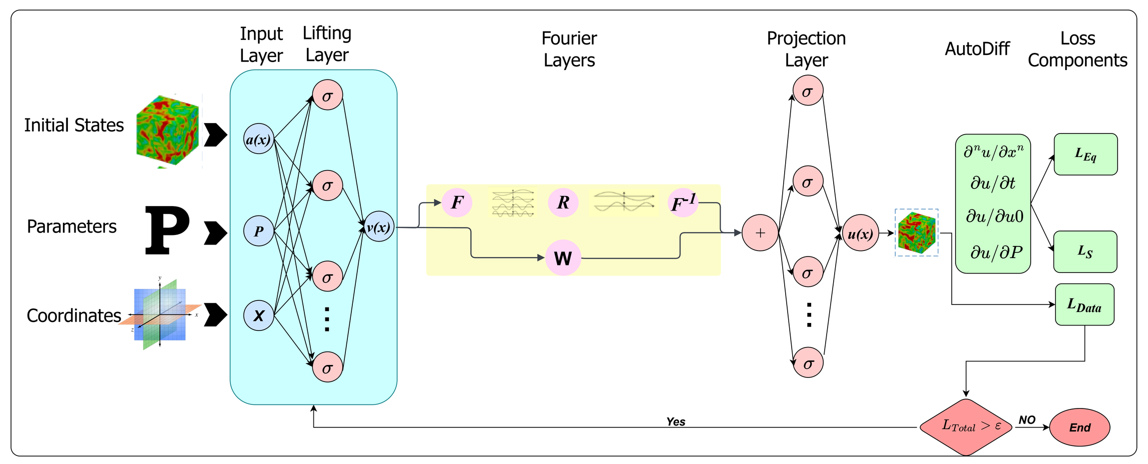
**Base Model:** Fourier Neural Operator (FNO)
**Objective:** Improve inversion, sensitivity, and robustness

**Loss Variants:**

- **FNO:** $L_u = \|\hat{u} - u\|^2$ (solution error)
- **FNO-PINN:** $L_u + L_{eq}$ (PDE residual)
- **SC-FNO:** $L_u + L_s$ (sensitivity loss)
- **SC-FNO-PINN:** $L_u + L_s + L_{eq}$

**Sensitivity Loss:** $L_s = \frac{1}{M}\sum_{j=1}^{M}\left\|\frac{\partial \hat{\mathbf{u}}}{\partial \mathbf{p}} - \frac{\partial u}{\partial \mathbf{p}}\right\|^2$

**Model Output:** $\mathbf{u} = \mathcal{F}(\mathbf{u}_0, x, t, \mathbf{p})$




*Schematic of SC-FNO architecture*

**Key Features:**

- Fourier-based neural operator architecture
- Sensitivity constraint enforces $\frac{\partial \hat{u}}{\partial \mathbf{p}}$
- Extends to other Neural Operators (WNO, MWNO, DeepONet)

## Test Problems

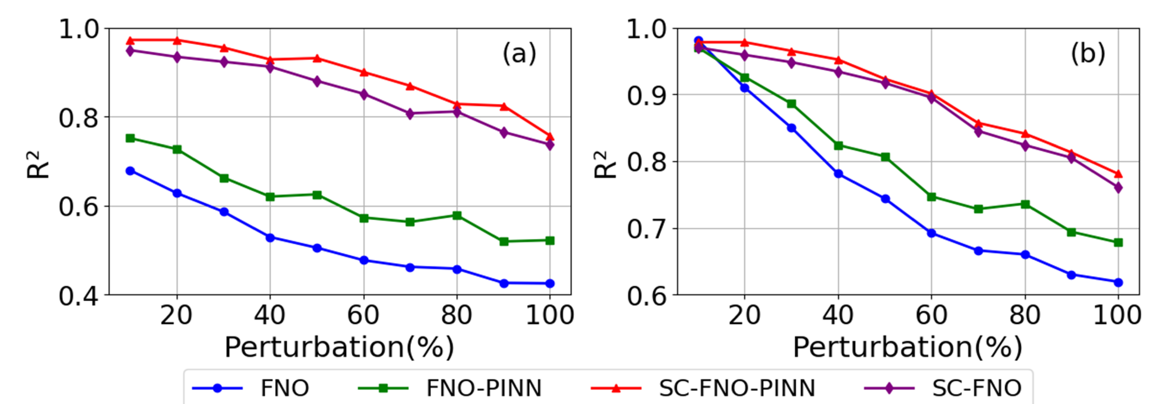
**ODEs:**
**ODE1: Composite Harmonic Oscillator** $du/dt = \alpha\sin(\alpha\pi t) + \beta\cos(\beta\pi t)$, $u(0) = \sin(\gamma\pi)$, Params: $\alpha, \beta, \gamma$
**ODE2: Duffing Oscillator** $d^2x/dt^2 + \delta dx/dt + \alpha x + \beta x^3 = \gamma\cos(\omega t)$, $x(0) = \epsilon$, $dx/dt(0) = \zeta$, Params: $\delta, \alpha, \beta, \gamma, \omega, \epsilon, \zeta$

**PDEs:**
**PDE1: Nonlinear Damped Wave** $\partial^2 u/\partial t^2 = c^2\partial^2 u/\partial x^2 + \alpha\partial u/\partial t + \beta u + \gamma\sin(\omega u)$, Params: $c, \alpha, \beta, \gamma, \omega$
**PDE2: Forced Burgers' Equation** $(1/\pi)\partial u/\partial t + \alpha u\partial u/\partial x = \gamma\partial^2 u/\partial x^2 + \delta\sin(\omega t)$, Params: $\alpha, \gamma, \delta, \omega, x_0, \sigma$
**PDE3: Navier-Stokes (Vorticity Form)** $\partial\omega/\partial t + \psi_y\partial\omega/\partial x - \psi_x\partial\omega/\partial y = (1/Re)\Delta\omega$, Params: $\alpha, \beta$
**PDE4: Allen-Cahn Equation** $\partial u/\partial t = \epsilon\partial^2 u/\partial x^2 + \alpha u - \beta u^3$, Params: $\epsilon, \alpha, \beta, c, \omega$

## Results 1: Generalization

### Performance Under Perturbed Parameter Ranges

- **SC-FNO maintains stability across perturbations, outperforming FNO and baseline models.**
- **Higher robustness demonstrated under extreme noise conditions, reducing sensitivity errors.**
- **Sensitivity constraints enable effective generalization, mitigating error amplification seen in FNO.**
- **Critical for real-world applications where parameter uncertainty is a challenge.**

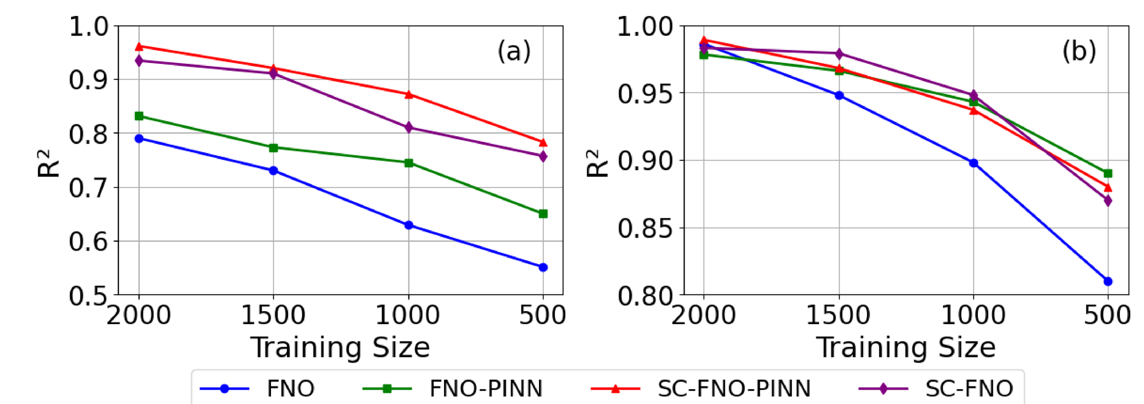



**Performance for PDE1 on perturbed data:**

**(a) Standardized $\frac{\partial \hat{\mathbf{u}}}{\partial \mathbf{p}}$, (b) $u(t)$.**

### Model Performance Across Training Data Volumes

- **SC-FNO achieves high accuracy with significantly fewer training samples compared to FNO.**
- **Gradient-informed learning enhances sample efficiency, reducing dependence on large datasets.**
- **Performance gap widens as training data decreases, emphasizing SC-FNO's advantage in data-limited scenarios.**
- **Demonstrates potential for application in cases where labeled data is scarce or expensive.**




**Performance of Models for PDE1 across training sizes:**

**(a) $\frac{\partial u}{\partial \omega}$, (b) $u(t)$.**

## Results 2: Sample Forward Prediction (With Perturbations)

- SC-FNO outperforms FNO in both standard and perturbed scenarios.
- SC constrained models demonstrate higher robustness to perturbations.
- SC-FNO achieves superior performance over PINN-loss models.
- Prediction accuracy remains stable despite parameter variations.
- Improvements in robustness lead to better generalization.

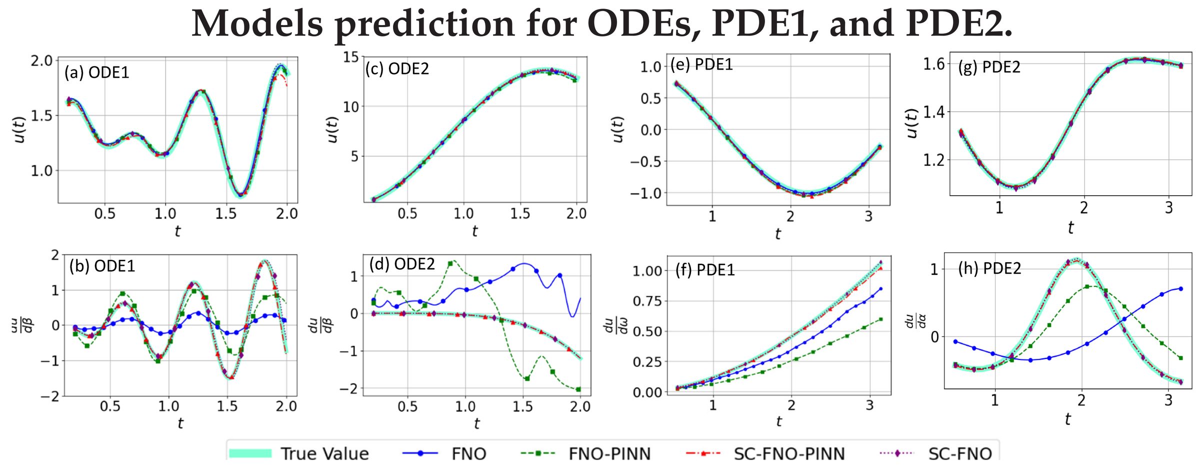
**Performance Comparison for Zoned PDE2**

| Metrics | N=500 | | N=100 | |
|---|---|---|---|---|
| | FNO | SC-FNO | FNO | SC-FNO |
| *State Value Metrics* | | | | |
| R² | 0.960 | 0.997 | 0.927 | 0.996 |
| Relative L² | 0.0282 | 0.0073 | 0.0387 | 0.0087 |
| *Mean Jacobian Metrics* | | | | |
| R² | -8.332 | 0.949 | -14.012 | 0.927 |
| Relative L² | 1.9627 | 0.1770 | 2.4623 | 0.2134 |

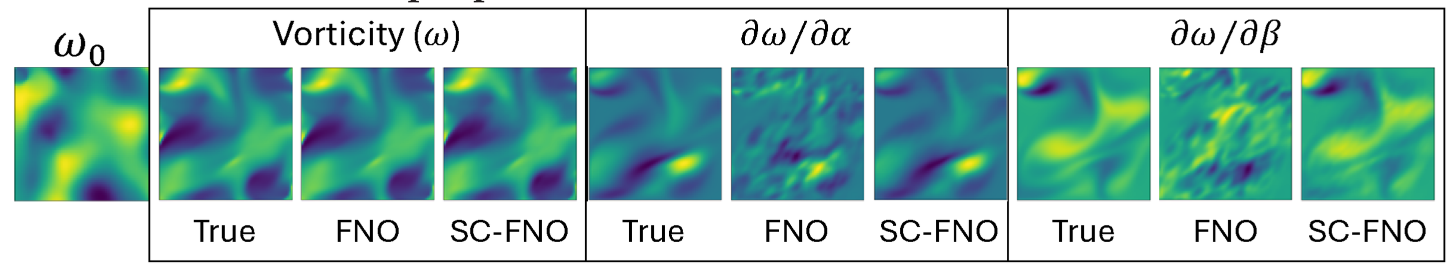
**Error for PDE2 with $2 \times 10^3$ training samples.**

| Value | Metric | Original range of parameters | | | | Perturbed range ($\lambda : 0.4$) | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | FNO | SC-FNO | SC-FNO-PINN | FNO-PINN | FNO | SC-FNO | SC-FNO-PINN | FNO-PINN |
| $u(t)$ | R² | **0.997** | **0.997** | 0.995 | 0.995 | 0.734 | 0.933 | 0.923 | 0.802 |
| | Relative L² | 0.0029 | **0.0016** | 0.0065 | 0.0073 | 0.0325 | 0.0112 | 0.0124 | 0.0287 |
| $\frac{\partial u}{\partial \alpha}$ | R² | 0.206 | **0.987** | 0.907 | 0.137 | 0.152 | 0.904 | 0.830 | 0.113 |
| | Relative L² | 0.2092 | **0.0135** | 0.0813 | 0.8545 | 1.1236 | 0.0755 | 0.0987 | 0.9865 |
| $\frac{\partial u}{\partial \gamma}$ | R² | 0.423 | **0.986** | 0.991 | 0.519 | 0.311 | 0.903 | 0.904 | 0.429 |
| | Relative L² | 0.8542 | **0.0540** | 0.0523 | 0.7566 | 0.9875 | 0.0767 | 0.0755 | 0.8244 |
| $\frac{\partial u}{\partial \delta}$ | R² | 0.821 | 0.912 | **0.957** | 0.871 | 0.604 | 0.835 | 0.876 | 0.719 |
| | Relative L² | 0.1245 | 0.0756 | **0.0567** | 0.1023 | 0.2544 | 0.1023 | 0.0888 | 0.1567 |
| $\frac{\partial u}{\partial \omega}$ | R² | 0.321 | **0.982** | 0.912 | 0.427 | 0.236 | 0.912 | 0.834 | 0.353 |
| | Relative L² | 0.8856 | **0.0567** | 0.0789 | 0.7899 | 1.0244 | 0.0722 | 0.0944 | 0.8878 |

**Models prediction for ODEs, PDE1, and PDE2.**




**Sample prediction for PDE 3 (Navier-Stokes).**

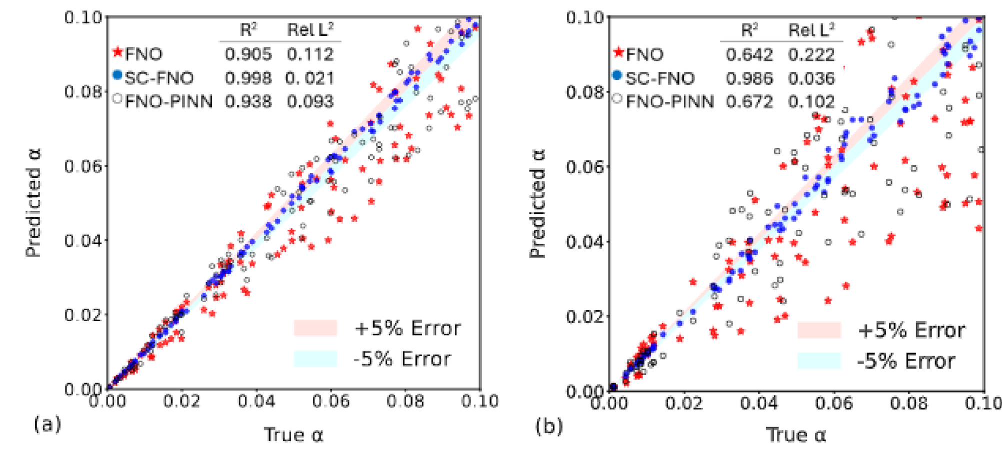



**Comparison of Model Training Time**

| Case | Average training time per epoch (s) | | | |
|---|---|---|---|---|
| | FNO | SC-FNO | FNO-PINN | SC-FNO-PINN |
| ODE1 | 1.10 | 1.94 | 1.53 | 2.46 |
| ODE2 | 1.58 | 2.13 | 1.76 | 2.86 |
| PDE1 | 35.24 | 53.32 | 52.13 | 82.13 |
| PDE2 | 32.66 | 44.92 | 39.11 | 73.06 |
| PDE2 (Zoned) | 5.37 | 7.23 | - | - |
| PDE2 (Zoned) | 8.09 | 11.23 | - | - |
| PDE3 | 47.16 | 109.43 | - | - |
| PDE4 | 11.54 | 19.12 | - | - |

## Results 3: Performance in Inversion Task

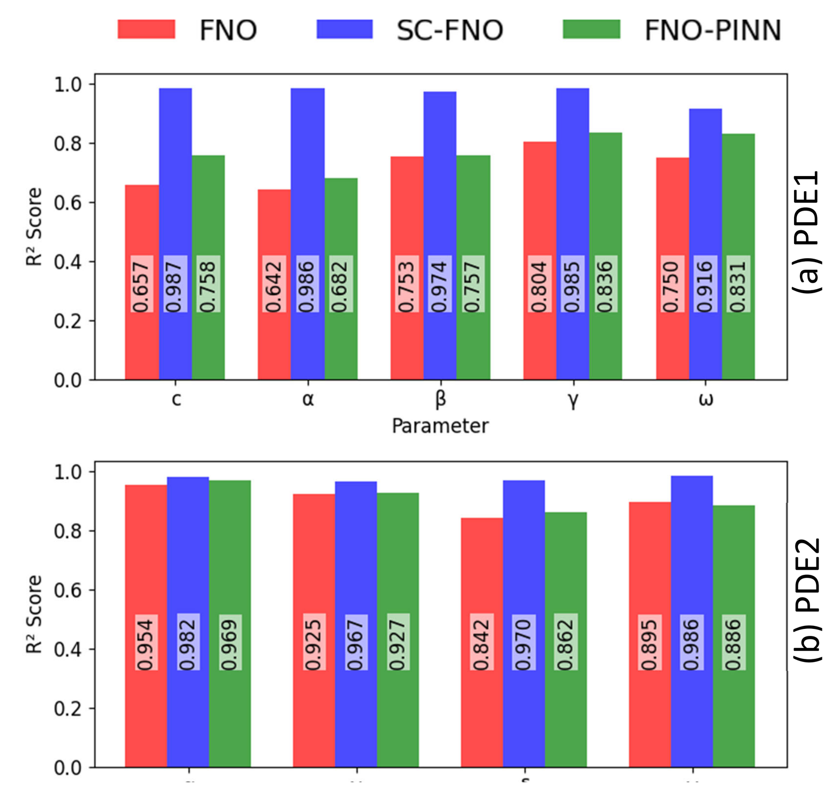
- Sensitivity-constrained neural operators achieve high accuracy in parameter inversion tasks.
- Sensitivity-constrained neural operators can be extended beyond SC-FNO.
- Sensitivity Constrains Enable robust parameter recovery for unseen scenarios.
- SC-FNO significantly reduces inversion errors compared to baseline models.




**Inversion of $\alpha$ in PDE1: (a) Single-parameter, (b) Multi-parameter.**

| Parameter | Fourier Neural Operators | | | | Other Neural Operators | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | FNO | | SC-FNO | | Without gradient supervision. | | | With gradient supervision. | | |
| | R² | Relative L² | R² | Relative L² | WNO | MWNO | DeepONet | SC-WNO | SC-MWNO | SC-DeepONet |
| c | 0.657 | 0.212 | 0.987 | 0.035 | 0.636 | 0.614 | 0.538 | 0.984 | 0.981 | 0.977 |
| $\alpha$ | 0.642 | 0.222 | 0.986 | 0.036 | 0.621 | 0.598 | 0.519 | 0.984 | 0.980 | 0.977 |
| $\beta$ | 0.753 | 0.183 | 0.974 | 0.042 | 0.738 | 0.723 | 0.668 | 0.969 | 0.963 | 0.956 |
| $\gamma$ | 0.804 | 0.165 | 0.985 | 0.037 | 0.792 | 0.780 | 0.736 | 0.982 | 0.978 | 0.975 |
| $\omega$ | 0.750 | 0.186 | 0.916 | 0.075 | 0.735 | 0.719 | 0.663 | 0.901 | 0.879 | 0.859 |

**Inversion performance for PDE1 across different neural operators.**




**Multi-parameter inversion for PDE1 & PDE2.**

## Future Directions

Sensitivity can now be obtained from differentiable solvers (Shen et al., 2023, *Nature Reviews*, https://doi.org/10.1038/s43017-023-00450-9), now used in hydrology (Song et al., 2024, *Water Resources Research*, https://doi.org/10.1029/2024WR038928), ecosystems, and water quality. Several frameworks support differentiable programming (Lonzarich et al., 2025; https://mhpi.github.io/codes/frameworks/).

## Contact Information

Chaopeng Shen is the editor of *Journal of Geophysical Research: Machine Learning and Computation*, a leading geoscience journal. Submissions welcome—contact him!


**Web:** https://mhpi.info/
**Email:** cshen@engr.psu.edu
**Phone:** +1 814-863-5844