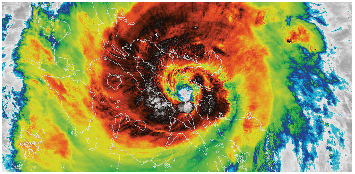
Continuous PDE Dynamics Forecasting with Implicit Neural Representations

ICLR 2023

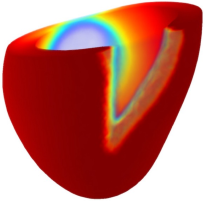
May 1st – 5th, 2023

Yuan Yin,[⋆1] Matthieu Kirchmeyer,[⋆1,2] Jean-Yves Franceschi,[⋆2] Alain Rakotomamonjy,[2] Patrick Gallinari[1,2]

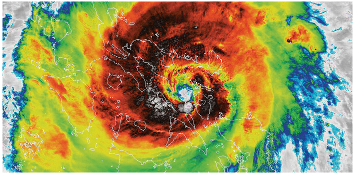
[⋆] *Equal Contribution* [1] *Sorbonne Université, CNRS, ISIR* [2] *Criteo AI Lab*



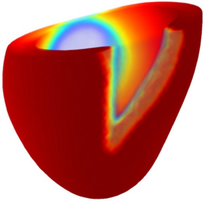
Weather forecasting



Heart electrical activities



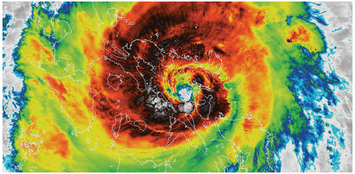
Weather forecasting



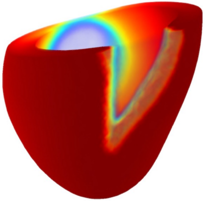
Heart electrical activities

Modeling Dynamics with DL: Domain on the Rise

➜ Goal: take advantage of DL to extract dynamics from data to predict the future.



Weather forecasting

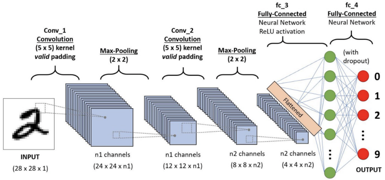


Heart electrical activities

Modeling Dynamics with DL: Domain on the Rise

- ➜ Goal: take advantage of DL to extract dynamics from data to predict the future.
- ➜ Predict a phenomenon in **space** and **time**.
- ➜ Effective models proposed with different properties.

Convolution (NODE)



Chen et al., *Neural Ordinary Differential Equations. NeurIPS 2018*

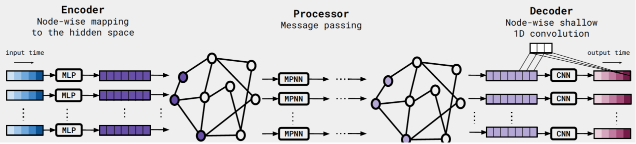
Forecast at any time in the future

Temporally continuous dynamics

Convolution (NODE)

Chen et al., *Neural Ordinary Differential Equations. NeurIPS 2018*

GNN (MP-PDE)

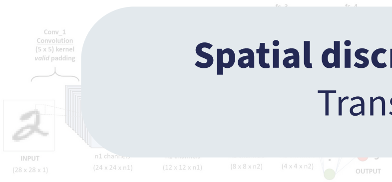


Brandstetter et al., *Message Passing Neural PDE Solvers. ICLR 2022*

No format requirements for the input

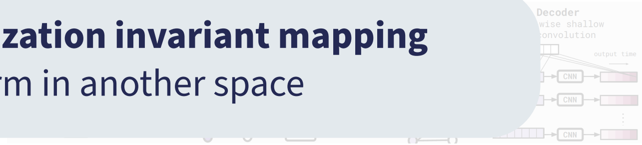
Point-cloud acceptable

Convolution (NODE)



Chen et al., *Neural Ordinary Differential Equations. NeurIPS 2018*

GNN (MP-PDE)

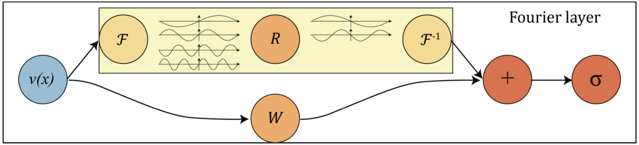


Brandstetter et al., *Message Passing Neural PDE Solvers. ICLR 2022*

Spatial discretization invariant mapping

Transform in another space

FFT (FNO)

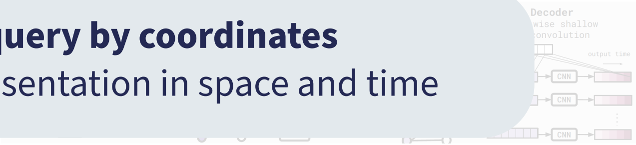


Li et al., *Fourier Neural Operator for Parametric Partial Differential Equations. ICLR 2021*

Convolution (NODE)

Chen et al., *Neural Ordinary Differential Equations. NeurIPS 2018*

GNN (MP-PDE)

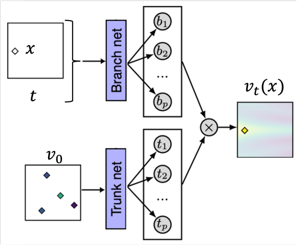


Brandstetter et al., *Message Passing Neural PDE Solvers. ICLR 2022*

Function query by coordinates

Continuous representation in space and time

Coordinate-based (DeepONet)

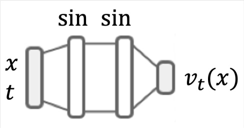


Lu et al., *Learning nonlinear operators via DeepONet. Nature Machine Intelligence 2021*

FFT (FNO)

Li et al., *Fourier Neural Operator for Parametric Partial Differential Equations. ICLR 2021*

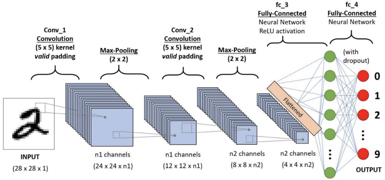
INR (SIREN)



Sitzmann et al., *Implicit Neural Representations with Periodic Activation Functions. NeurIPS 2020.*

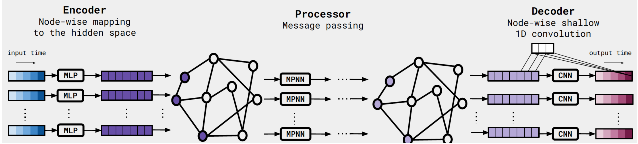
SCIENCES SORBONNE UNIVERSITÉ CRITEO AI Lab

Convolution (NODE)



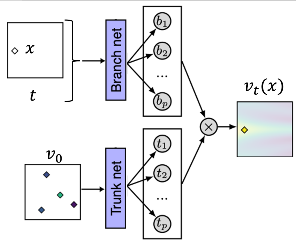
Chen et al., *Neural Ordinary Differential Equations. NeurIPS 2018*

GNN (MP-PDE)



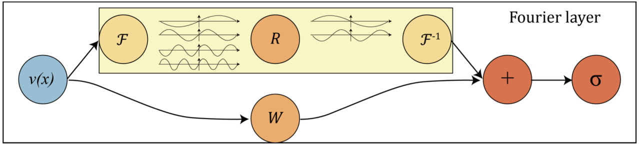
Brandstetter et al., *Message Passing Neural PDE Solvers. ICLR 2022*

Coordinate-based (DeepONet)



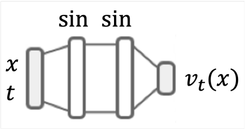
Lu et al., *Learning nonlinear operators via DeepONet. Nature Machine Intelligence 2021*

FFT (FNO)



Li et al., *Fourier Neural Operator for Parametric Partial Differential Equations. ICLR 2021*

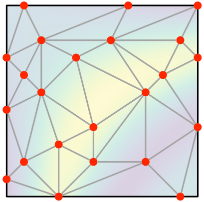
INR (SIREN)

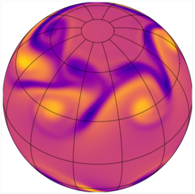


Sitzmann et al., *Implicit Neural Representations with Periodic Activation Functions. NeurIPS 2020.*

➜ **Spatial flexibility:**

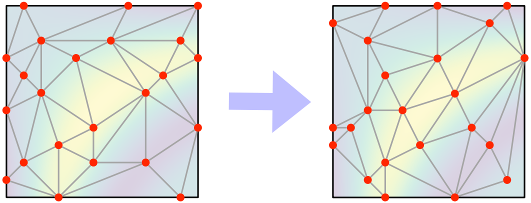
- **Spatial flexibility:**
  - *Handling **free-form input and domains** with the same general architecture.*





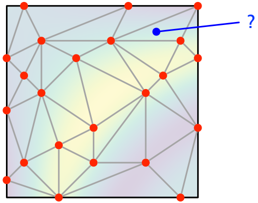
→ **Spatial flexibility:**

- *Handling **free-form input and domains** with the same general architecture.*
- *Generalize to **new input grids** by removing architectural constraints.*



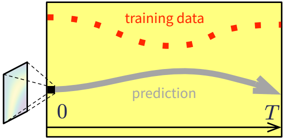
➜ Spatial flexibility:

- ➥ *Handling **free-form input and domains** with the same general architecture.*
- ➥ *Generalize to **new input grids** by removing architectural constraints.*
- ➥ *Arbitrary **coordinate query** for spatial interpolation.*

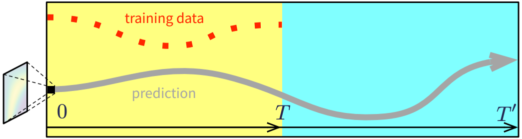


- **Spatial flexibility:**
  - *Handling **free-form input and domains** with the same general architecture.*
  - *Generalize to **new input grids** by removing architectural constraints.*
  - *Arbitrary **coordinate query** for spatial interpolation.*
- **Temporal flexibility:**

- **Spatial flexibility:**
  - *Handling **free-form input and domains** with the same general architecture.*
  - *Generalize to **new input grids** by removing architectural constraints.*
  - *Arbitrary **coordinate query** for spatial interpolation.*
- **Temporal flexibility:**
  - *Given time-discrete training data, produce **time-continuous solutions** with **new initial conditions**.*



- **Spatial flexibility:**
  - *Handling **free-form input and domains** with the same general architecture.*
  - *Generalize to **new input grids** by removing architectural constraints.*
  - *Arbitrary **coordinate query** for spatial interpolation.*
- **Temporal flexibility:**
  - *Given time-discrete training data, produce **time-continuous solutions** with **new initial conditions**.*
  - ***Extrapolation beyond train horizon** through dynamics modeling.*

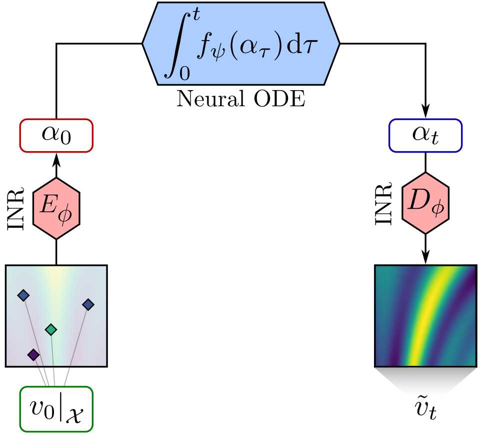


- **Spatial flexibility:**
  - *Handling **free-form input and domains** with the same general architecture.*
  - *Generalize to **new input grids** by removing architectural constraints.*
  - *Arbitrary **coordinate query** for spatial interpolation.*
- **Temporal flexibility:**
  - *Given time-discrete training data, produce **time-continuous solutions** with **new initial conditions**.*
  - ***Extrapolation beyond train horizon** through dynamics modeling.*

We introduce DINo

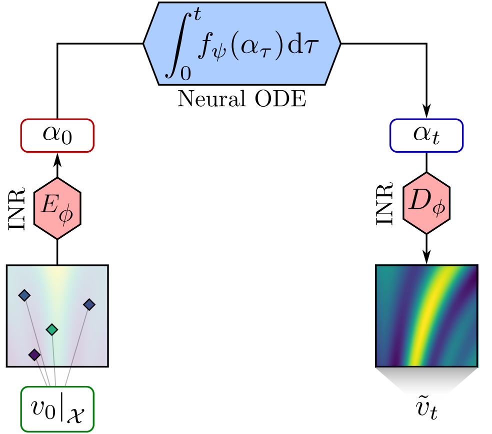
Space and time-continuous neural PDE forecaster.

→ (ENC) Encode free-form observations into a latent vector.

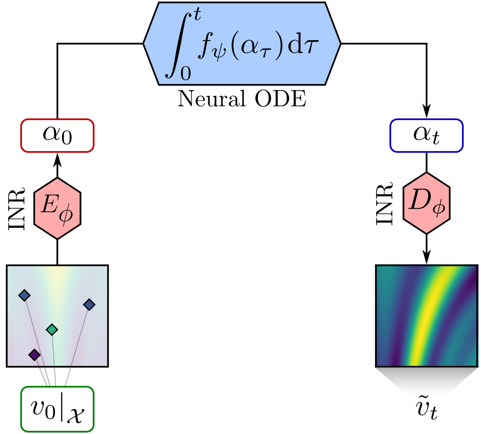


➜ (ENC) Encode free-form observations into a latent vector.

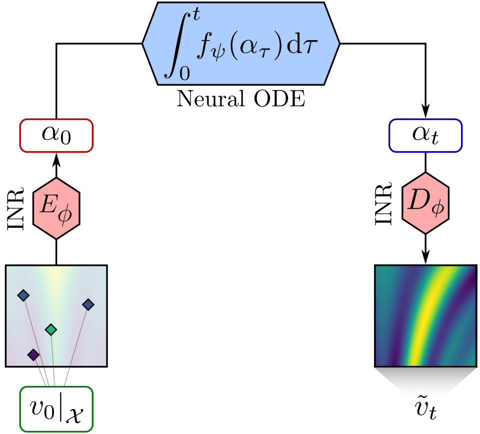
➜ (DYN) Unroll dynamics with time-continuous Neural ODE.



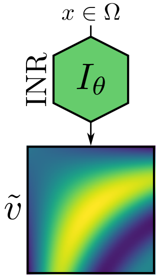
- (ENC) Encode free-form observations into a latent vector.
- (DYN) Unroll dynamics with time-continuous Neural ODE.
- (DEC) Decode with space-continuous emission function.



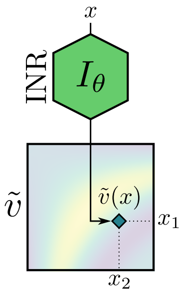
- (ENC) Encode free-form observations into a latent vector.
- (DYN) Unroll dynamics with time-continuous Neural ODE.
- (DEC) Decode with space-continuous emission function.
- (ENC)(DEC) with implicit neural representations.



➜ Represent continuous data.

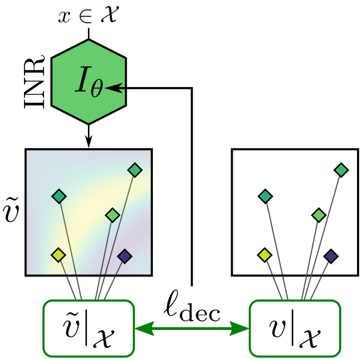


- Represent continuous data.
- With coordinate-based NN $I_\theta : \Omega \to \mathbb{R}^{d_c}$ with periodic activations.



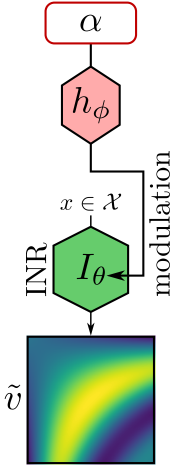
- Represent continuous data.
- With coordinate-based NN $I_\theta : \Omega \to \mathbb{R}^{d_c}$ with periodic activations.
- Learn θ by gradient descent over MSE:

$$\min_\theta \sum_{x \in \mathcal{X}} \left\| v(x) - I_\theta(x) \right\|_2^2 .$$



➜ Decoding latent vector α via a hypernetwork h_ϕ:

$$I_{h_\phi(\alpha)} = \tilde{v}.$$

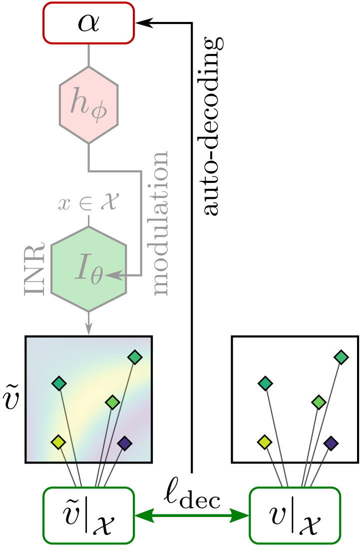


➜ Decoding latent vector α via a hypernetwork h_ϕ:

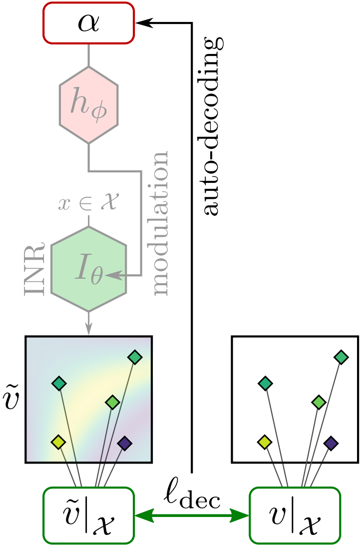
$$I_{h_\phi(\alpha)} = \tilde{v}.$$

➜ Auto-decoding to infer α given $v|_\mathcal{X}$:

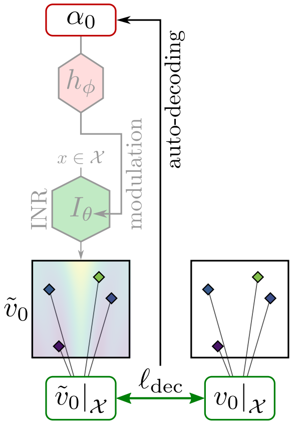
$$\alpha = \text{auto-dec}\left(v|_\mathcal{X}, h_\phi\right).$$



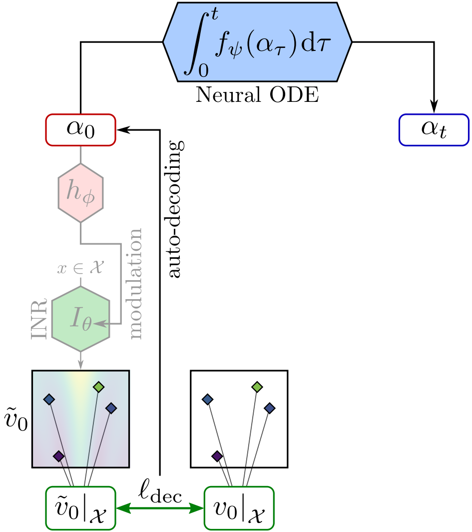
- Decoding latent vector α via a hypernetwork h_ϕ:
$$I_{h_\phi(\alpha)} = \tilde{v}.$$
- Auto-decoding to infer α given $v|_\mathcal{X}$:
$$\alpha = \text{auto-dec}\left(v|_\mathcal{X}, h_\phi\right).$$
- Encodes multiple samples using the same decoder.



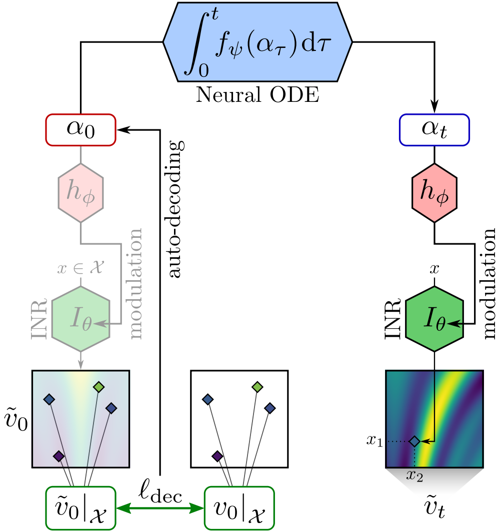
$$\text{(ENC)}\ \alpha_0 = \text{auto-dec}(\, v_0|_{\mathcal{X}}, h_\phi),$$

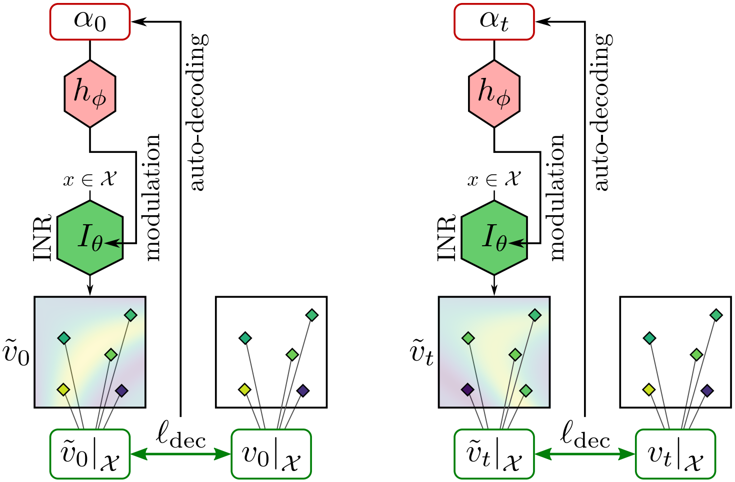


$$(\text{ENC})\ \alpha_0 = \text{auto-dec}(v_0|_{\mathcal{X}}, h_\phi), \qquad (\text{DYN})\ \frac{d\alpha_t}{dt} = f_\psi(\alpha_t),$$



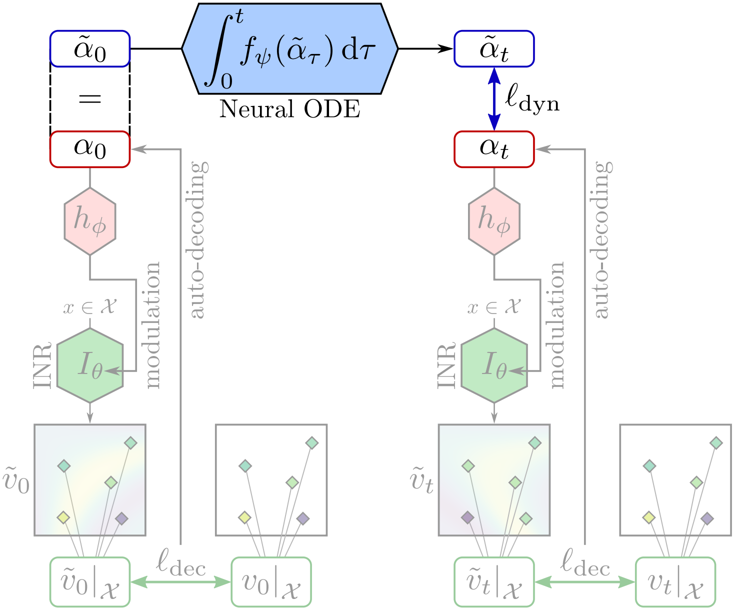
(ENC) $\alpha_0 = \text{auto-dec}(v_0|_{\mathcal{X}}, h_\phi)$, (DYN) $\frac{d\alpha_t}{dt} = f_\psi(\alpha_t)$, (DEC) $\forall t, \tilde{v}_t = I_{h_\phi(\alpha_t)}$.

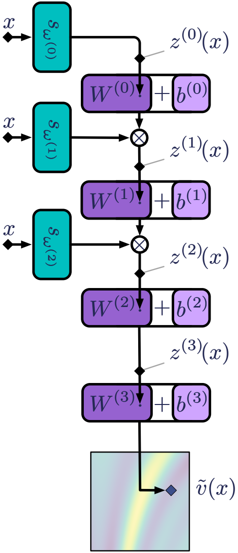




α_0
h_ϕ
auto-decoding
modulation
$x \in \mathcal{X}$
INR
I_θ
$\tilde{v}_0$
ℓ_{dec}
$\tilde{v}_0|_\mathcal{X}$
$v_0|_\mathcal{X}$
α_t
h_ϕ
auto-decoding
modulation
$x \in \mathcal{X}$
INR
I_θ
$\tilde{v}_t$
ℓ_{dec}
$\tilde{v}_t|_\mathcal{X}$
$v_t|_\mathcal{X}$

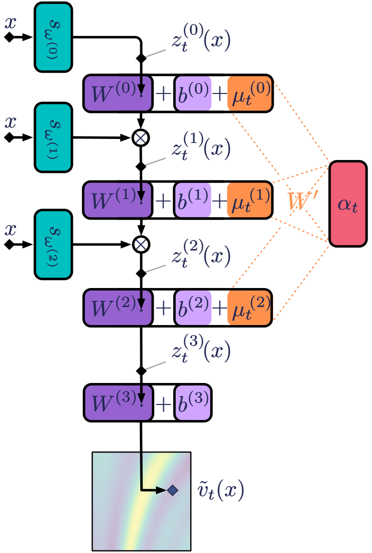
SCIENCES SORBONNE UNIVERSITÉ CRITEO AI Lab





Multiplicative Filter Nets (MFN, Fathony et al., 2021)

- ➜ Combination of spatial basis functions.
- ➜ MFN have interpretable parameters:
  - ➥ parameters for *basis functions and coefficients*.

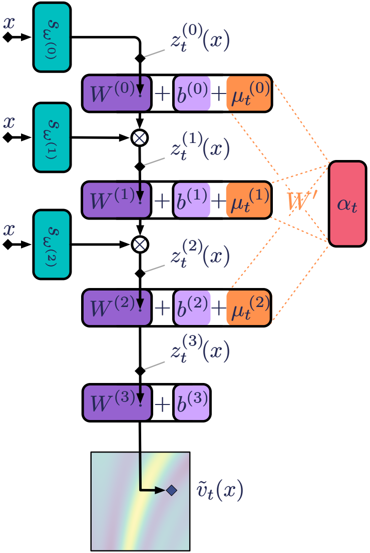


Multiplicative Filter Nets (MFN, Fathony et al., 2021)

- ➜ Combination of spatial basis functions.
- ➜ MFN have interpretable parameters:
  - ➥ parameters for *basis functions* and *coefficients*.

Fitting Samples with Latent Shift Modulation

- ➜ Modulate INR with latent vector (Dupont et al., 2022).
- ➜ Add shift modulation to coefficients via a hypernet.



Multiplicative Filter Nets (MFN, Fathony et al., 2021)

- Combination of spatial basis functions.
- MFN have interpretable parameters:
  - parameters for *basis functions* and *coefficients*.

Fitting Samples with Latent Shift Modulation

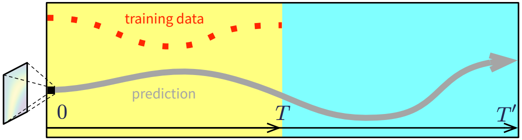
- Modulate INR with latent vector (Dupont et al., 2022).
- Add shift modulation to coefficients via a hypernet.

Space-Time Variable Separation

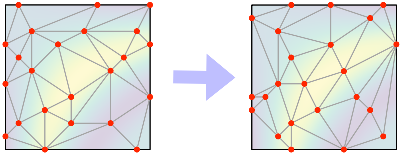
$$\tilde{v}_t(x) = \sum_m \overbrace{c^{(m)}(\alpha_t)}^{\text{time-dependent coefficient}} \times \underbrace{s_{\gamma^{(m)}}(x)}_{\text{spatial basis element}}.$$

→ Diverse set of evaluation scenarios.

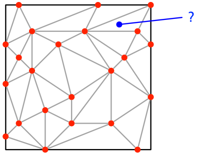
➥ New initial condition
➥ Temporal extrapolation
➥ Time continuity



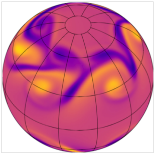
➥ Changing observation grid



➥ Spatial interpolation



➥ Data on manifold

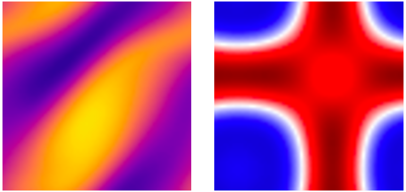


Experimental Setting

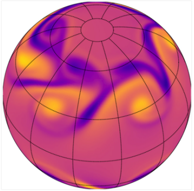
➜ Diverse set of evaluation scenarios.

➜ Various time-dependent PDEs.

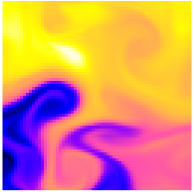
➥ 2D planar PDEs
(Navier-Stokes, Wave)



➥ 3D spherical PDE
(Shallow-Water)



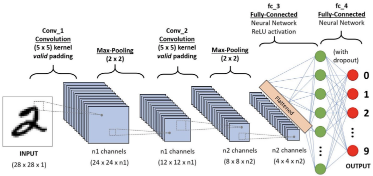
➥ Real-world data
(Sea Surface Temperature)

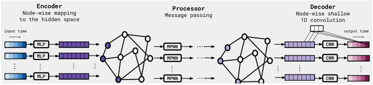


Experimental Setting

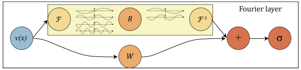
- ➜ Diverse set of evaluation scenarios.
- ➜ Various time-dependent PDEs.
- ➜ Comparison to recent neural PDE forecasters.

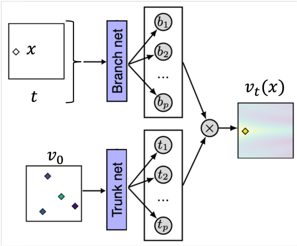
➥ Discretized
(NODE, MP-PDE)



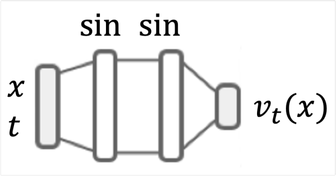


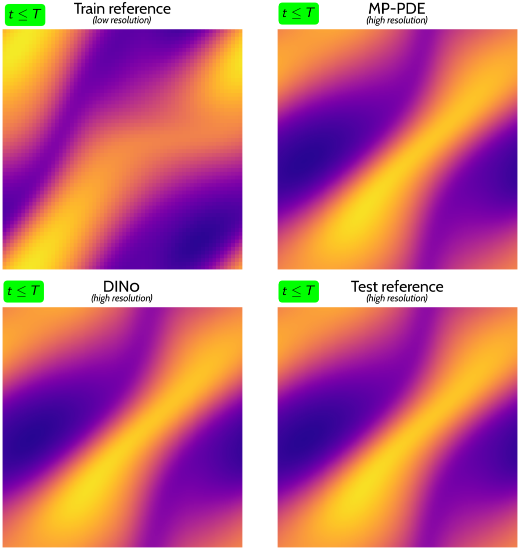
➥ Neural Operator
(Markov FNO, DeepONet)





➥ Temporal INRs
(SIREN, MFN)



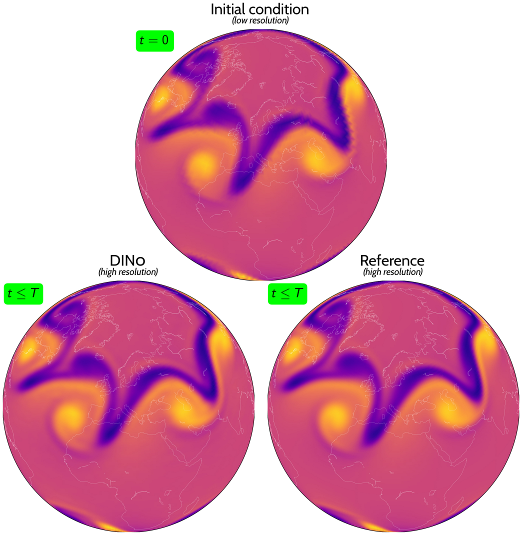


Main Results

State-of-the-art prediction performance in various generalization settings:

- ➜ better temporal extrapolation;
- ➜ better adaptation to new grids;
- ➜ better spatial interpolation.

Animation: zero-shot super-resolution and temporal extrapolation on Navier-Stokes.



Results generalize to PDEs on manifolds thanks to the spatial flexibility of INRs.

Animation: zero-shot super-resolution and temporal extrapolation on Shallow-Water.

Take-Home Messages

→ New time and space continuous PDE forecaster.

Take-Home Messages

- ➜ New time and space continuous PDE forecaster.
- ➜ Combines flexibility of INRs + ODEs.

Take-Home Messages

- ➜ New time and space continuous PDE forecaster.
- ➜ Combines flexibility of INRs + ODEs.
- ➜ Spatiotemporal generalization.

Take-Home Messages

- ➜ New time and space continuous PDE forecaster.
- ➜ Combines flexibility of INRs + ODEs.
- ➜ Spatiotemporal generalization.

Paper `https://openreview.net/forum?id=B73niNjbPs`
Code `https://github.com/mkirchmeyer/DINo`
Email

- ➜ yuan.yin@isir.upmc.fr
- ➜ m.kirchmeyer@criteo.com
- ➜ jycja.franceschi@criteo.com

Paper

Code