ENMA: Tokenwise Autoregression for Generative Neural PDE Operators

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NEURAL INFORMATION PROCESSING SYSTEMS

Problem & Context

★ Solving **parametric** PDEs

$$
\begin{aligned}
\mathcal{N}\left[\boldsymbol{u};\boldsymbol{c},\boldsymbol{f}\right](x,t) &= 0, && \text{for } (x,t)\in\Omega\times(0,T],\\
\mathcal{B}\left[\boldsymbol{u};\boldsymbol{b}\right](x,t) &= 0, && \text{for } (x,t)\in\partial\Omega\times[0,T],\\
\boldsymbol{u}(x,0) &= \boldsymbol{u}^0(x), && \text{for } x\in\Omega,
\end{aligned}
$$

c: PDE coefficients
f: forcing terms
b: boundary conditions
$\mathbf{u^0}$: initial condition

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★ Deterministic neural surrogate

– Modeling complex/chaotic physical behavior
– Modeling uncertainty
– Partially observed systems

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★ Generative neural surrogate

Diffusion

\+ Continuous at pixel level
\+ Uncertainty quantification

– Expensive training stage
– Requires a high number of denoising steps

Auto-regressive

\+ In-context learning
\+ Causality aligned generation

– Requires quantization
– Uncalibrated uncertainty quantification

How to create a generative model for PDE solving that keeps the advantages and consistency of autoregressive modeling while being continuous in space?

Problem & Context

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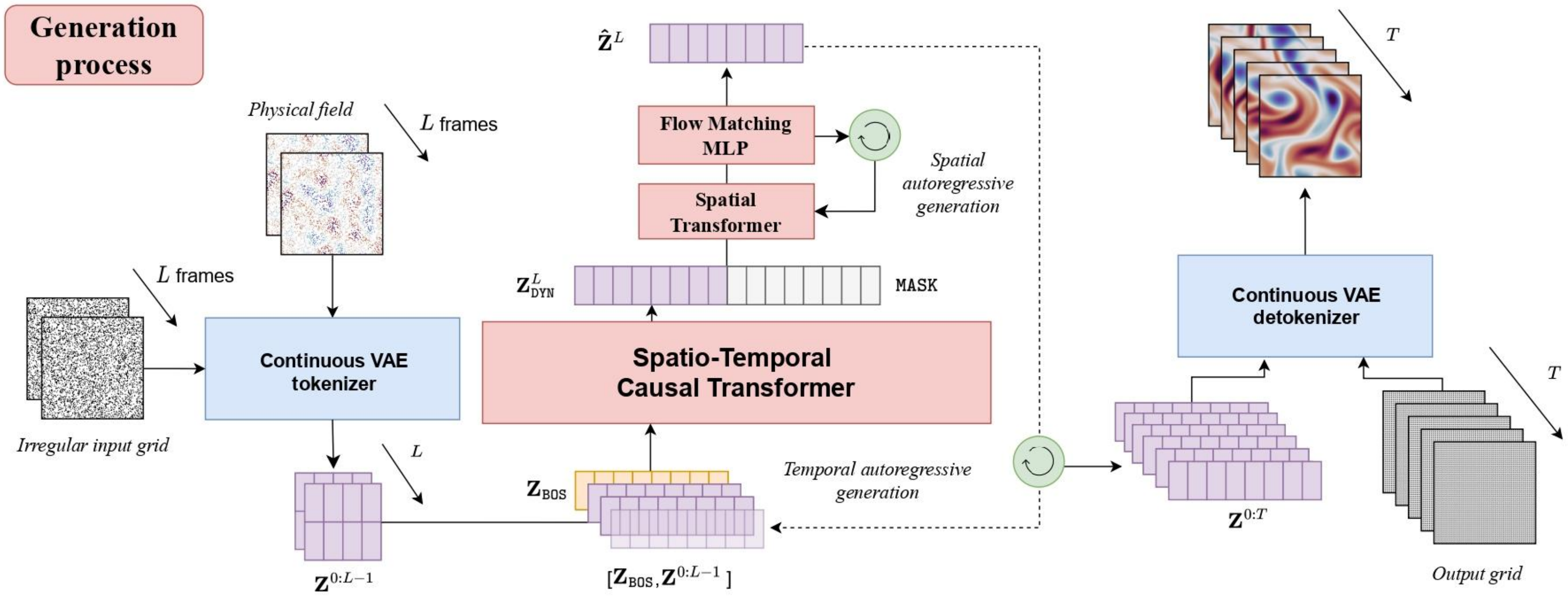
We propose:

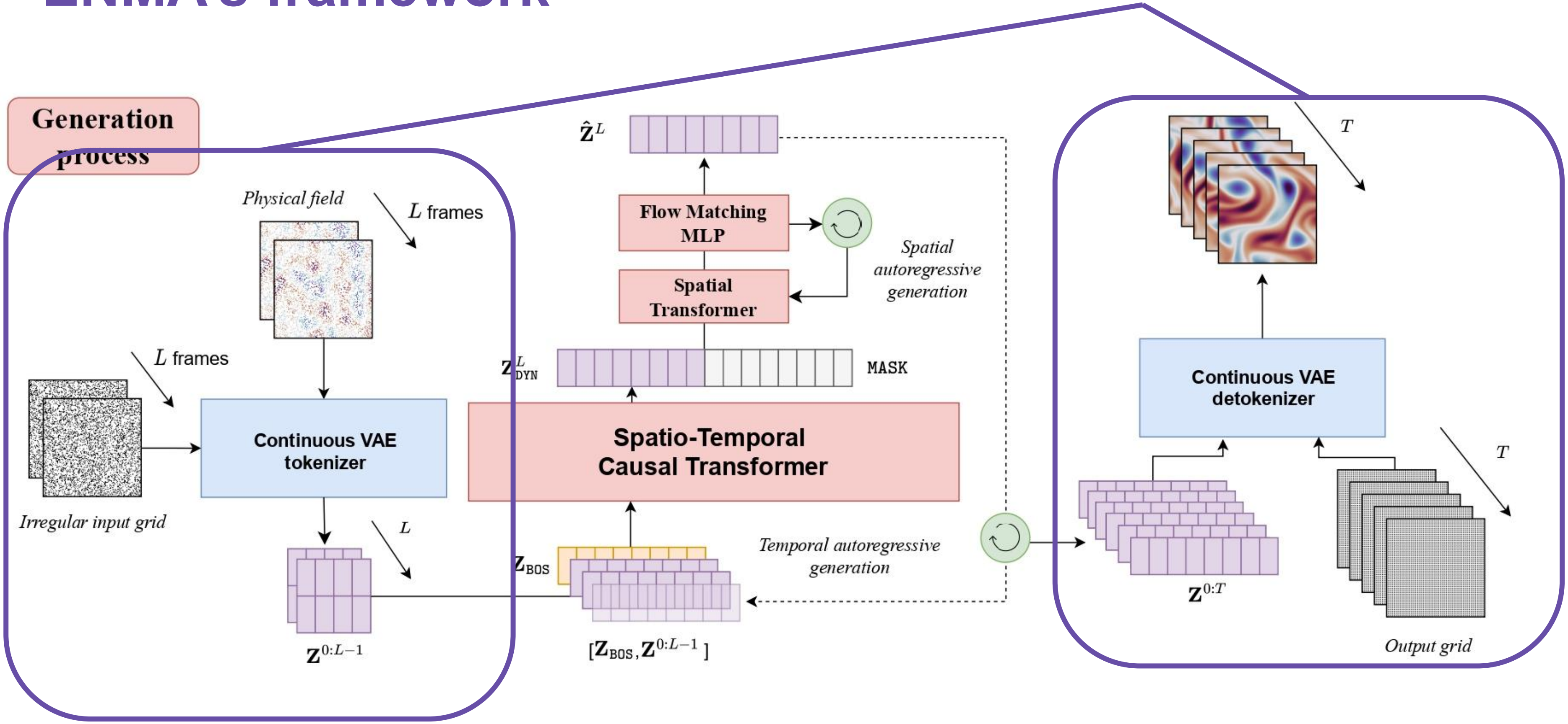
ENMA

ENMA's framework



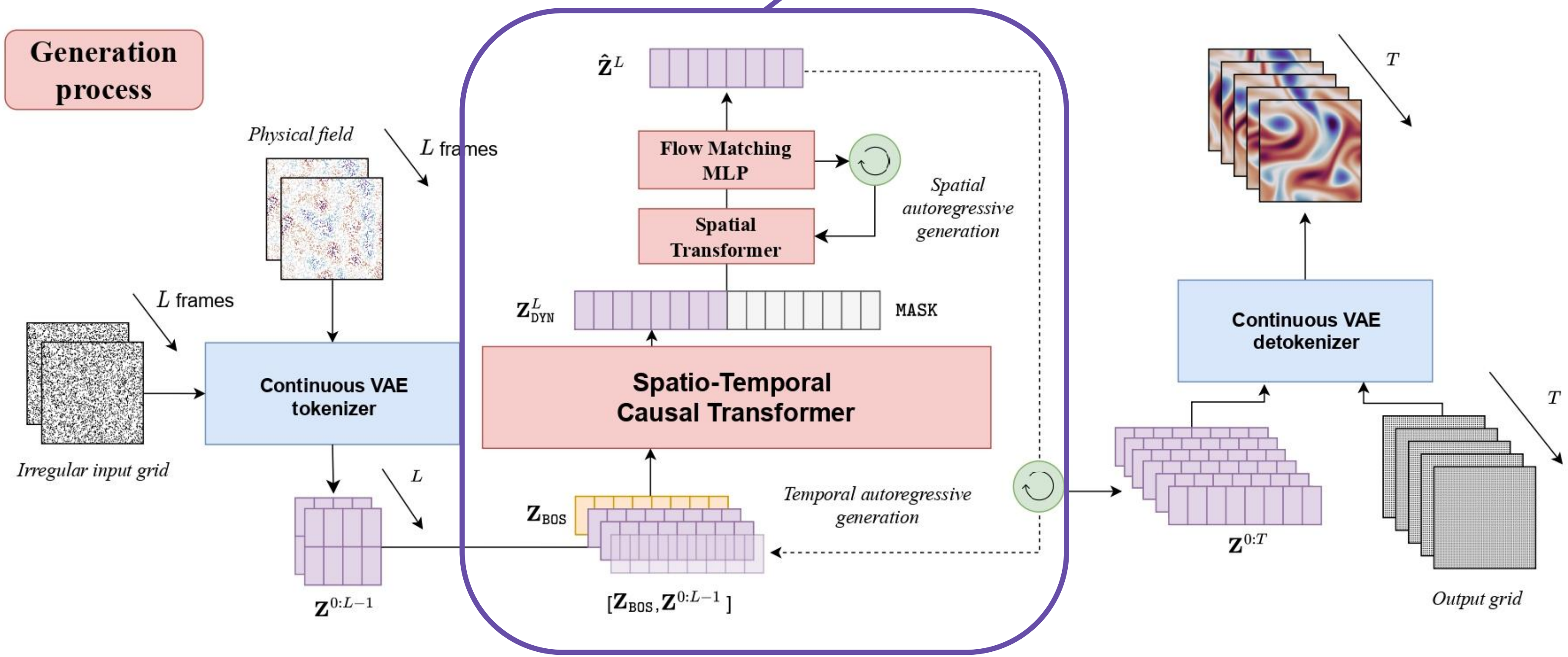
ENMA's framework

Causal & continuous Encoder/decoder
+ Continuous at pixel level
+ arbitrary domain encoding

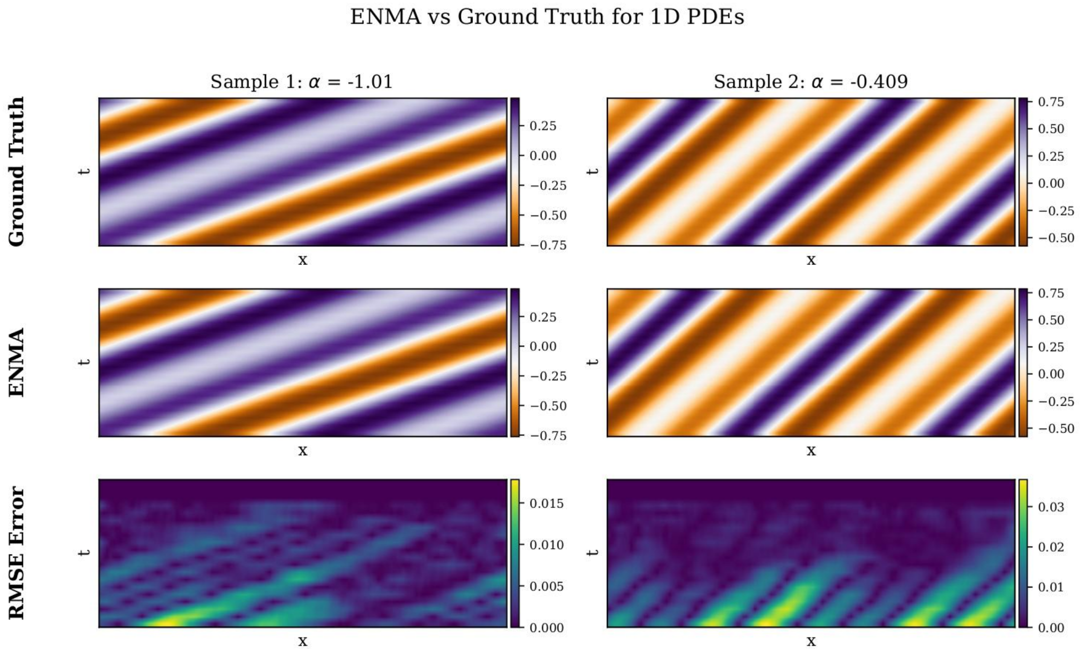


ENMA’s framework

Generative Model
+ Uncertainty quantification
+ Causality aligned generation



Some results on the Advection PDE



More results in the paper!

★ Experiment on the encoder/decoder

$\downarrow \mathcal{X}_{te}$	**Dataset →** / **Model ↓**	**Advection** *Reconstruction*	*Time-stepping*	*Compression rate*
$\pi = 100\%$	OFormer	1.70e-1	1.11e+0	×0.25
	GINO	3.15e-1	8.55e-1	×2
	AROMA	5.41e-3	2.23e-1	×2
	CORAL	1.34e-2	9.64e-1	×2
	ENMA	**1.83e-3**	**1.64e-1**	**×4**
$\pi = 50\%$	OFormer	1.79e-1	1.11e+0	-
	GINO	3.21e-1	8.64-1	-
	AROMA	2.34e-2	2.29e-1	-
	CORAL	7.57e-2	9.74e-1	-
	ENMA	**4.60e-3**	**1.72e-1**	-
$\pi = 20\%$	OFormer	2.50e-1	1.13e+0	-
	GINO	3.54e-1	9.11e-1	-
	AROMA	1.67e-1	3.21e-1	-
	CORAL	4.77e-1	1.06e+0	-
	ENMA	**3.05e-2**	**3.13e-1**	-

★ Experiment on the generative process

Setting ↓	**Dataset →** / **Model ↓**	**Advection** *In-D*	*Out-D*
Temporal Conditioning	FNO	2.47e-1	7.95e-1
	BCAT	5.55e-1	9.23e-1
	AVIT	1.64e-1	**5.02e-1**
	AR-DiT	2.36e-1	8.56e-1
	Zebra	2.04e-1	1.39e+0
	ENMA	**3.95e-2**	5.30e-1
Initial Value Problem	In-Context ViT	1.15e+0	1.20e+0
	[CLS] ViT	1.15e+0	1.36e+0
	Zebra	3.16e-1	1.47e+0
	ENMA	**2.02e-1**	**8.07e-1**

More about ENMA !

Project Page

Paper

Code

ENMA's generative training and inference