Vectorized Conditional Neural Fields: A Framework for Solving Time-dependent Parametric PDEs

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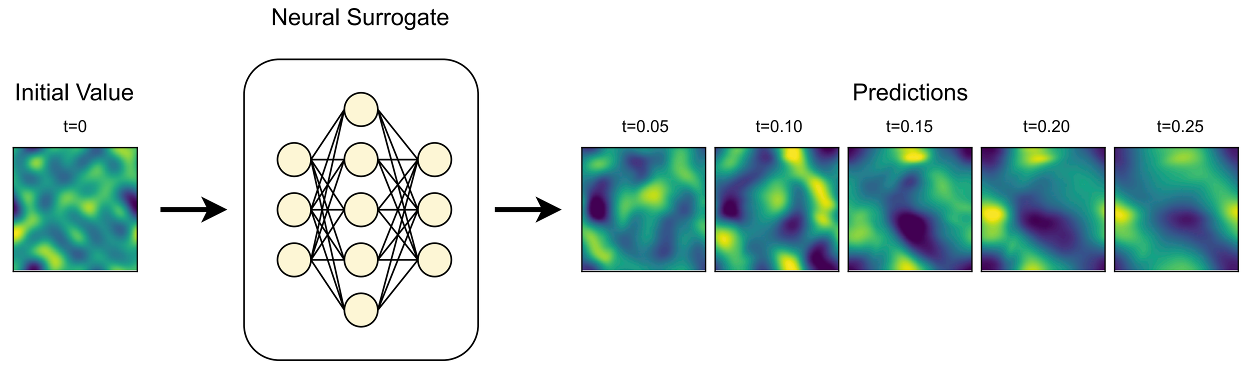
Introduction

- Simulation of physical systems (e.g., fluid dynamics and weather forecasting) relies on solving PDEs
- Machine learning is increasingly used for solving PDEs



Partial Differential Equations

- Burgers' equation models diffusive waves in fluid dynamics over time

$$\partial_t u(t,\boldsymbol{x}) + u(t,\boldsymbol{x})\partial_x u(t,\boldsymbol{x}) = \frac{\nu}{\pi}\partial_{xx} u(t,\boldsymbol{x})$$

t: Temporal coordinate
$\boldsymbol{x}$: Spatial coordinate

- Solving PDEs: Finding function $u(t, \boldsymbol{x})$ that satisfies the equation and constraints (initial and boundary condition)

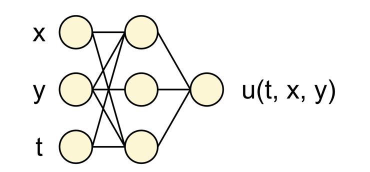
Motivation

- Neural surrogates lack desirable properties:
  - x Spatial- and temporal **super-resolution**
  - x Generalization to **PDE parameter** values
  - x **Efficiency** and **accuracy**
- Vectorized Conditional Neural Field (VCNeF):
  - ✓ Learns solution as a function $u(t, x)$
  - ✓ Incorporates PDE parameter values
  - ✓ Parallel generation of queried solutions
- VCNeF is based on Linear Transformers and Neural Fields

Background Knowledge

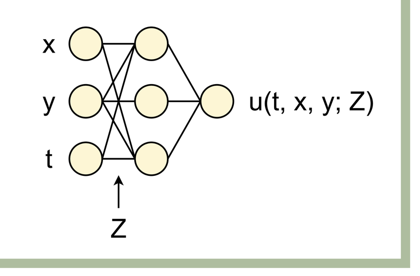
- Neural Field (e.g., PINN):

$$f_\theta: (\mathbb{R}_+ \times \mathbb{R}^d) \to \mathbb{R}^c$$
$$(t, \boldsymbol{x}) \mapsto u(t, \boldsymbol{x})$$



- Conditional Neural Field:

$$f_\theta: (\mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^n) \to \mathbb{R}^c$$
$$(t, \boldsymbol{x}; Z) \mapsto u(t, \boldsymbol{x}; Z)$$



Method

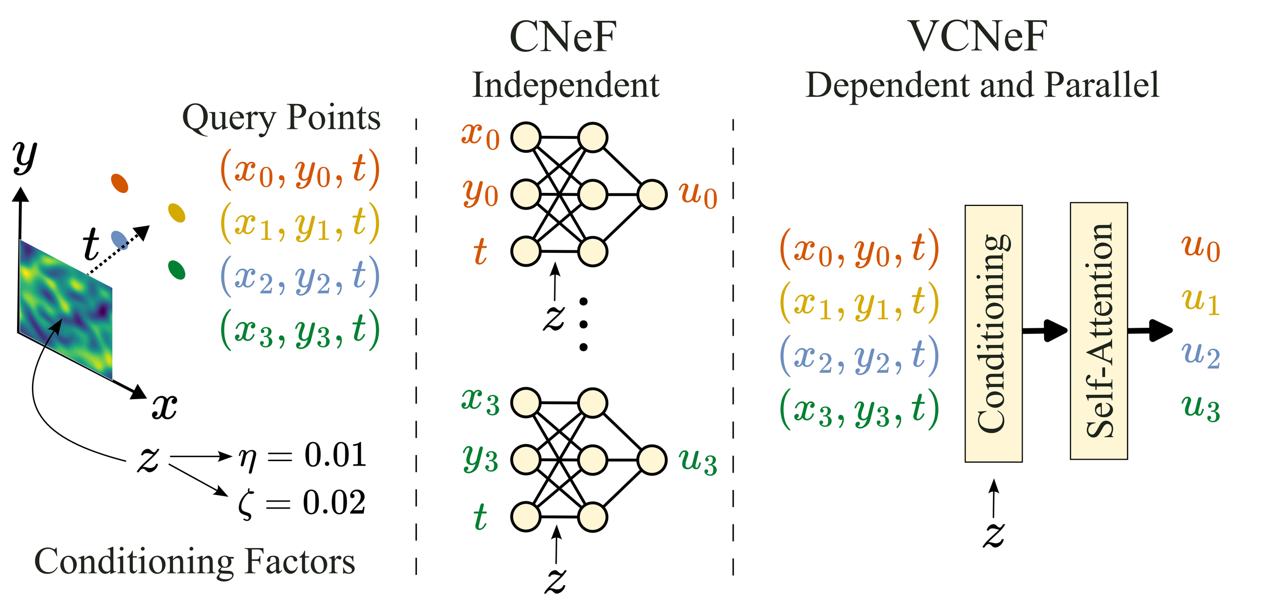
Vectorized Conditional Neural Field

- Takes a **vector** of spatial coordinates
- Exploits **spatial dependencies** between coordinates with attention
- Generates all outputs in **one forward pass**
- Conditioned on **initial value** and **PDE parameter**

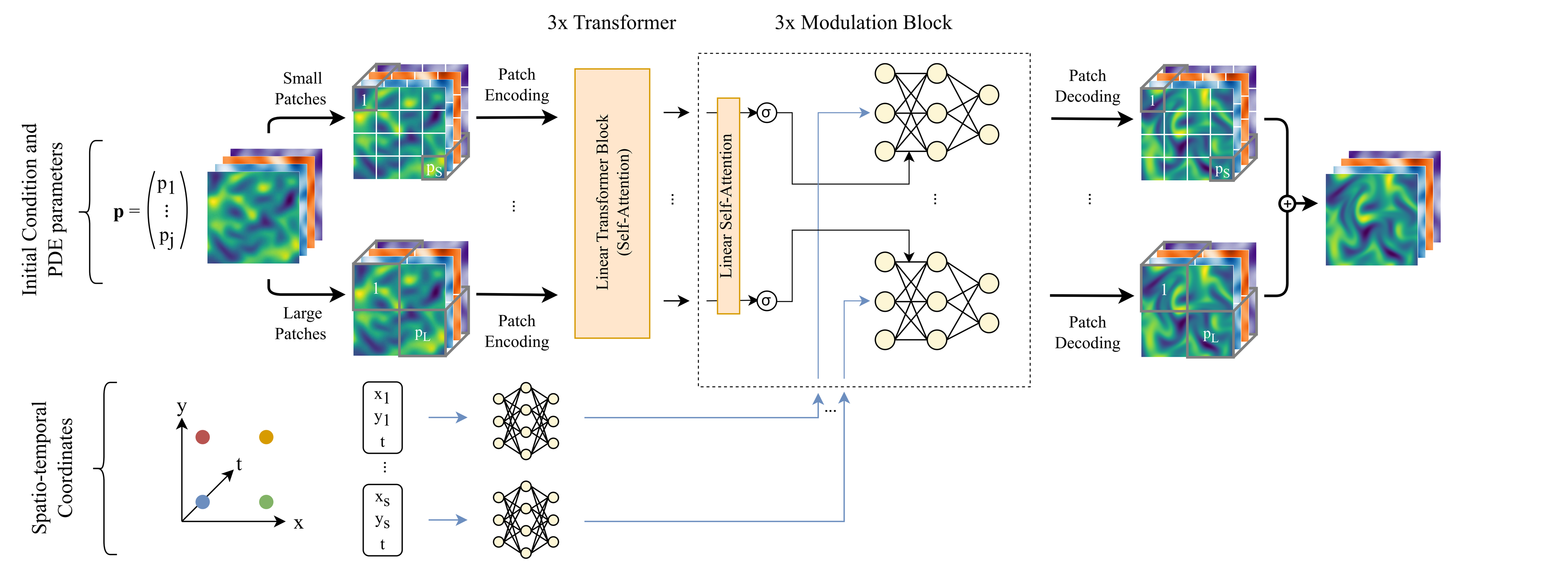
Properties:

- Spatial and temporal **super-resolution**
- **Accelerated** training and inference
- Allows including **physics-aware loss**

Conditional Neural Field vs VCNeF



Neural Architecture



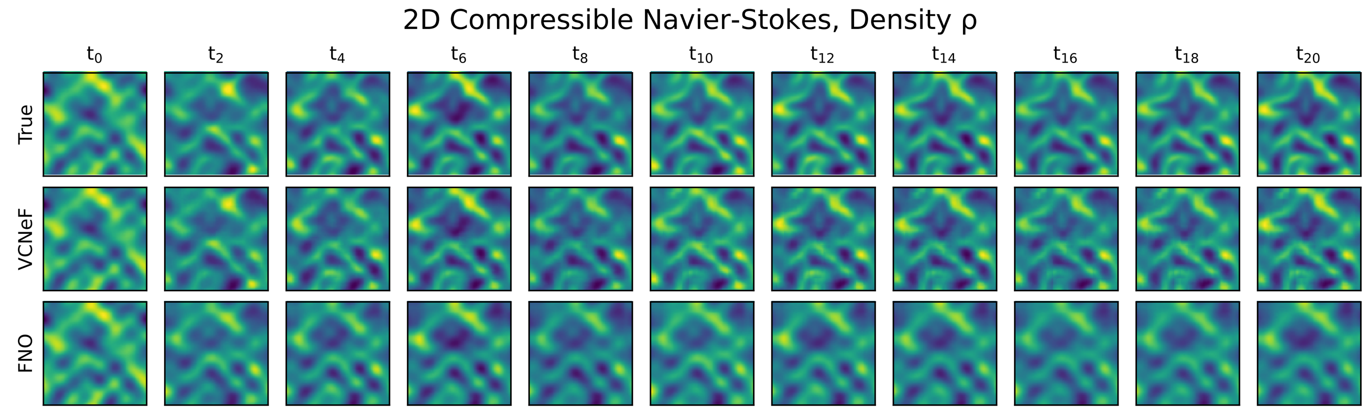
Experiments

- Focus on initial value problems for **1D Burgers'**, **1D Advection**, and **Compressible Navier-Stokes** (CNS) equations from PDEBench
- Baselines: Fourier Neural Operator (FNO), MP-PDE, CORAL, OFormer, and Galerkin Transformer

Proposed VCNeF:

- Performs competitively with the baselines and often outperforms them
- Has spatial and temporal zero-shot super-resolution capabilities
- Generalizes to unseen PDE parameter values

Qualitative Result



Comparison to SOTA Baselines for Fixed PDE Parameter Value and Resolutions

PDE	Model	nRMSE (↓)	bRMSE (↓)
Burgers	FNO	0.0987	0.0225
	MP-PDE	0.3046 (+208.7%)	0.0725 (+221.7%)
	CORAL	0.2221 (+125.1%)	0.0515 (+128.2%)
	OFormer	0.1035 (+4.9%)	**0.0215** (-4.5%)
	Galerkin	0.1651 (+67.3%)	0.0366 (+62.3%)
	VCNeF	**0.0824** (-16.5%)	0.0228 (+1.3%)
Advection	FNO	0.0190	0.0239
	MP-PDE	0.0195 (+2.7%)	0.0283 (+18.4%)
	CORAL	0.0198 (+4.3%)	0.0127 (-46.8%)
	OFormer	**0.0118** (-38.0%)	**0.0073** (-69.6%)
	Galerkin	0.0621 (+227.1%)	0.0349 (+46.2%)
	VCNeF	0.0165 (-13.0%)	0.0088 (-63.2%)
1D CNS	FNO	0.5722	1.9797
	CORAL	0.5993 (+4.7%)	1.5908 (-19.6%)
	OFormer	0.4415 (-22.9%)	2.0478 (+3.4%)
	Galerkin	0.7019 (+22.7%)	3.0143 (+52.3%)
	VCNeF	**0.2943** (-48.6%)	**1.3496** (-31.8%)
2D CNS	FNO	0.5625	0.2332
	Galerkin	0.6702 (+19.2%)	0.8219 (+252.4%)
	VCNeF	**0.1994** (-64.6%)	**0.0904** (-61.2%)
3D CNS	FNO	0.8138	6.0407
	VCNeF	**0.7086** (-12.9%)	**4.8922** (-19.0%)

Spatial and Temporal Zero-Shot Super-Resolution

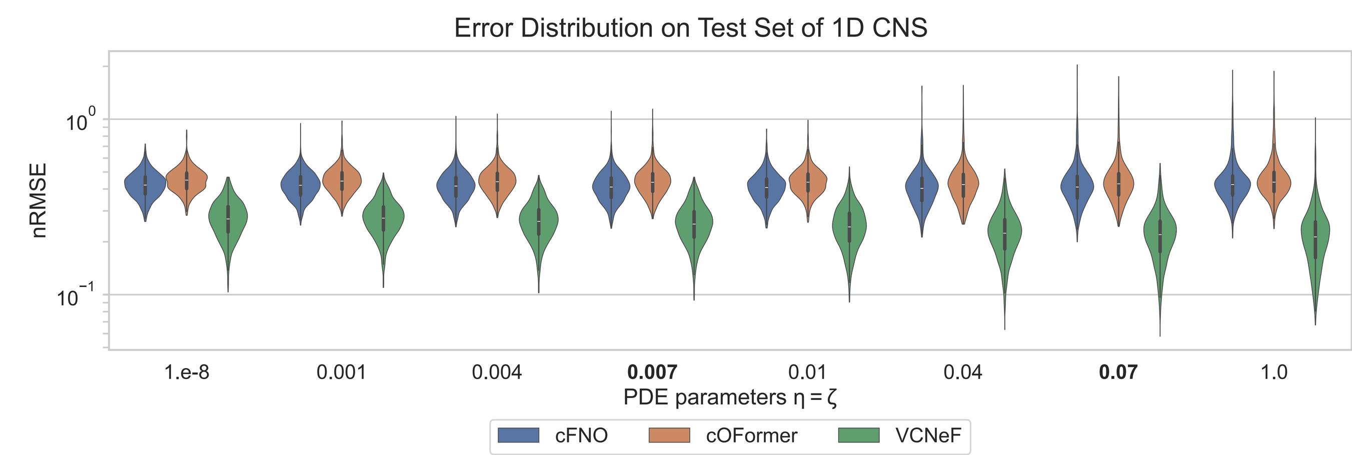
Trained on lower resolution and tested on higher resolutions

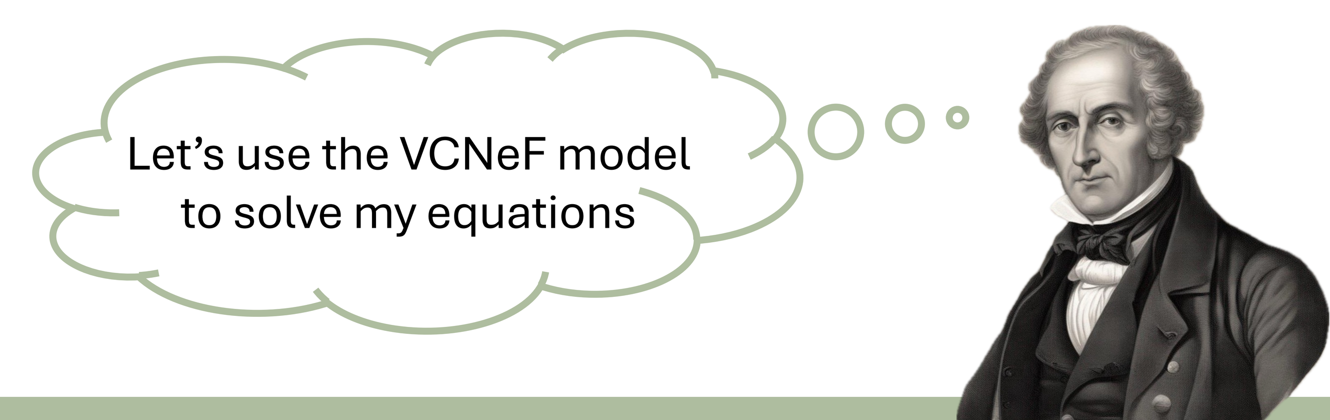
PDE	Spatial res.	Model	nRMSE (↓)	bRMSE (↓)
1D CNS	256	FNO	0.5722	1.9797
		OFormer	0.4415	2.0478
		VCNeF	**0.2943**	**1.3496**
	512	FNO	0.6610	2.7683
		OFormer	0.4657	2.5618
		VCNeF	**0.2943**	**1.3502**
	1024	FNO	0.7320	3.5258
		OFormer	0.4655	2.5526
		VCNeF	**0.2943**	**1.3510**
3D CNS	$32 \times 32 \times 32$	FNO	0.8138	6.0407
		VCNeF	**0.7086**	**4.8922**
	$64 \times 64 \times 64$	FNO	0.9452	8.7068
		VCNeF	**0.7228**	**5.1495**
	$128 \times 128 \times 128$	FNO	1.0077	9.8633
		VCNeF	**0.7270**	**5.3208**

PDE	Temporal res.	Model	nRMSE (↓)	bRMSE (↓)
1D CNS	41	FNO	0.5722	1.9797
		CORAL	0.5993	1.5908
		VCNeF	**0.2943**	**1.3496**
	82	FNO + Interp.	0.5667	1.9639
		CORAL	1.1524	3.7960
		VCNeF	**0.2965**	**1.3741**
3D CNS	11	FNO	0.8138	6.0407
		VCNeF	**0.7086**	**4.8922**
	21	FNO + Interp.	0.8099	6.1938
		VCNeF	**0.7106**	**5.1446**

Generalization to Unseen PDE Parameter Values

Trained on set of PDE parameter values and tested on unseen values (boldfaced)





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Project page: https://jhagnberger.github.io/vectorized-conditional-neural-field
Code: https://github.com/jhagnberger/vcnef