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Multifidelity, domain decomposition, and stacking for improving training for physics-informed networks

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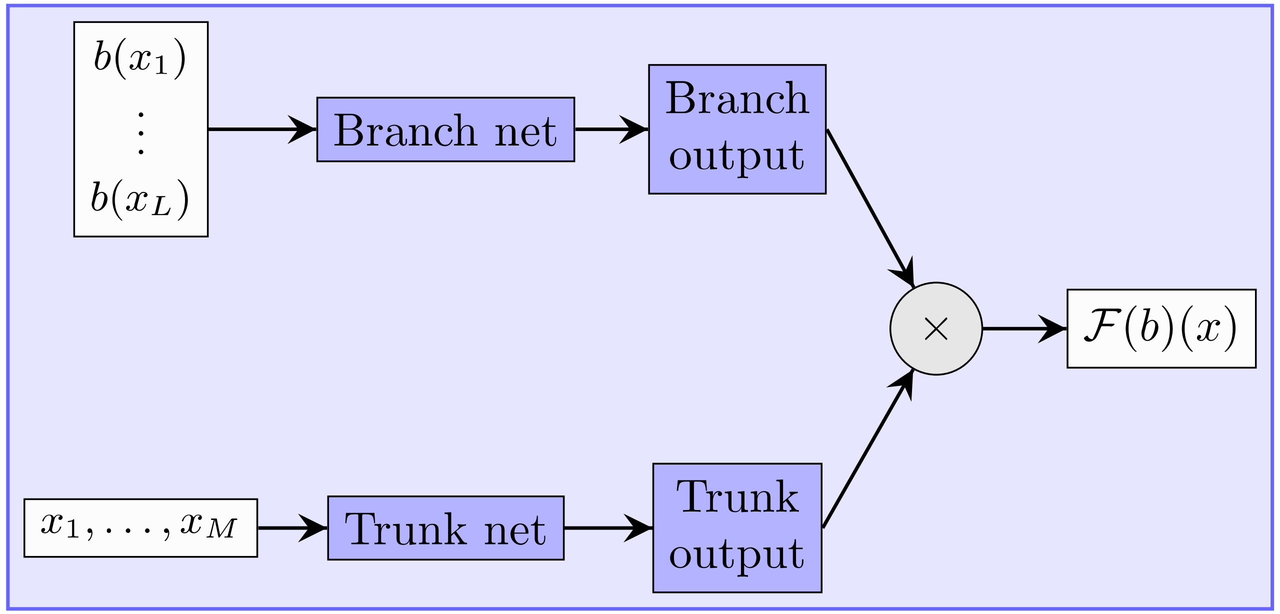
Deep Operator Networks (DeepONets)

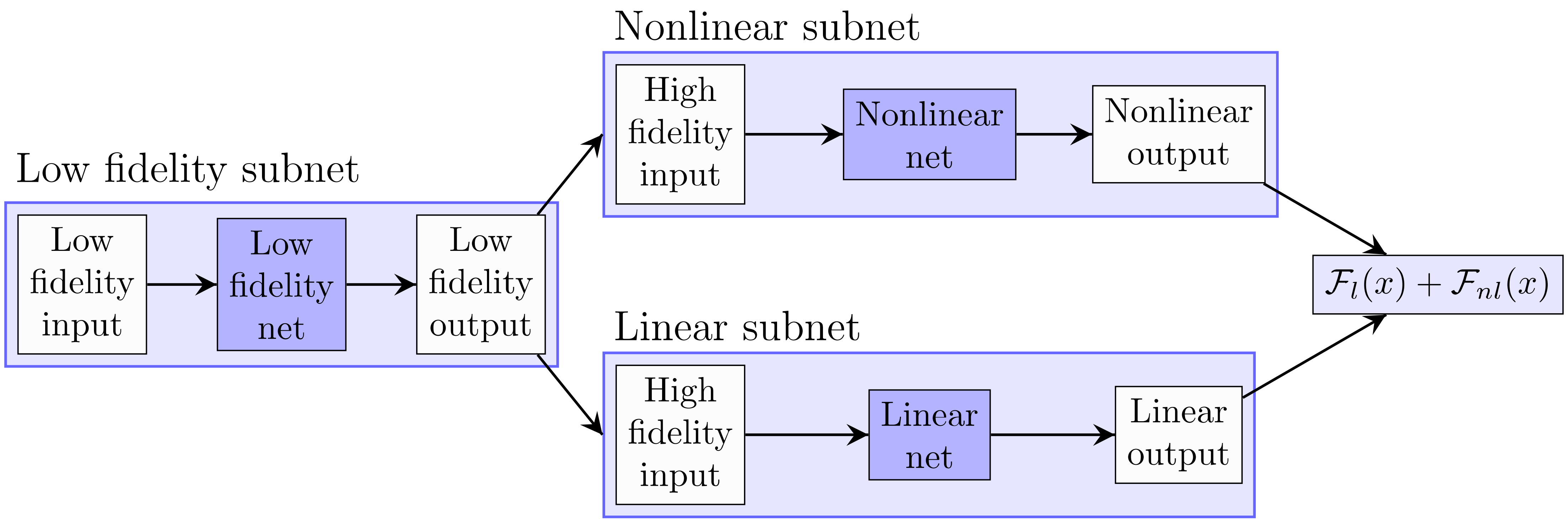
- PINNs map one input to one output
- PI-DeepONets map a *space* of inputs to a *space* of outputs
- PI-DeepONets are much more powerful, but therefore much more difficult to train.



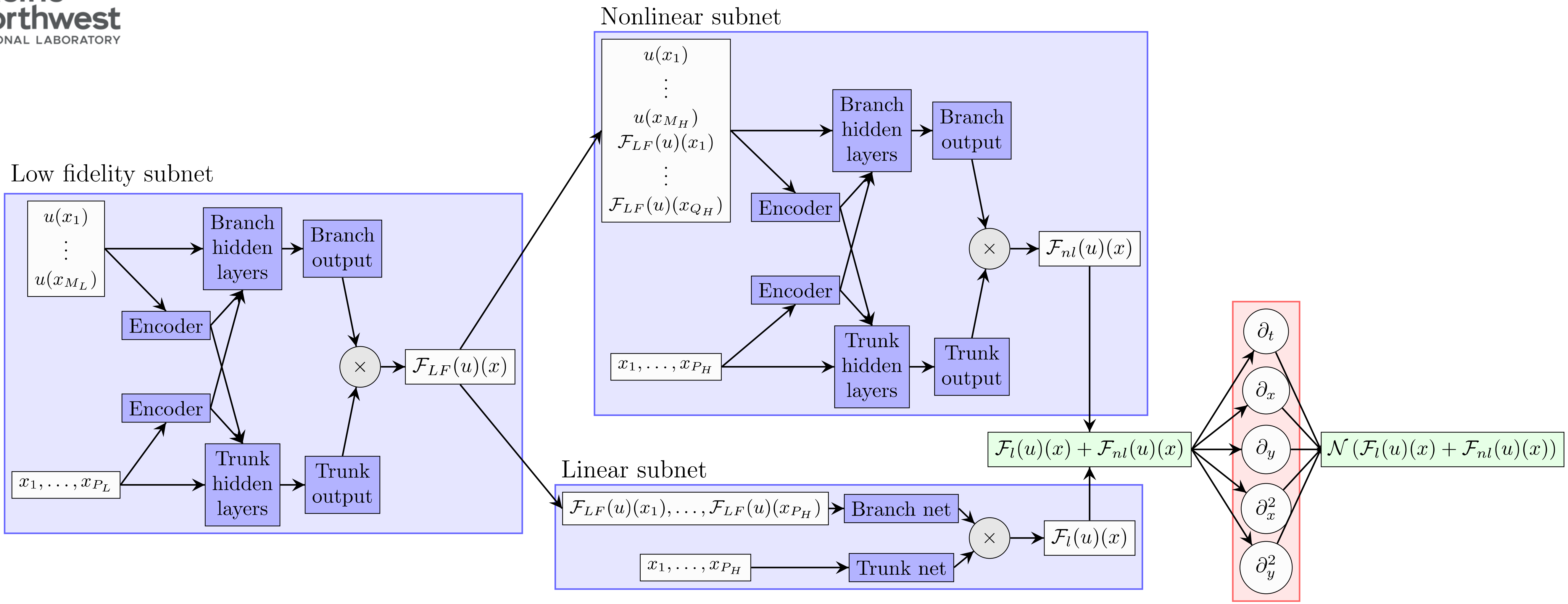
Lu, Lu, et al. "Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators." *Nature machine intelligence* 3.3 (2021): 218-229.
Wang, Sifan, Hanwen Wang, and Paris Perdikaris. "Learning the solution operator of parametric partial differential equations with physics-informed DeepONets." *Science advances* 7.40 (2021): eabi8605.

Multifidelity

- Allows the use of one or more dataset and physics to enhance training
- Specific structure allows for exploiting correlations between the data



General framework



$$\mathcal{L}(\theta) = \lambda_1 \mathcal{L}_{HF}(\theta_{nl}, \theta_l) + \lambda_2 \mathcal{L}_{LF}(\theta_{LF}) + \lambda_3 \left(\sum w_{nl}^2 + \sum b_{nl}^2 \right) + \lambda_4 \left(\sum w_{LF}^2 + \sum b_{LF}^2 \right)$$
$$+ \lambda_5 \mathcal{L}_{IC}(\theta_{nl}, \theta_l) + \lambda_6\, \mathcal{L}_{BC}(\theta_{nl}, \theta_l) + \lambda_7 \mathcal{L}_{physics}(\theta_{nl}, \theta_l)$$

AAH, et al. "Multifidelity deep operator networks." *Journal of Computational Physics* (2023).

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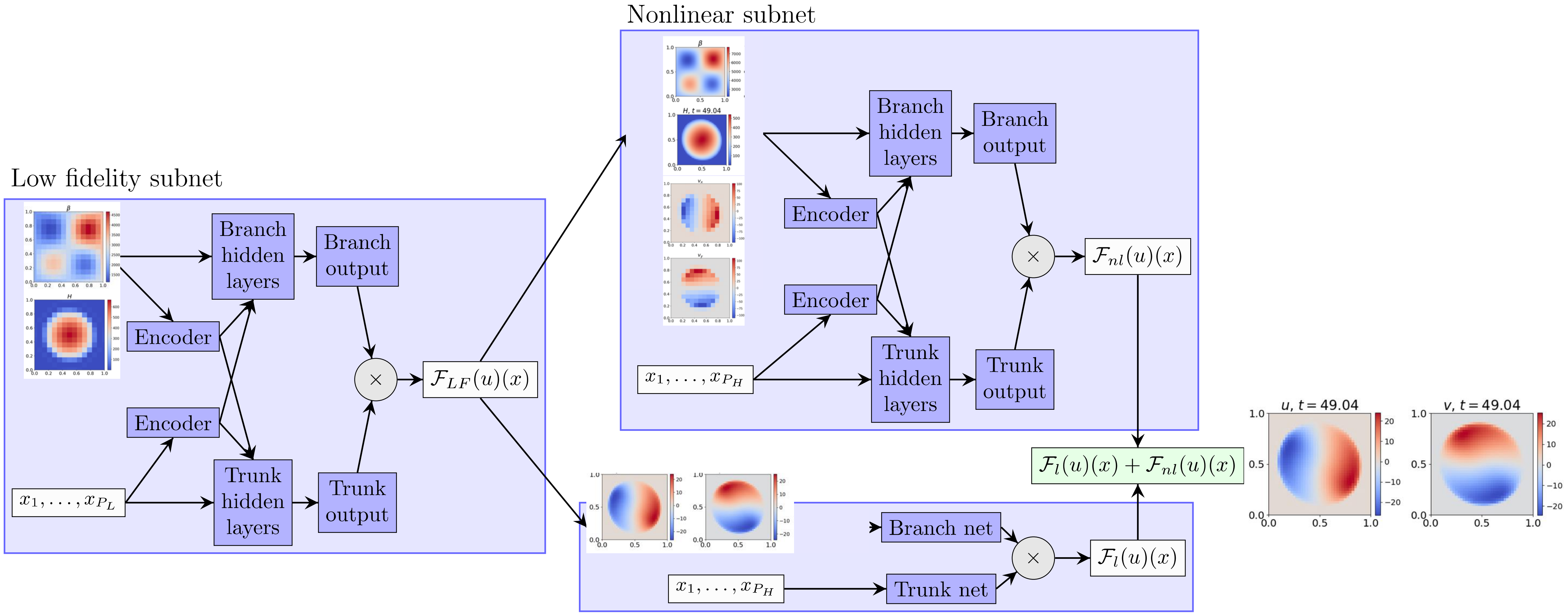

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One-dimensional jump function

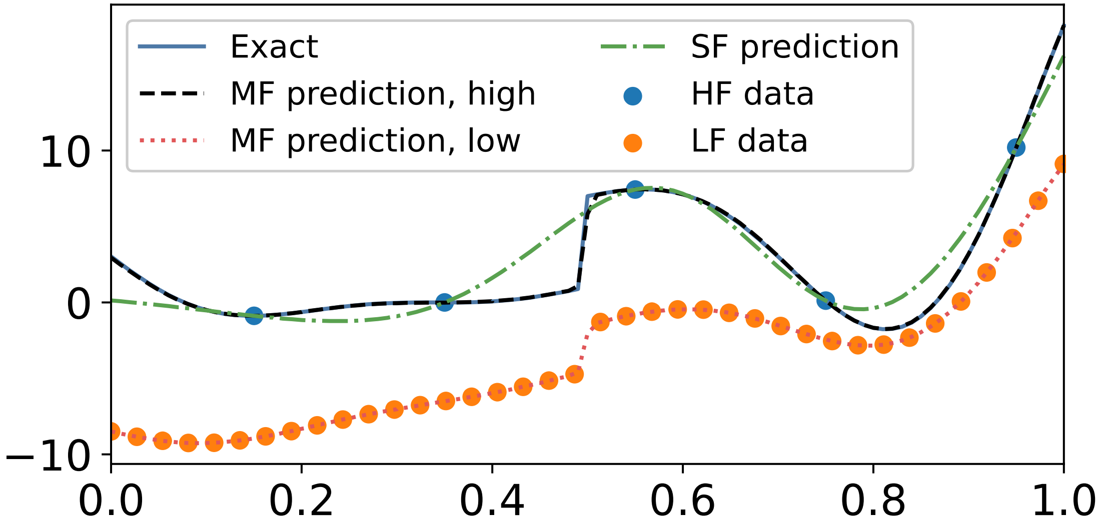
$$y_L(u)(x) = \begin{cases} 0.5(6x-2)^2\sin(u) + 10(x-0.5) - 5 & x \le 0.5 \\ 0.5(6x-2)^2\sin(u) + 10(x-0.5) - 2 & x > 0.5 \end{cases}$$

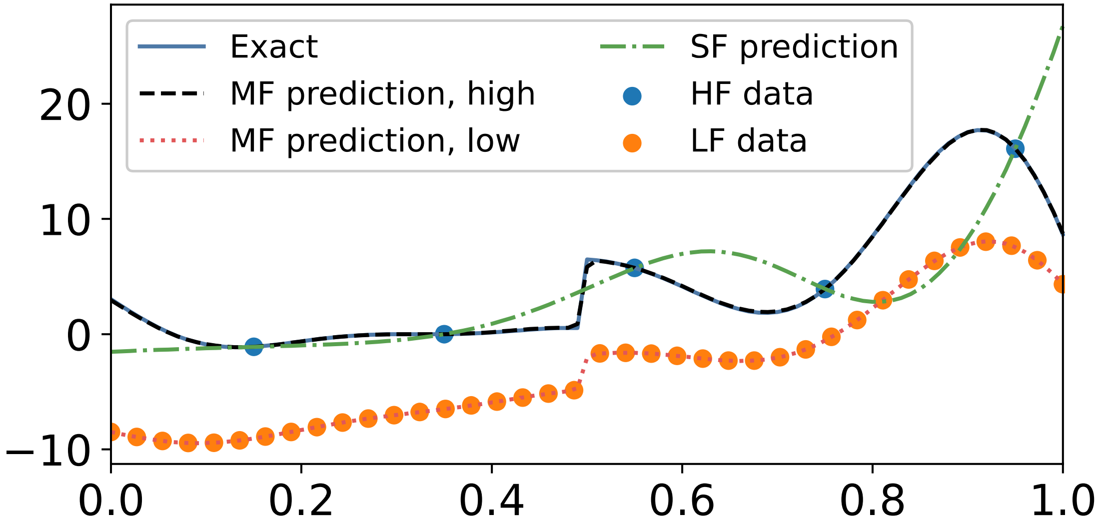
$$y_H(u)(x) = 2y_L(u)(x) - 20x + 20$$

$$u = ax - 4$$

$N_L = 20$
$M_L = \mathrm{P_L} = 38$
$N_H = 10$
$M_H = P_H = 5$

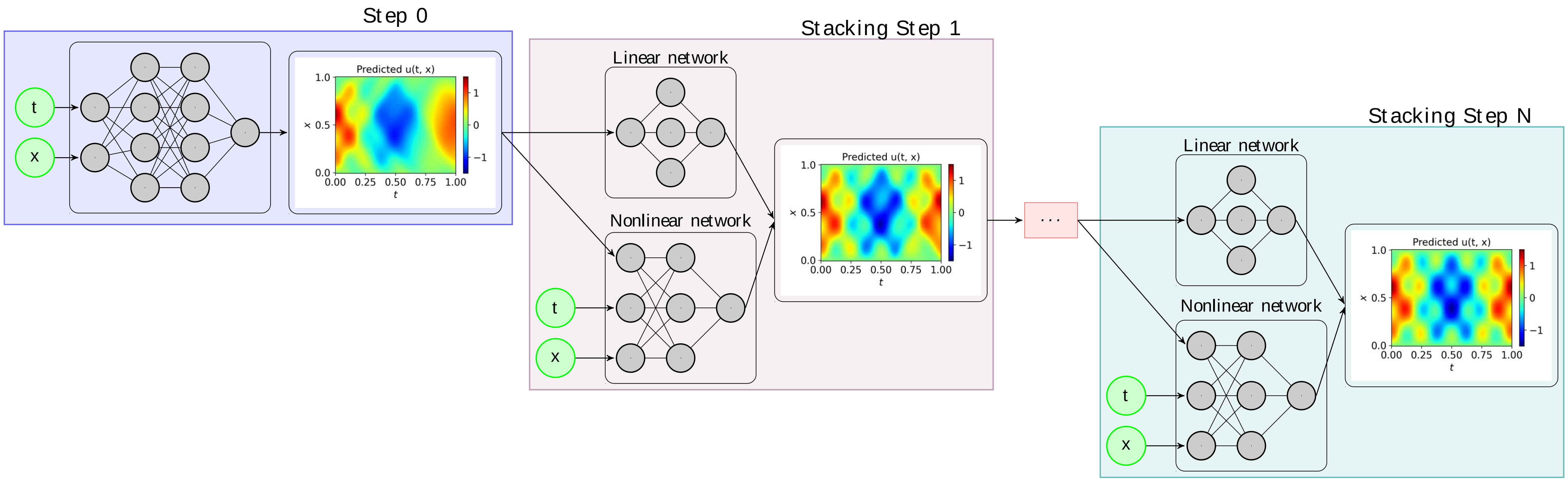
$$\mathcal{F}_l(u)(x) = 1.9479\mathcal{F}_{LF}(u)(x) - 19.1719x + 19.3459 - 0.04870x\mathcal{F}_{LF}(u)(x)$$





Stacking multifidelity networks improves predictions

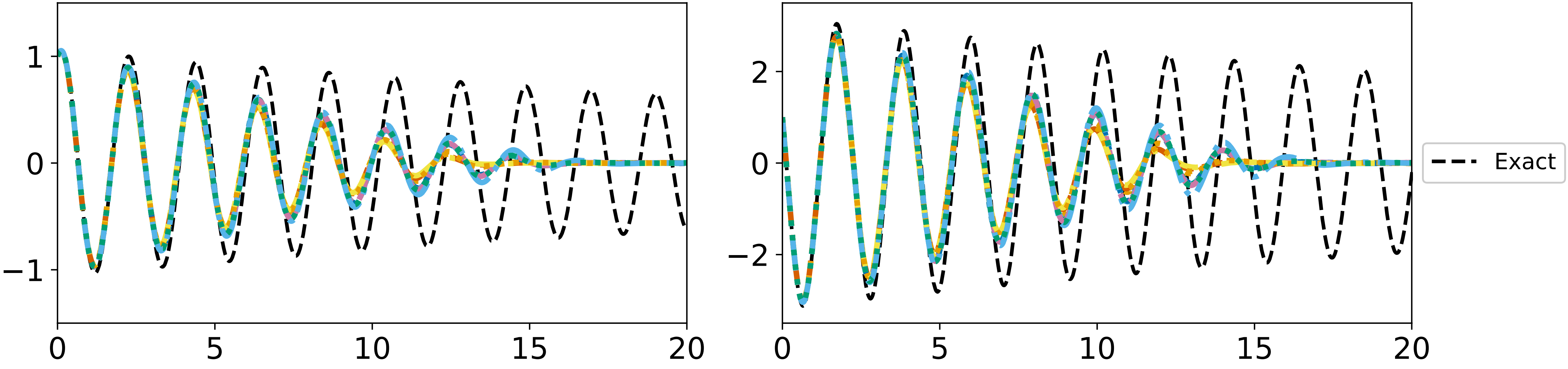
- Train a vanilla PINN/DeepONet
- Continually train MF networks until the desired accuracy is reached



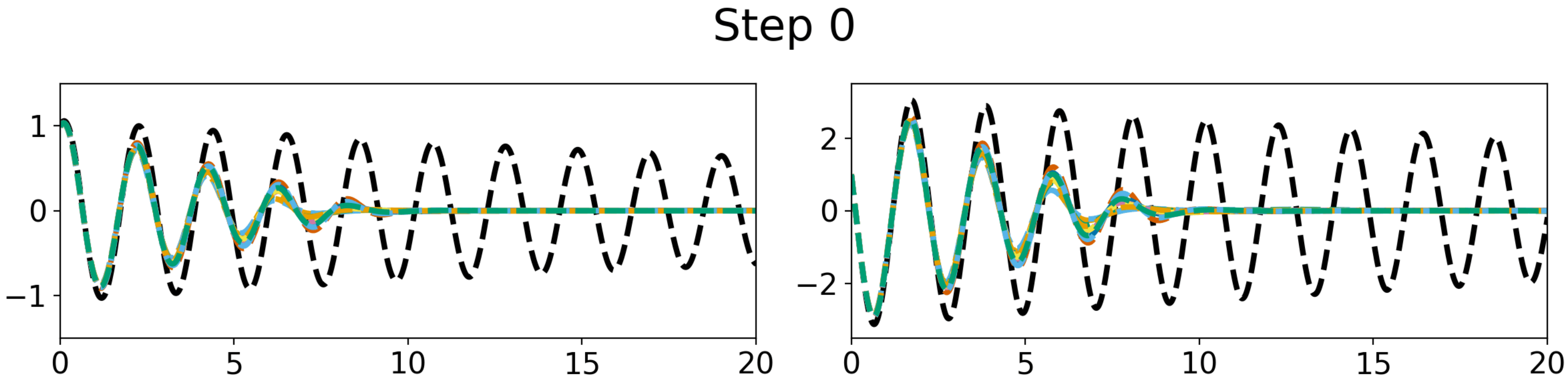
Pendulum

$$\frac{ds_1}{dt} = s_2$$
$$\frac{ds_s}{dt} = -\frac{b}{m}s_2 - \frac{g}{L}\sin(s_1)$$

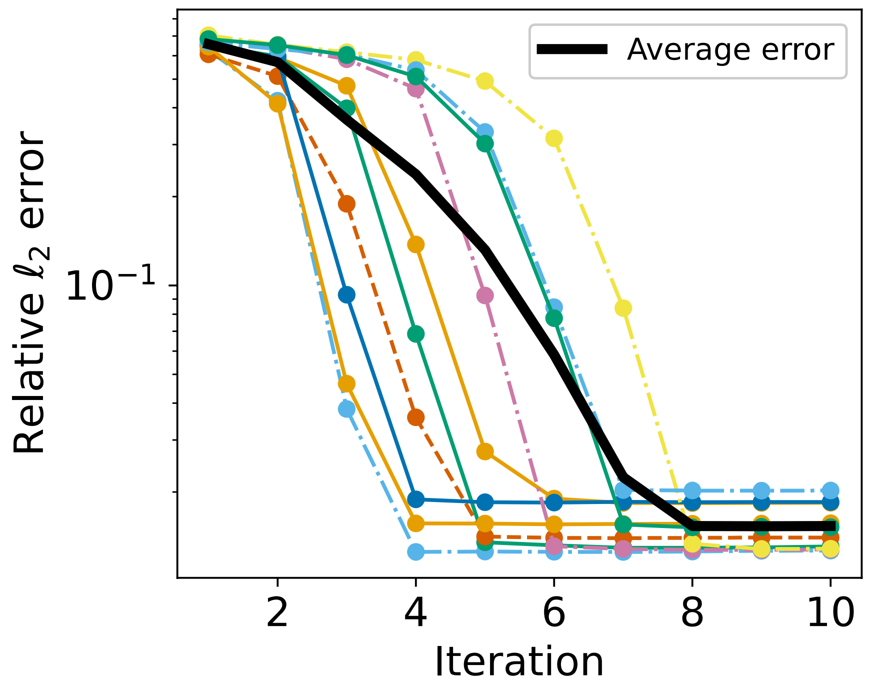
$$s_1(0) = 1$$
$$s_2(0) = 1$$



Pendulum



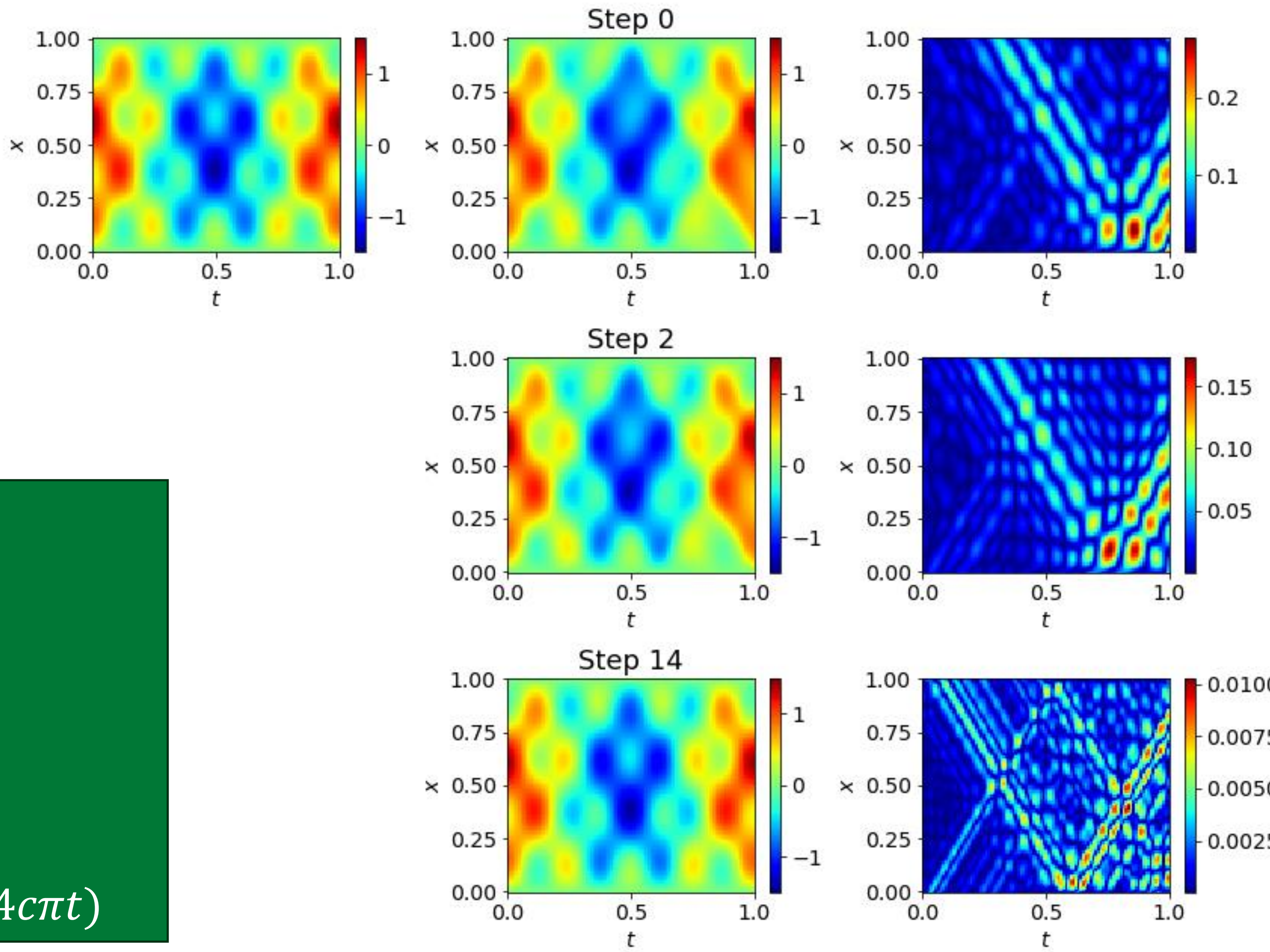
Step 0
1
0
−1
0
5
10
15
20
2
0
−2
0
5
10
15
20



Average error
Relative ℓ_2 error
10^{-1}
2
4
6
8
10
Iteration

Wave equation

$c = 2$



$$s_{tt}(x,t) - c^2 s_{xx}(x,t) = 0$$

$$s(x,0) = \sin(\pi x) + 0.5\sin(4\pi x)$$
$$s_t(x,0) = 0$$
$$s(0,t) = s(1,t) = 0$$

$$s(x,t) = \sin(\pi x)\cos(c\pi t) + 0.5\sin(4\pi x)\cos(4c\pi t)$$

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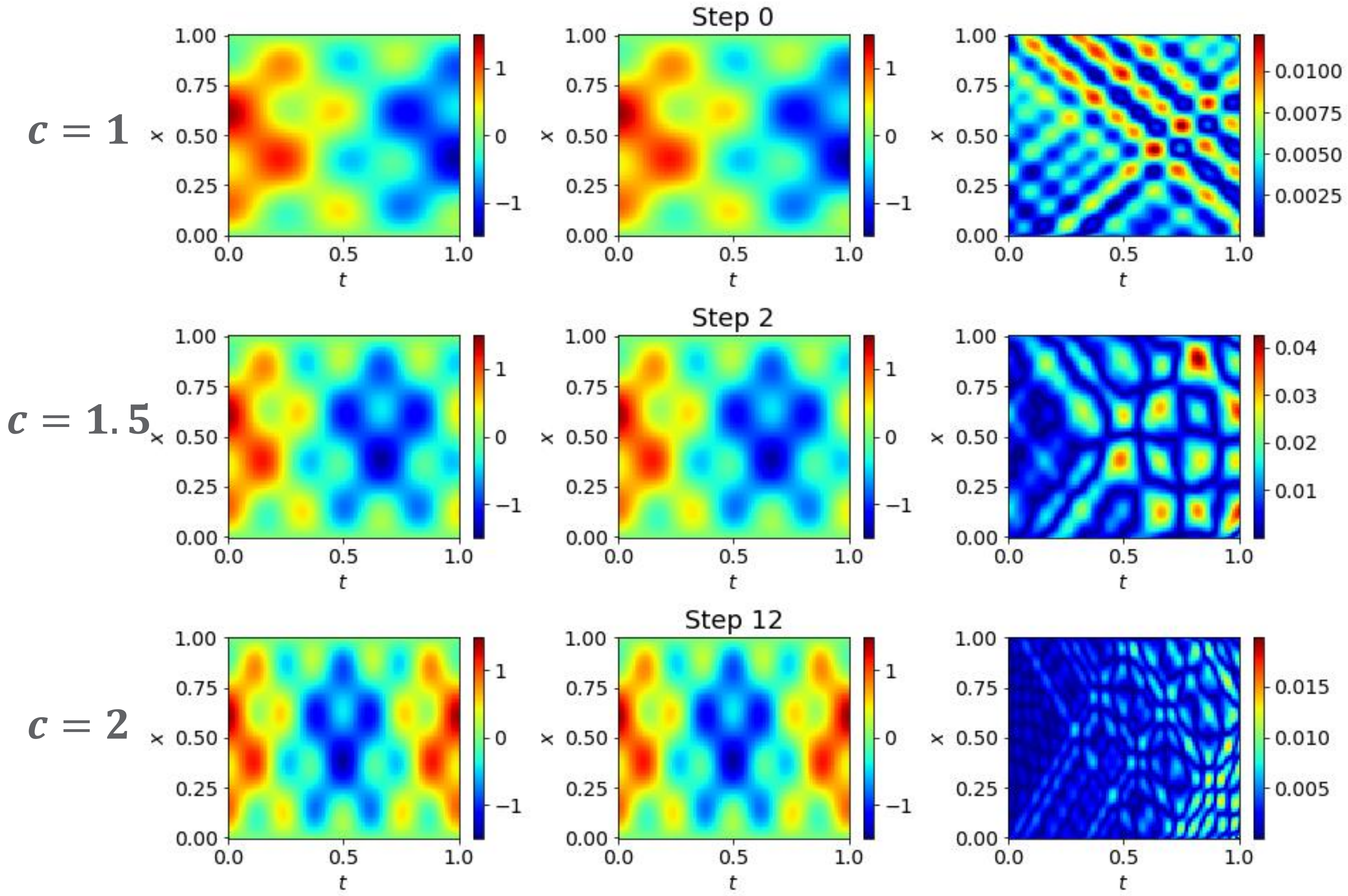
Wave equation



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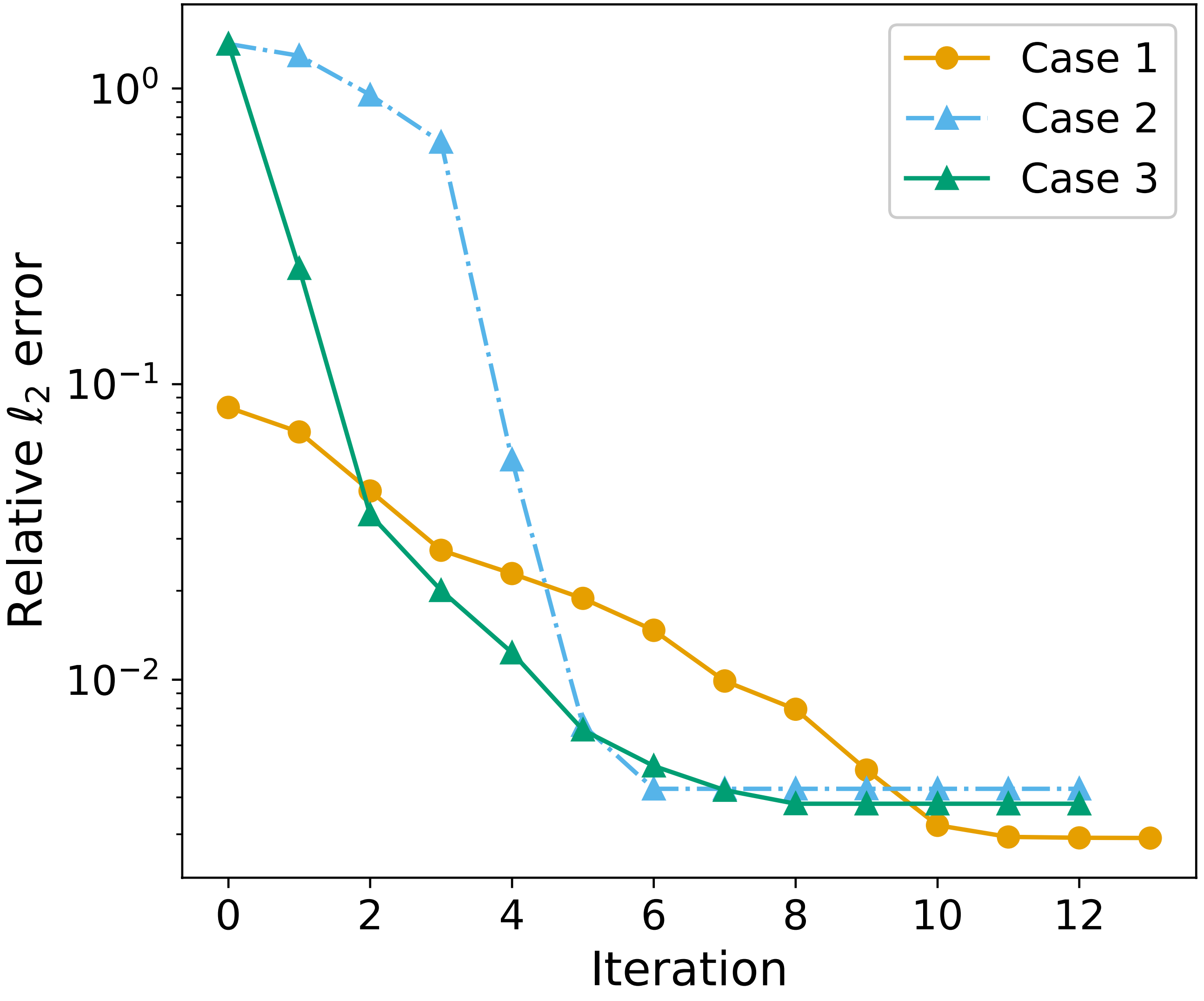
Wave equation

Case 1: $c = 2$
Case 2: $c = [1, 1.25, 1.5, 1.75, 2, 2 \ldots]$
Case 3: $c = [1, 2, 2 \ldots]$



$$s_{tt}(x,t) - c^2 s_{xx}(x,t) = 0$$

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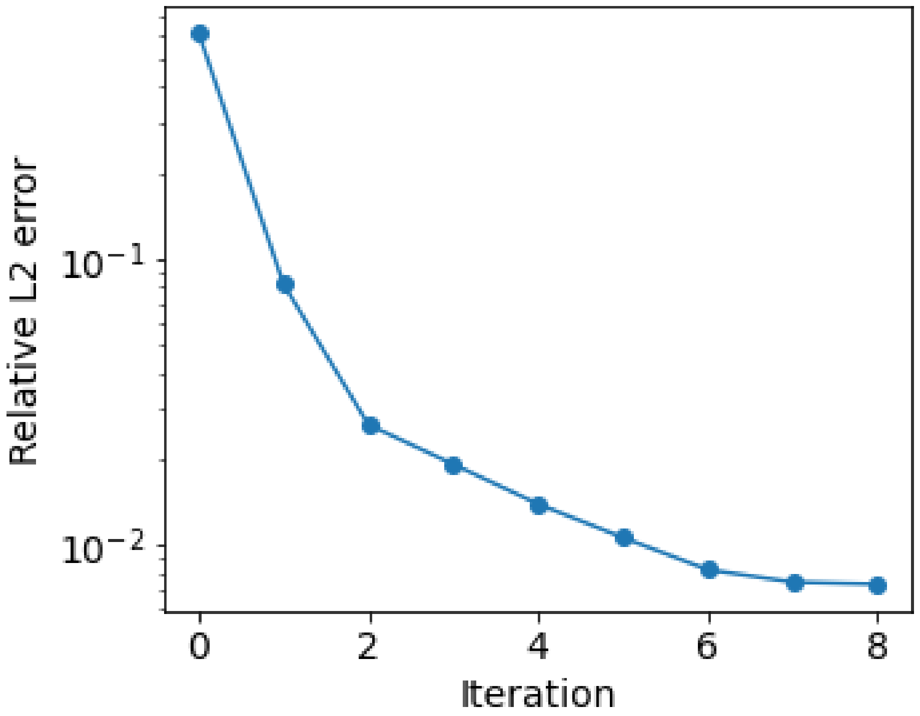
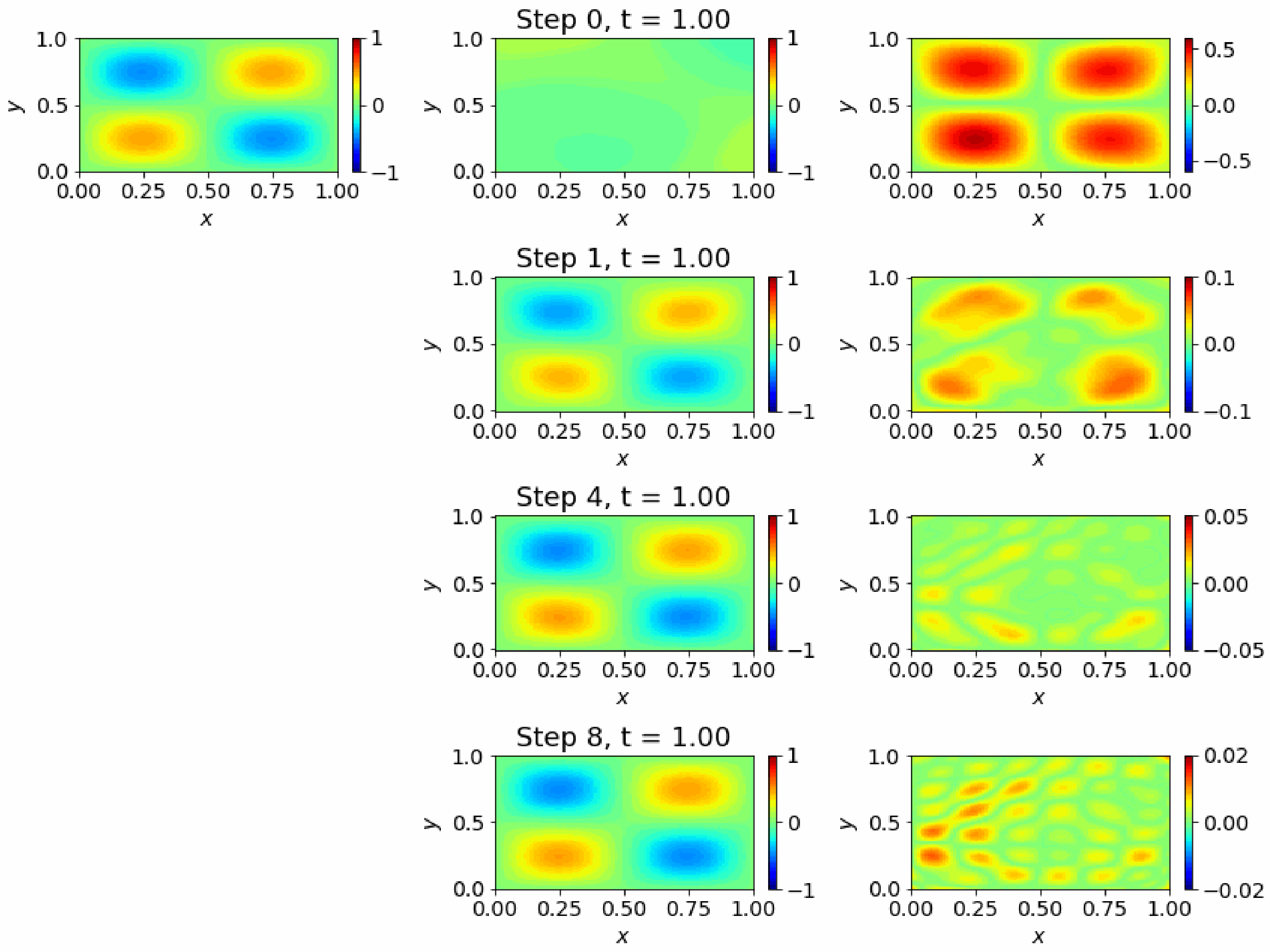
$$s_t(x,0) = 0$$
$$s(0,t) = s(1,t) = 0$$

Wave equation, 2d

$$s_{tt}(x,y,t) - c^2 s_{xx}(x,t) - c^2 s_{yy}(x,y,t) = 0$$

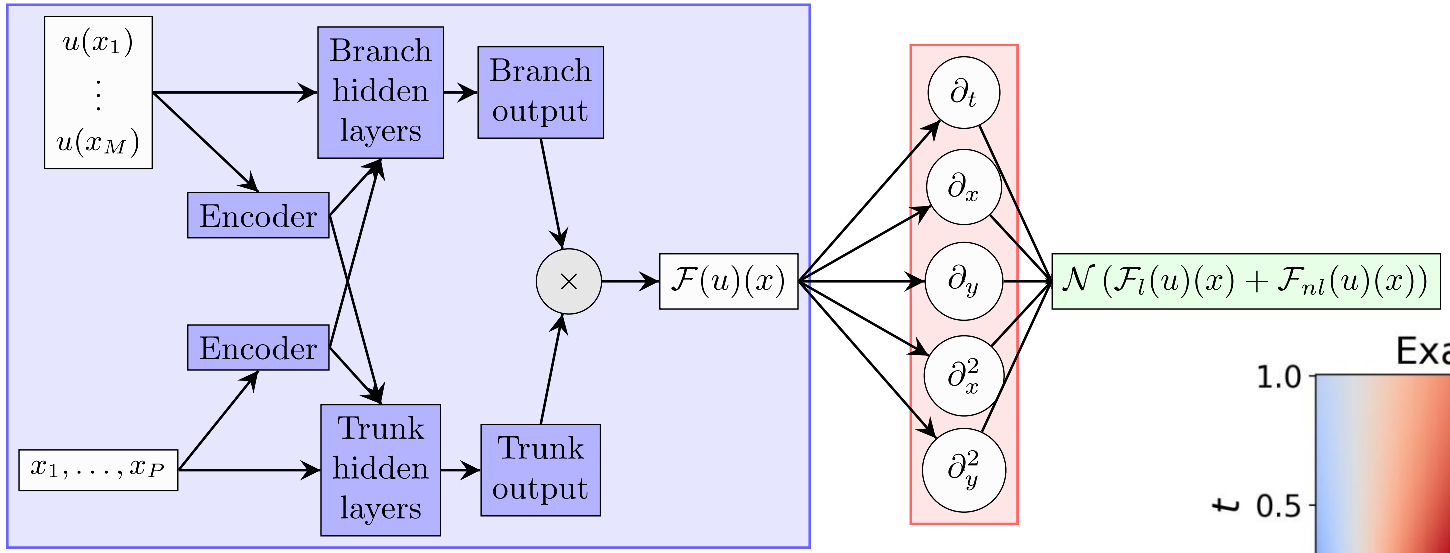
$$s(x,y,0) = \sin(\pi x)\sin(\pi y)$$
$$s_t(x,y,0) = 0$$
$$s(0,y,t) = s(1,y,t) = 0$$
$$s(x,0,t) = s(x,1,t) = 0$$

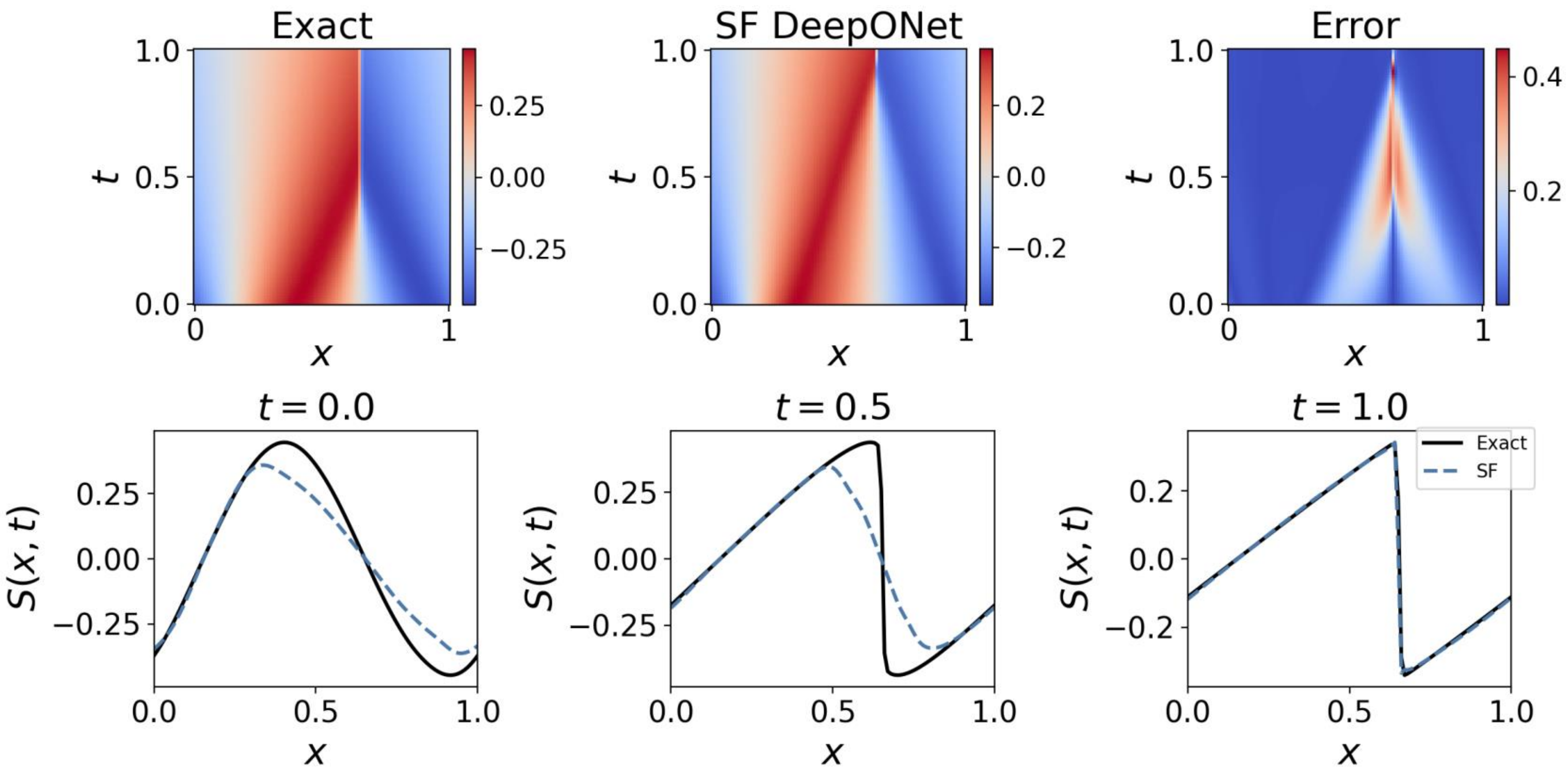




Stacking DeepONets

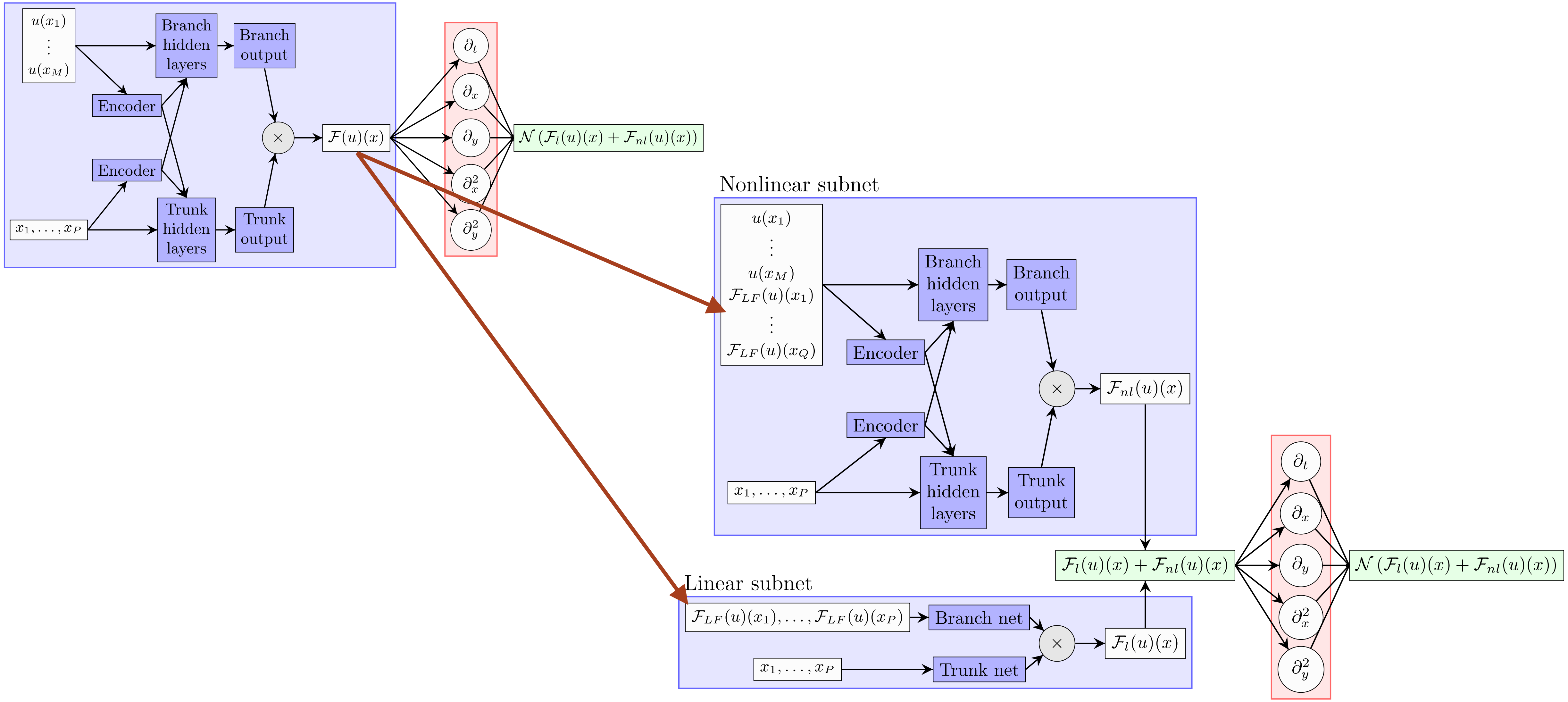
1) Train a single fidelity physics-informed DeepONet





Stacking DeepONets

2) Train a non-composite multifidelity physics-informed DeepONet



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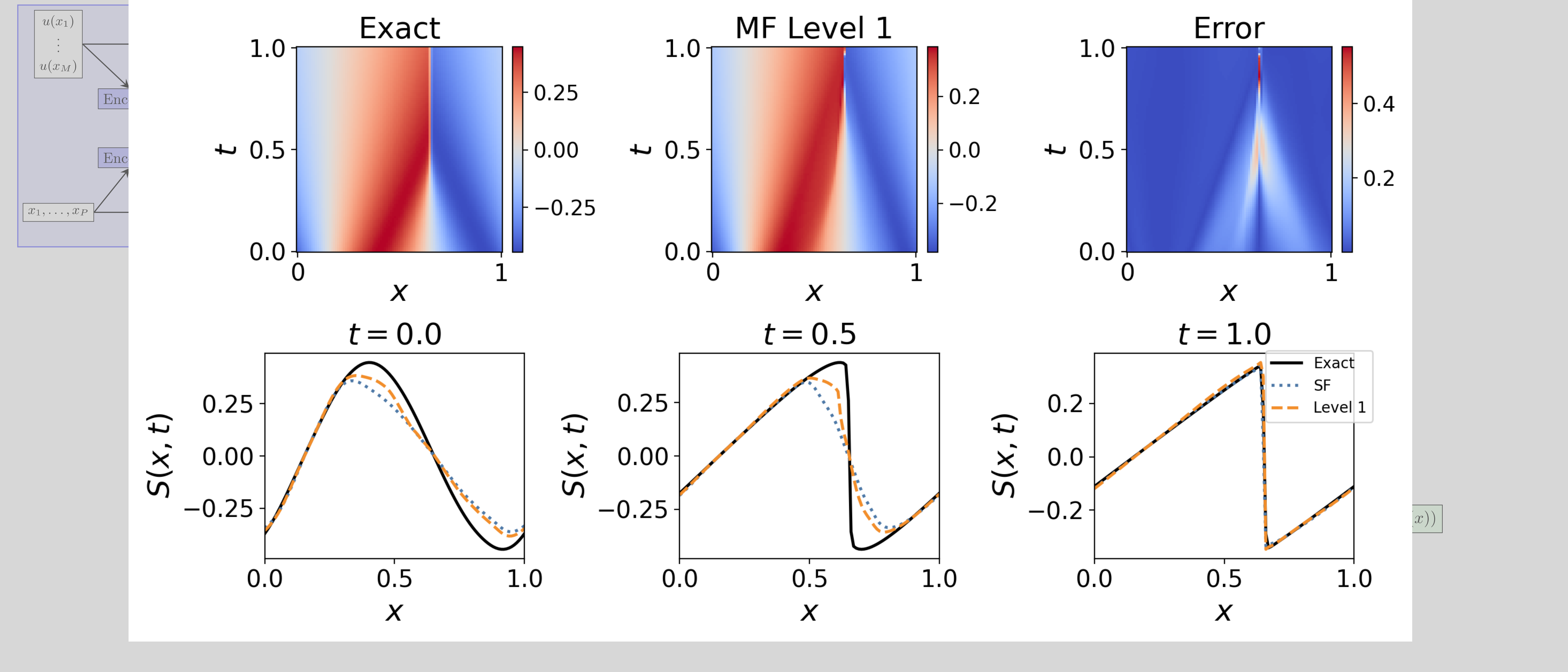
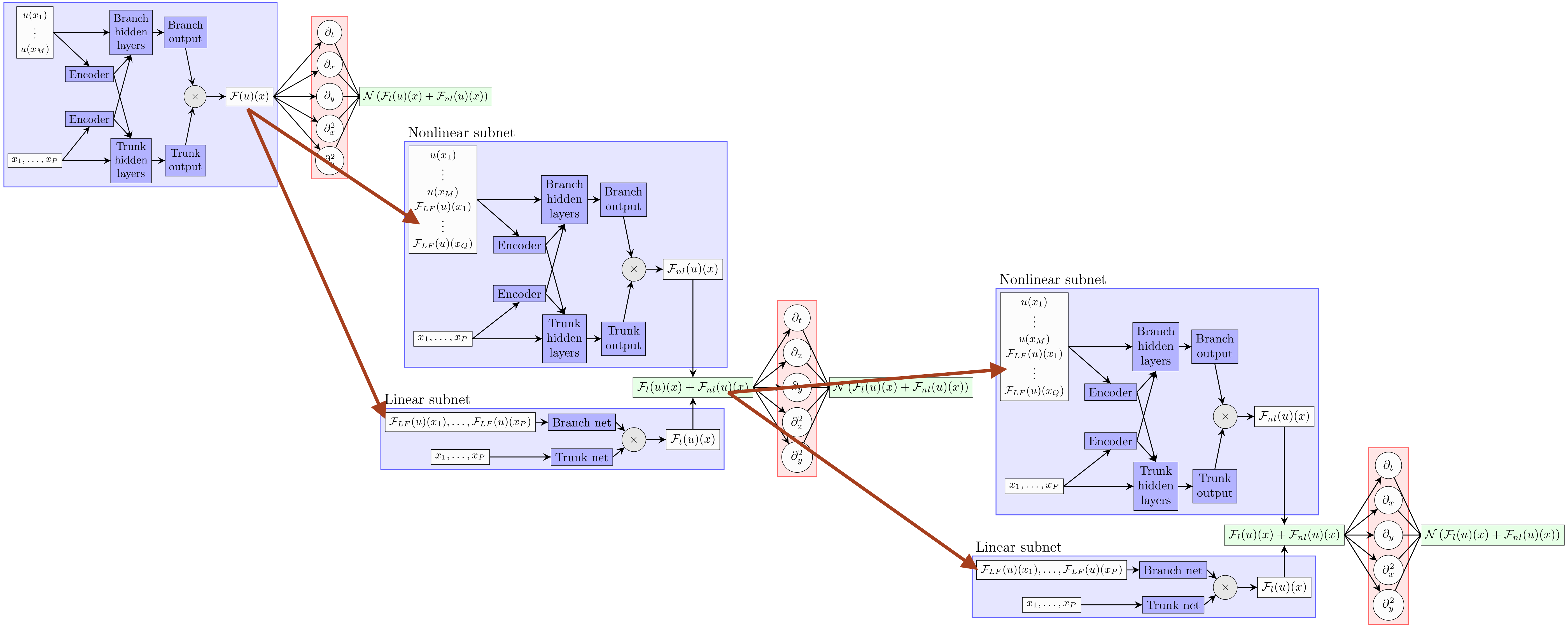


Stacking DeepONets

3) Train another non-composite multifidelity physics-informed DeepONet



Stacking DeepONets

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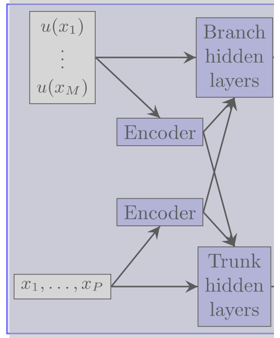
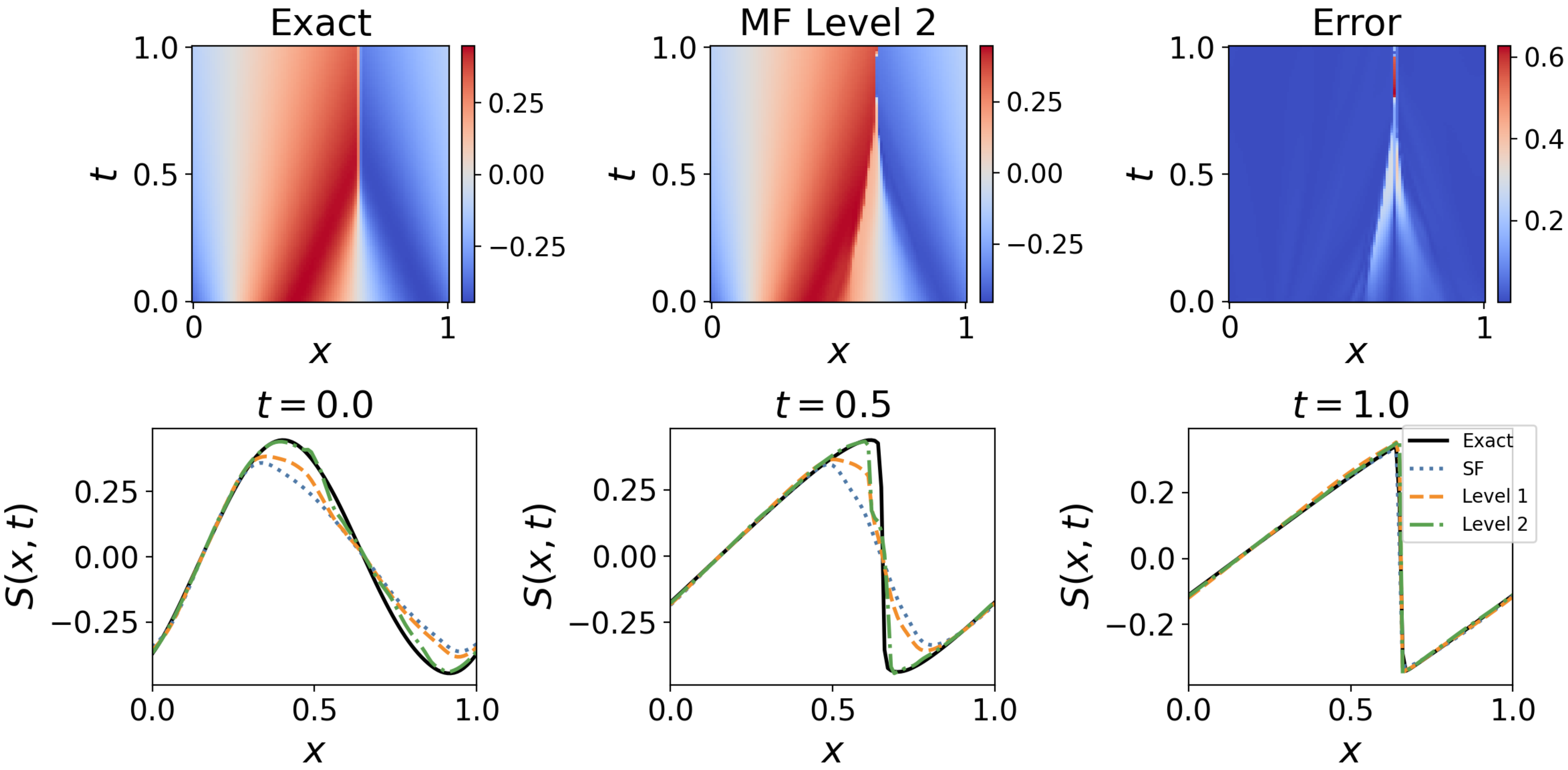
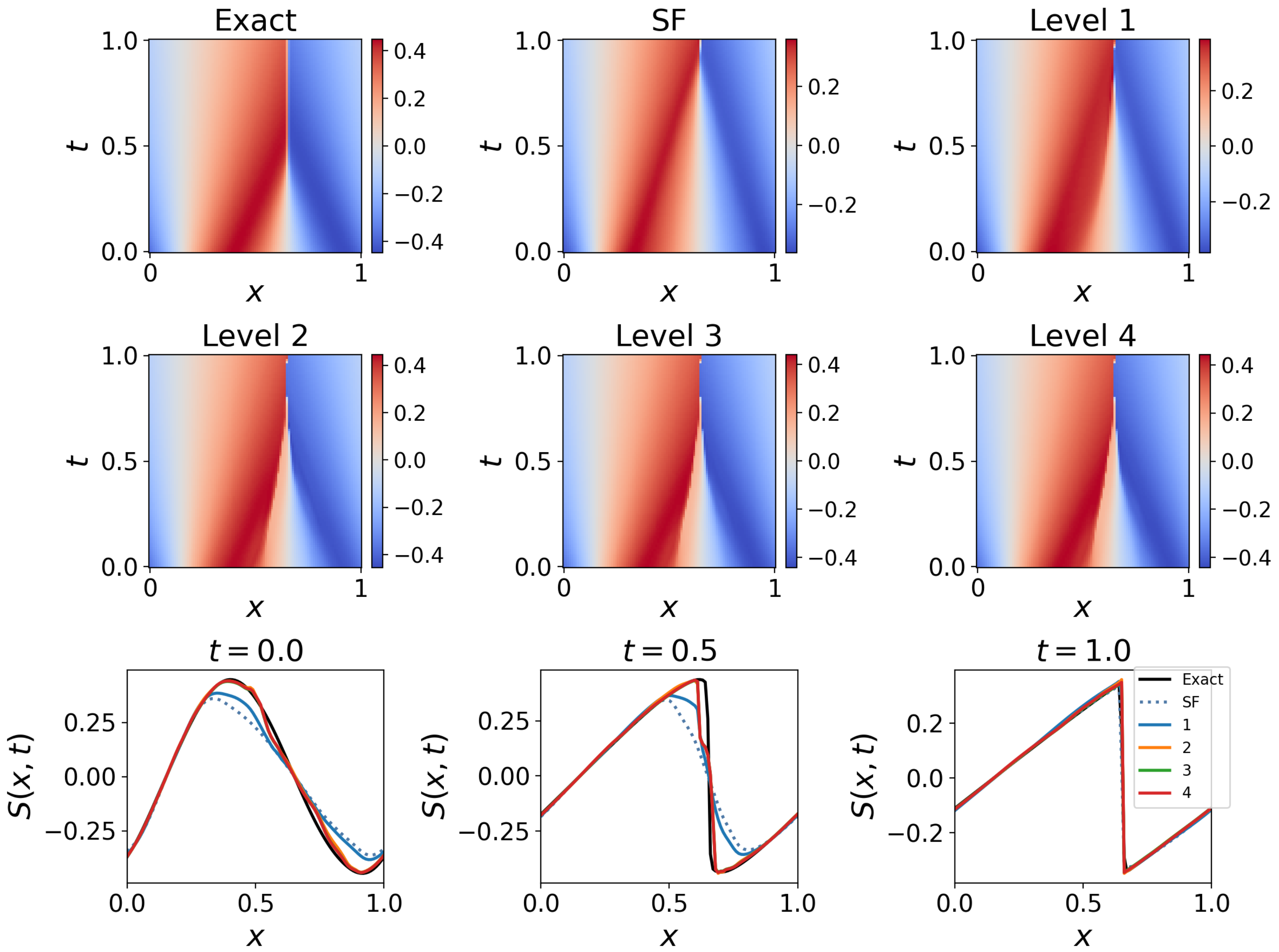
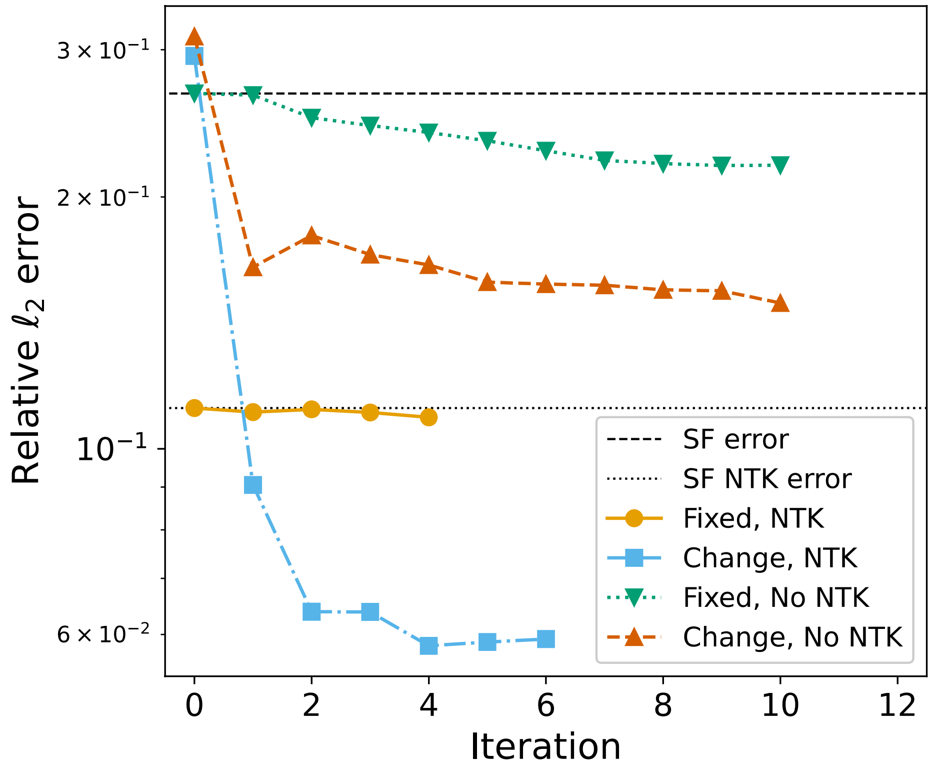


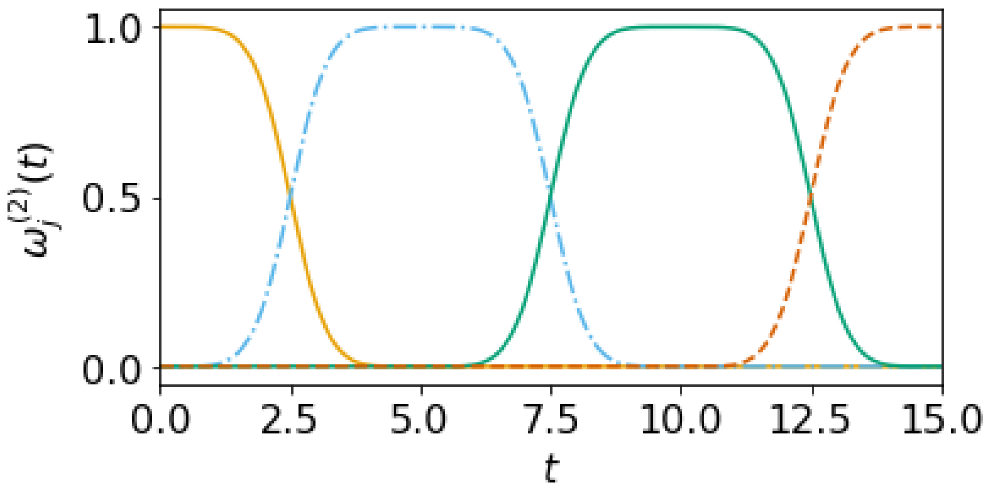


Stacking DeepONet





Finite basis PINNs



- Finite basis PINNs elegantly allow for domain decomposition through a weighted sum using partition of unity functions

$$u^{(l)}(x,\theta^{(l)}) = \sum_{j=1}^{J^{(l)}} \omega_j^{(l)} u_{j,MF}^{(l)}(x,\theta_j^{(l)},u^{(l-1)})$$

$$u_{j,MF}^{(l)}\left(x,\theta_j^{(l)}\right) = (1-|\alpha|)\,u_{j,linear}^{(l)}\left(x,\theta_j^{(l)}\right) + |\alpha|\,u_{j,nonlinear}^{(l)}\left(x,\theta_j^{(l)}\right)$$

Finite basis PINNs

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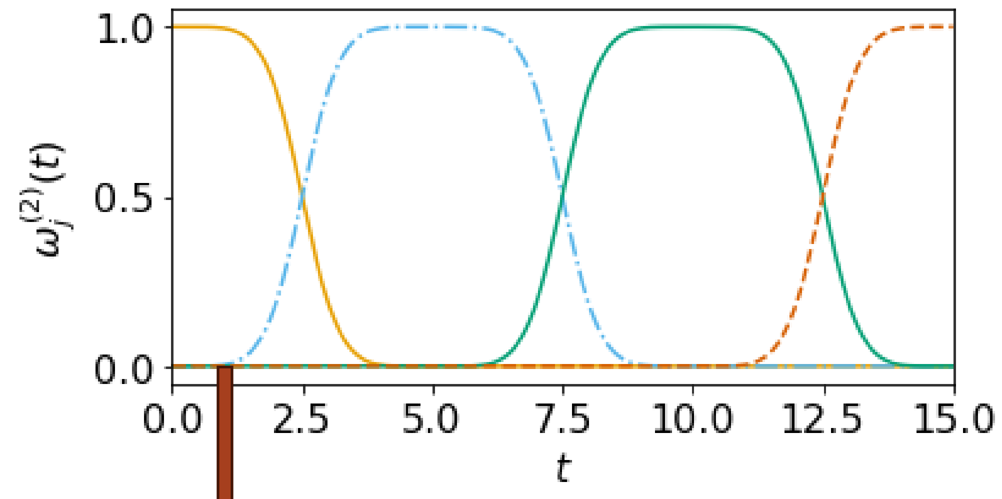

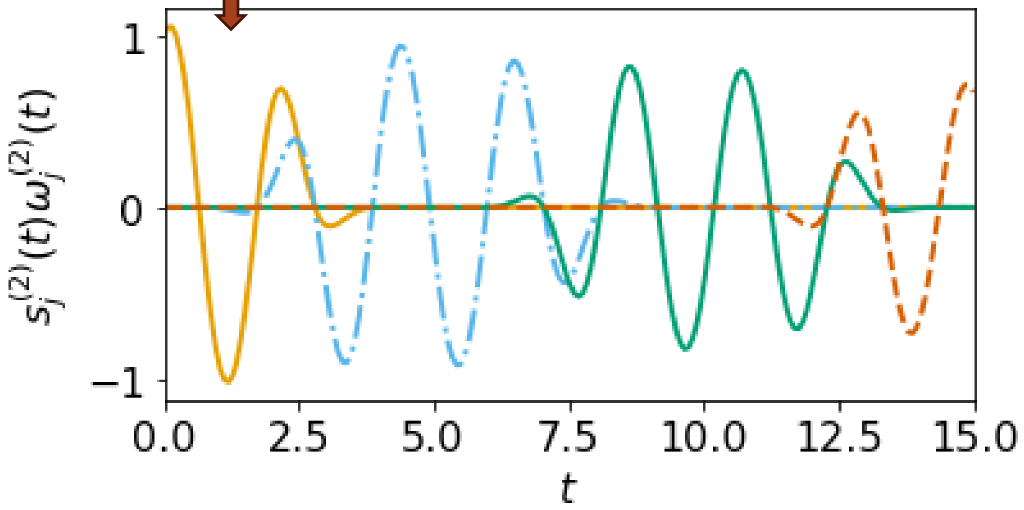

Finite basis PINNs

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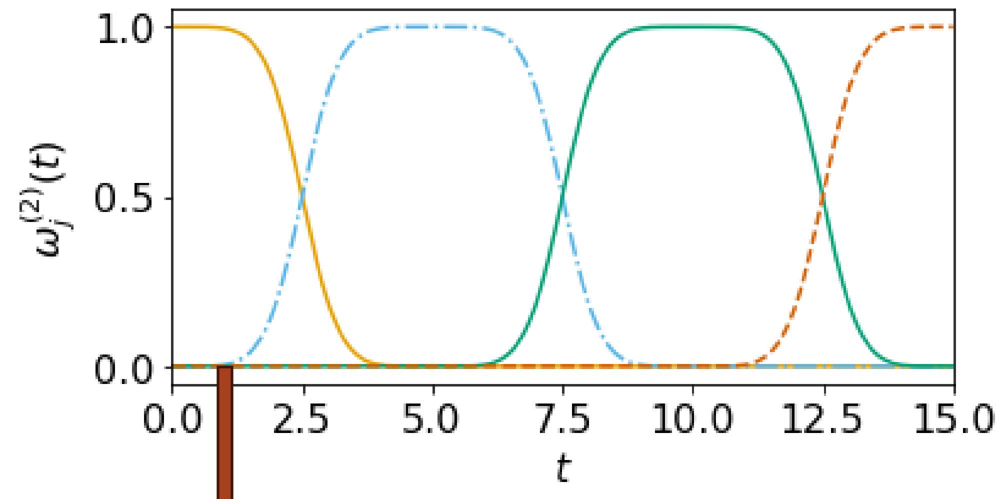
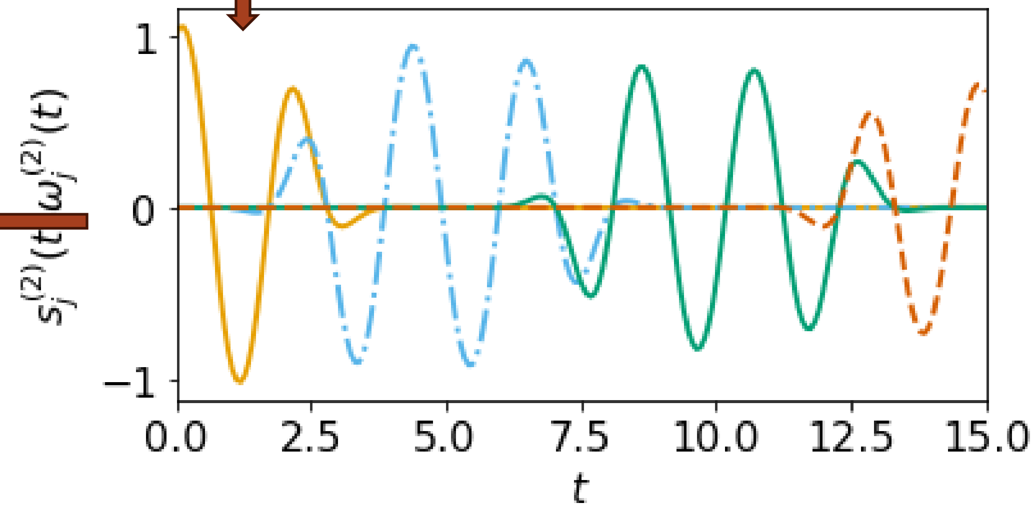
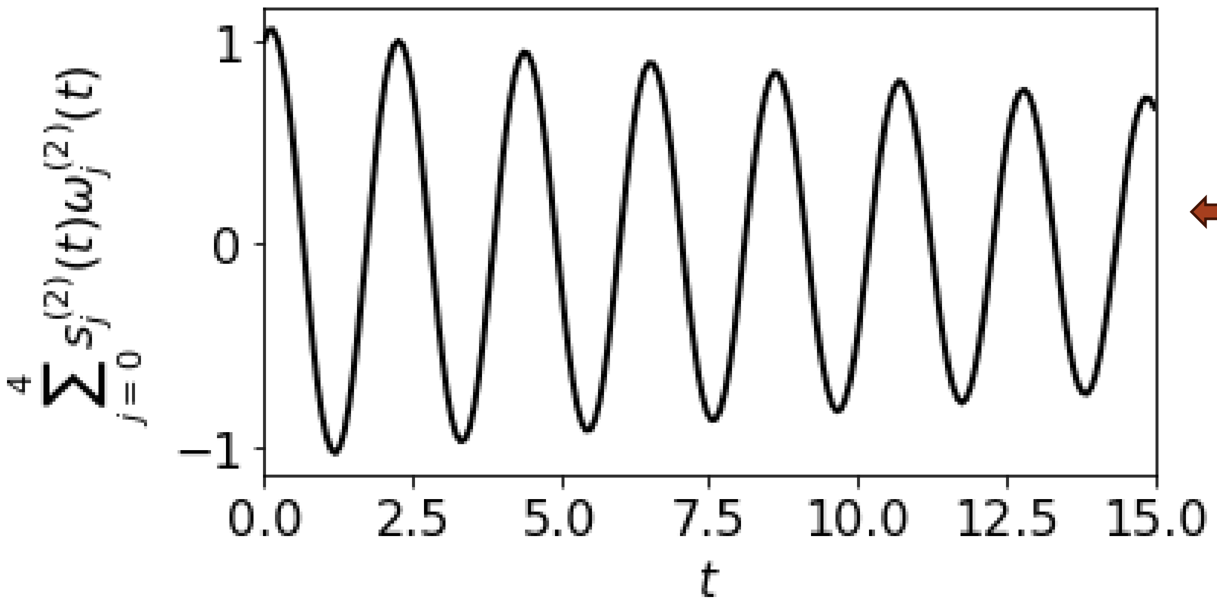
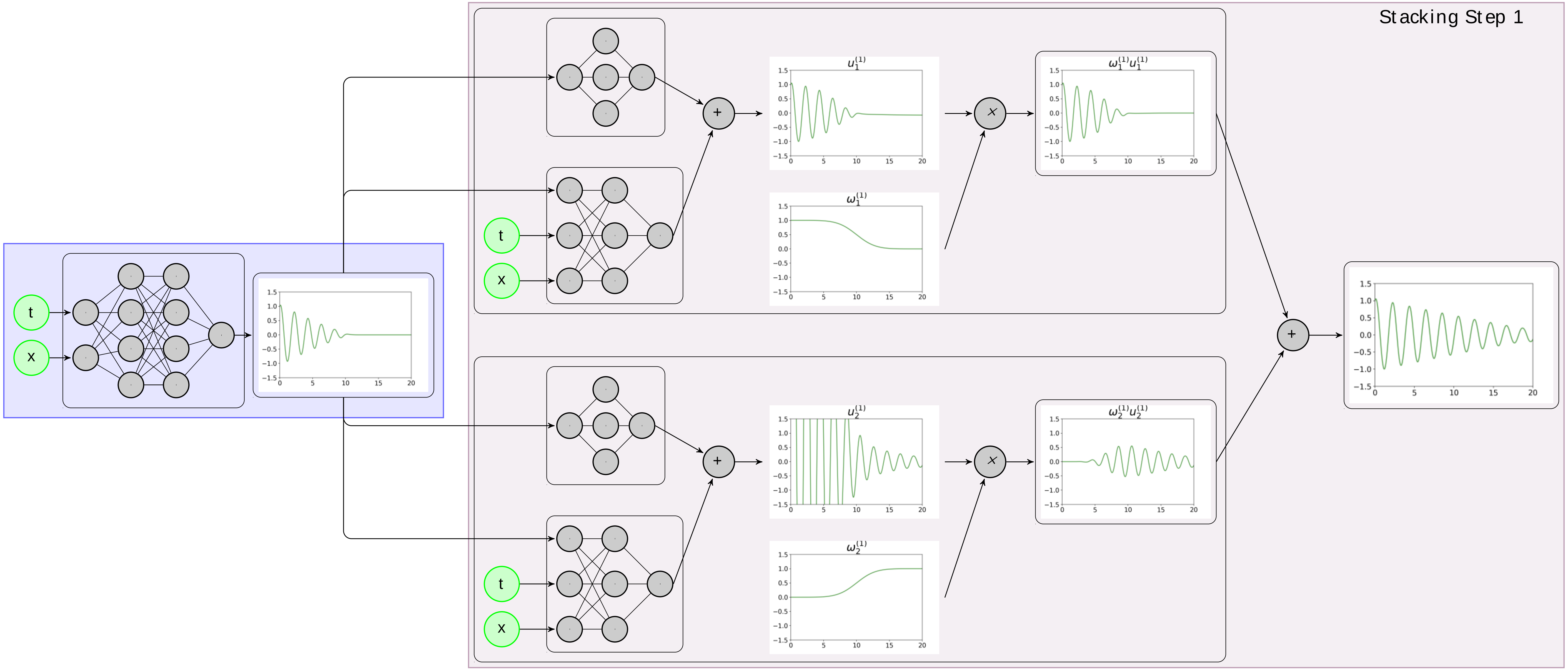


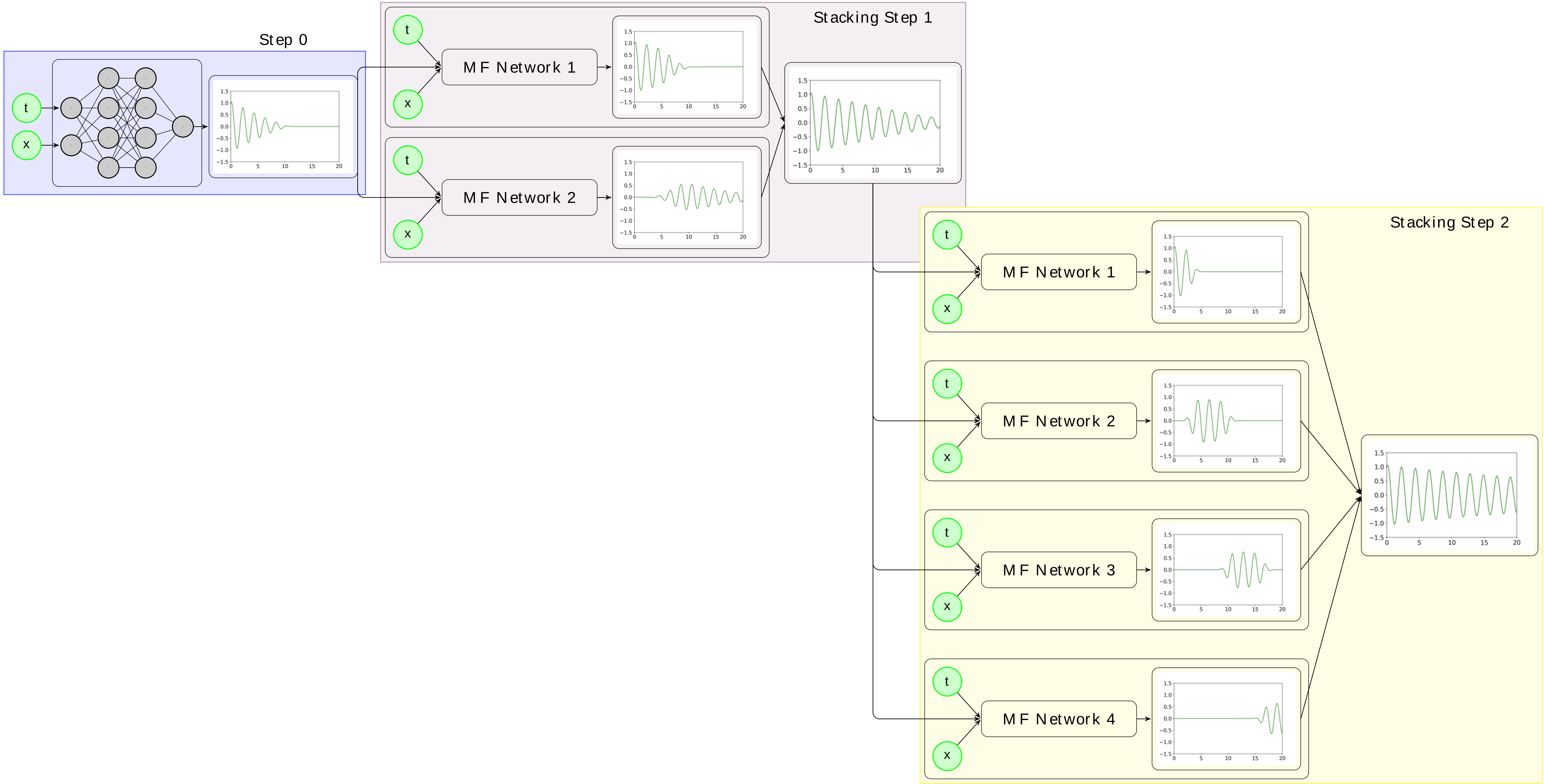




Stacking FBPINNs



Stacking FBPINNs



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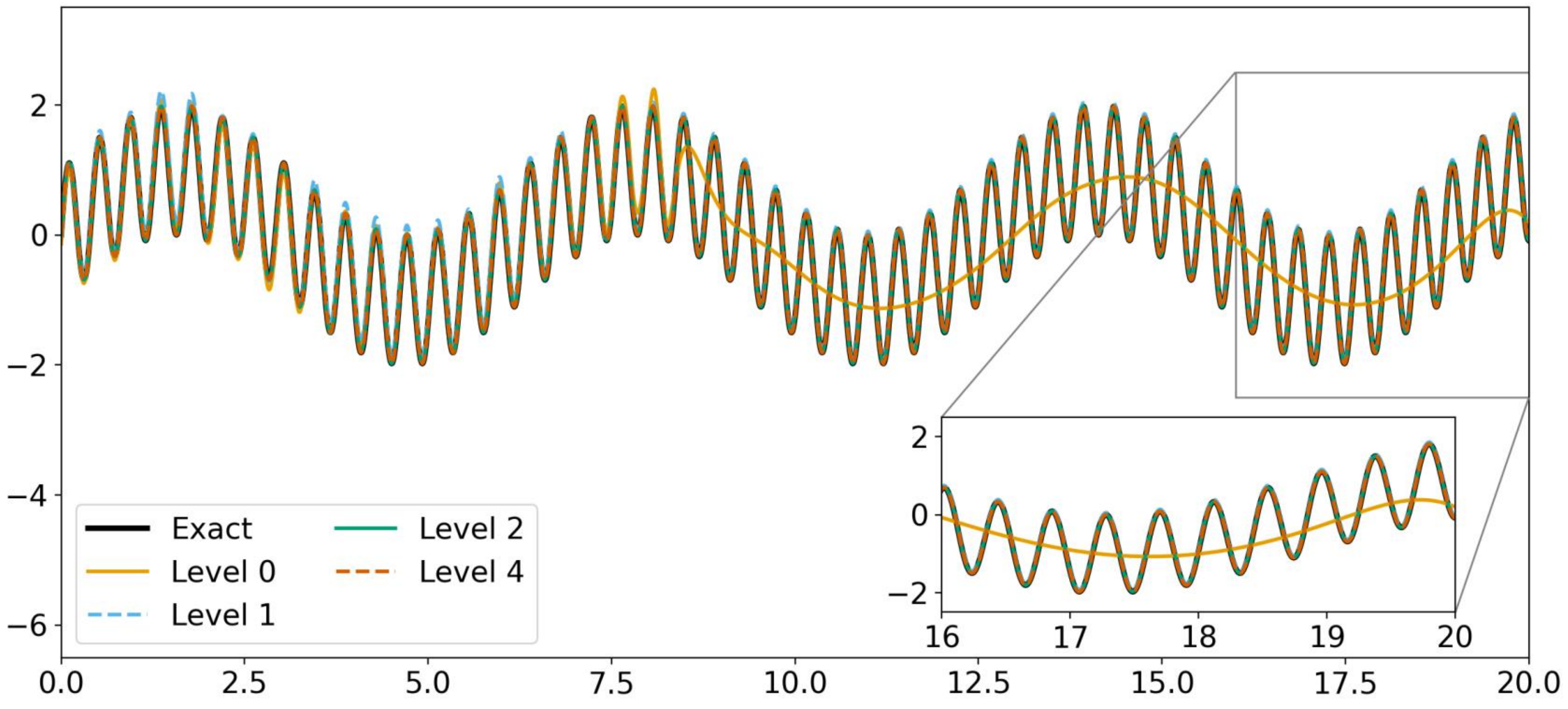
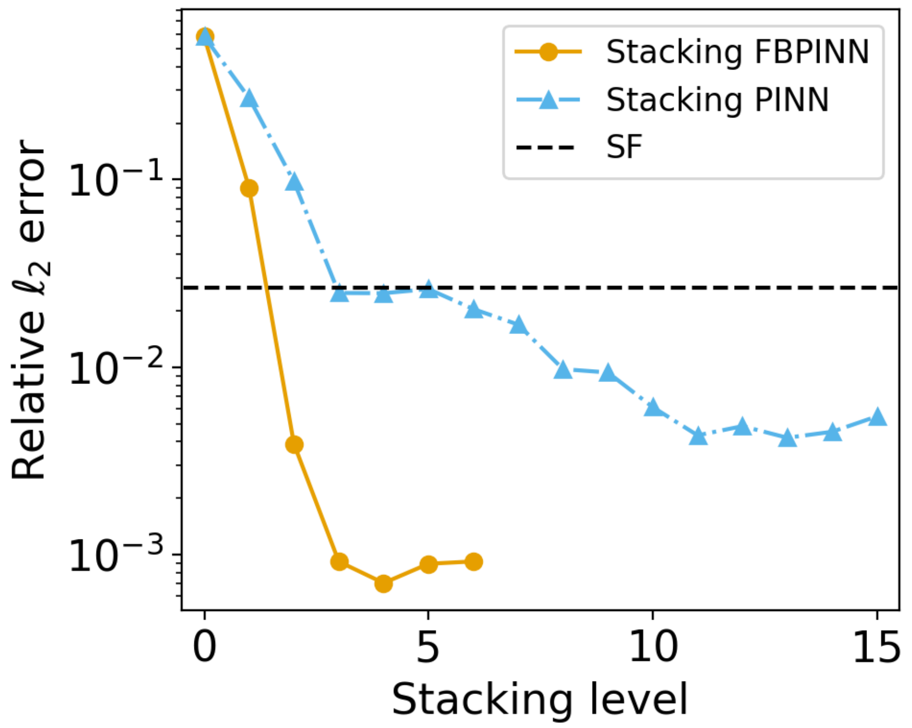
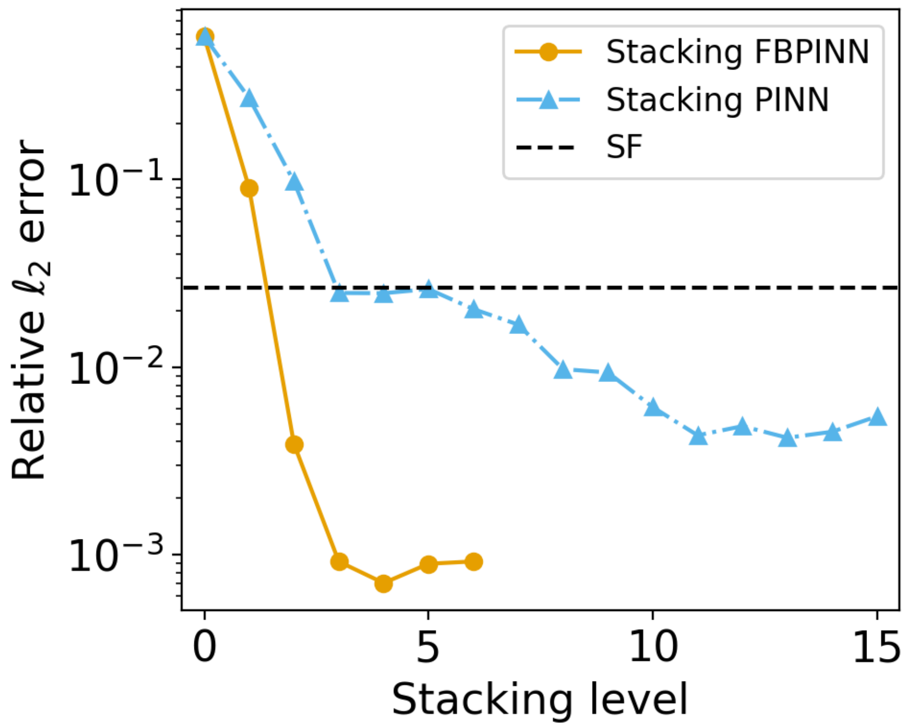
Multiscale



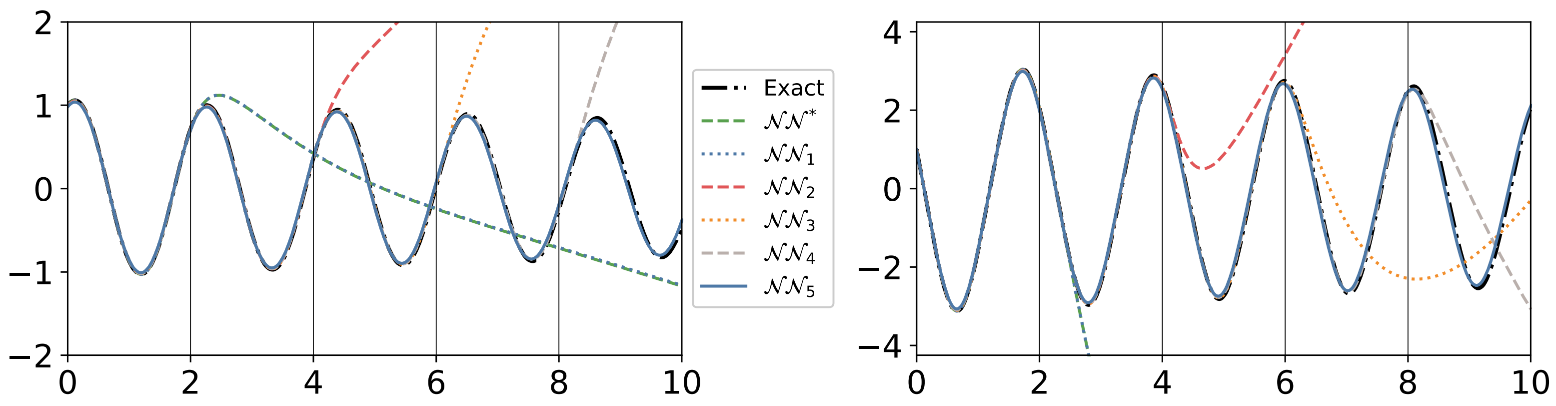


Multiscale

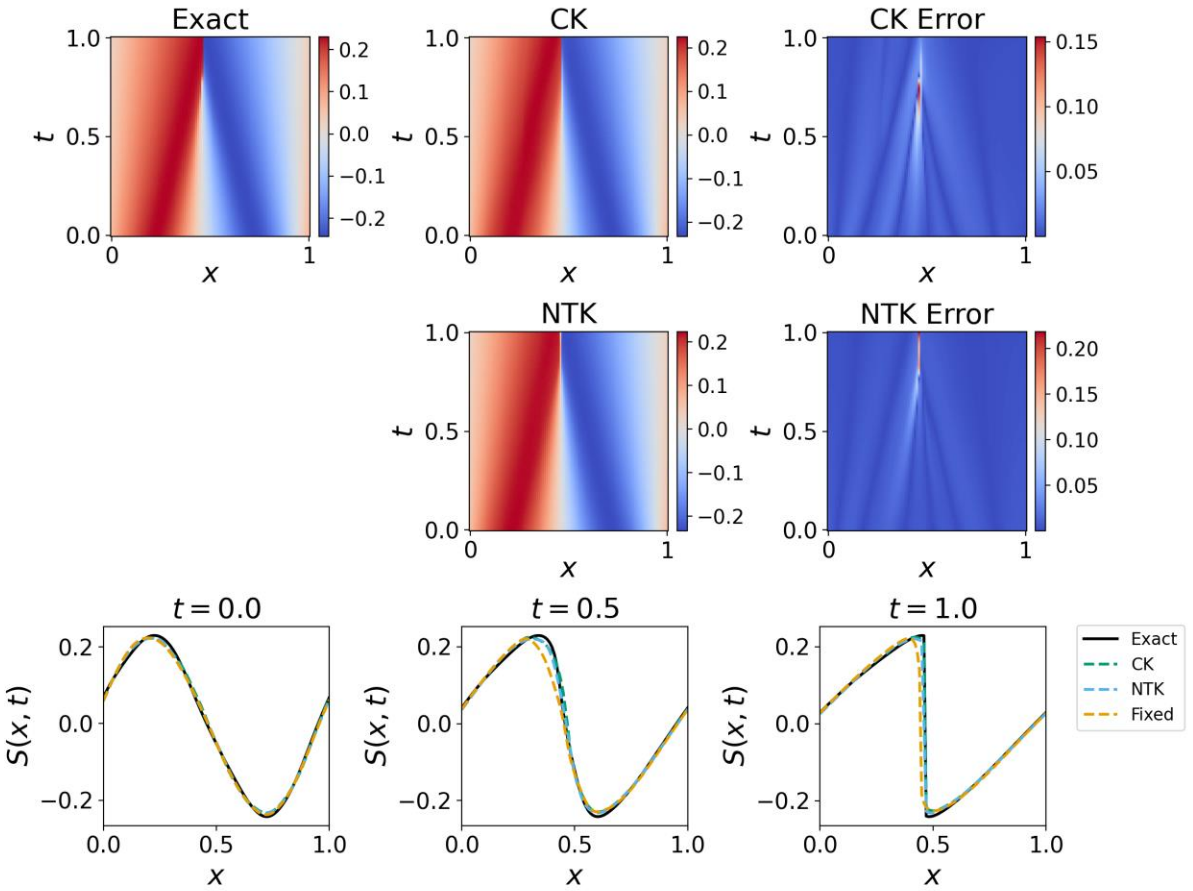
Method	Network size	Parameters	Error
PINN	4x64	12673	0.6543
PINN	5x64	16833	0.0265
Stacking PINN	4x16, 1x5, 3 levels	4900	0.0249
Stacking PINN	4x16, 1x5, 10 levels	11179	0.0061
Stacking FBPINN	**4x16, 1x5, 2 levels**	**7822**	**0.00415**
Stacking FBPINN	4x16, 1x5, 5 levels	59902	0.00083



Multifidelity methods can improve training of physics- and data-informed networks

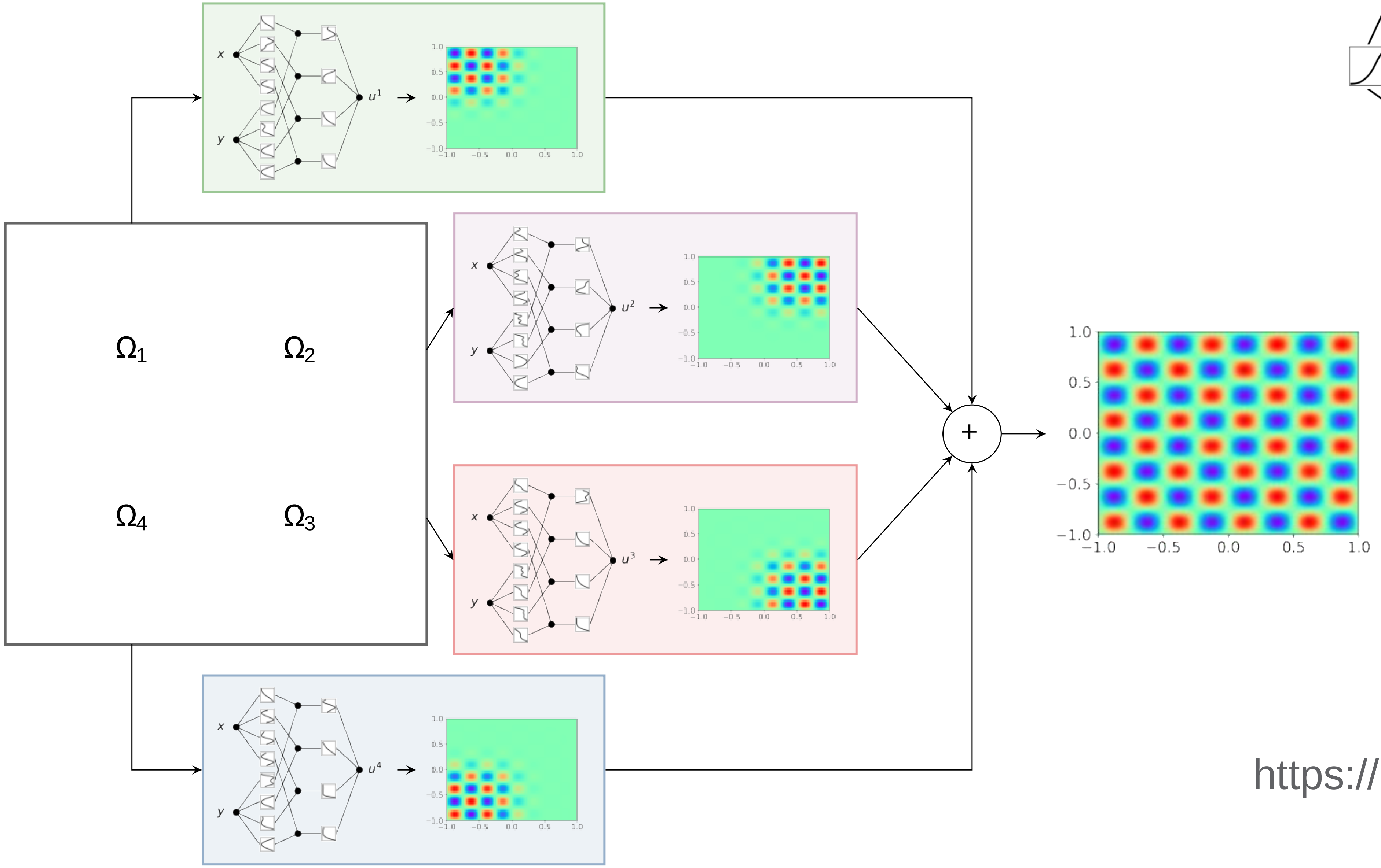


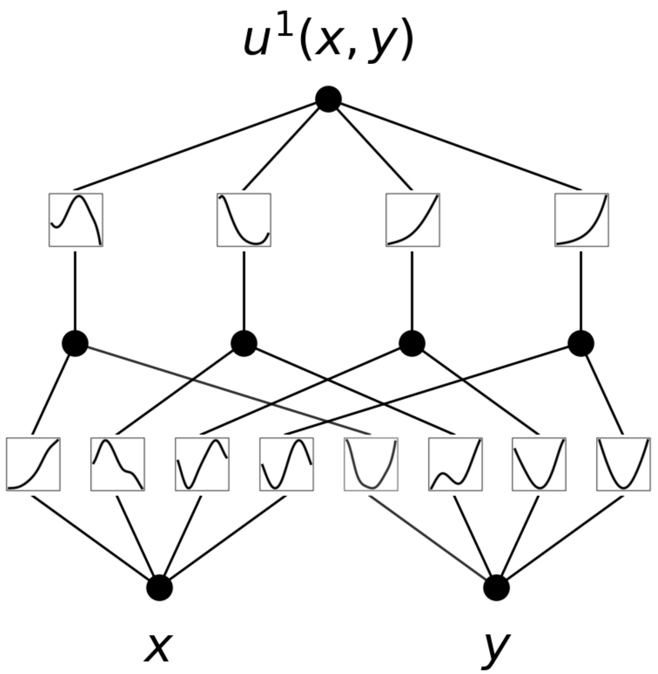
Continual learning with multifidelity arXiv:2304.03894



Conjugate kernel for accurate and fast training arXiv:2310.18612

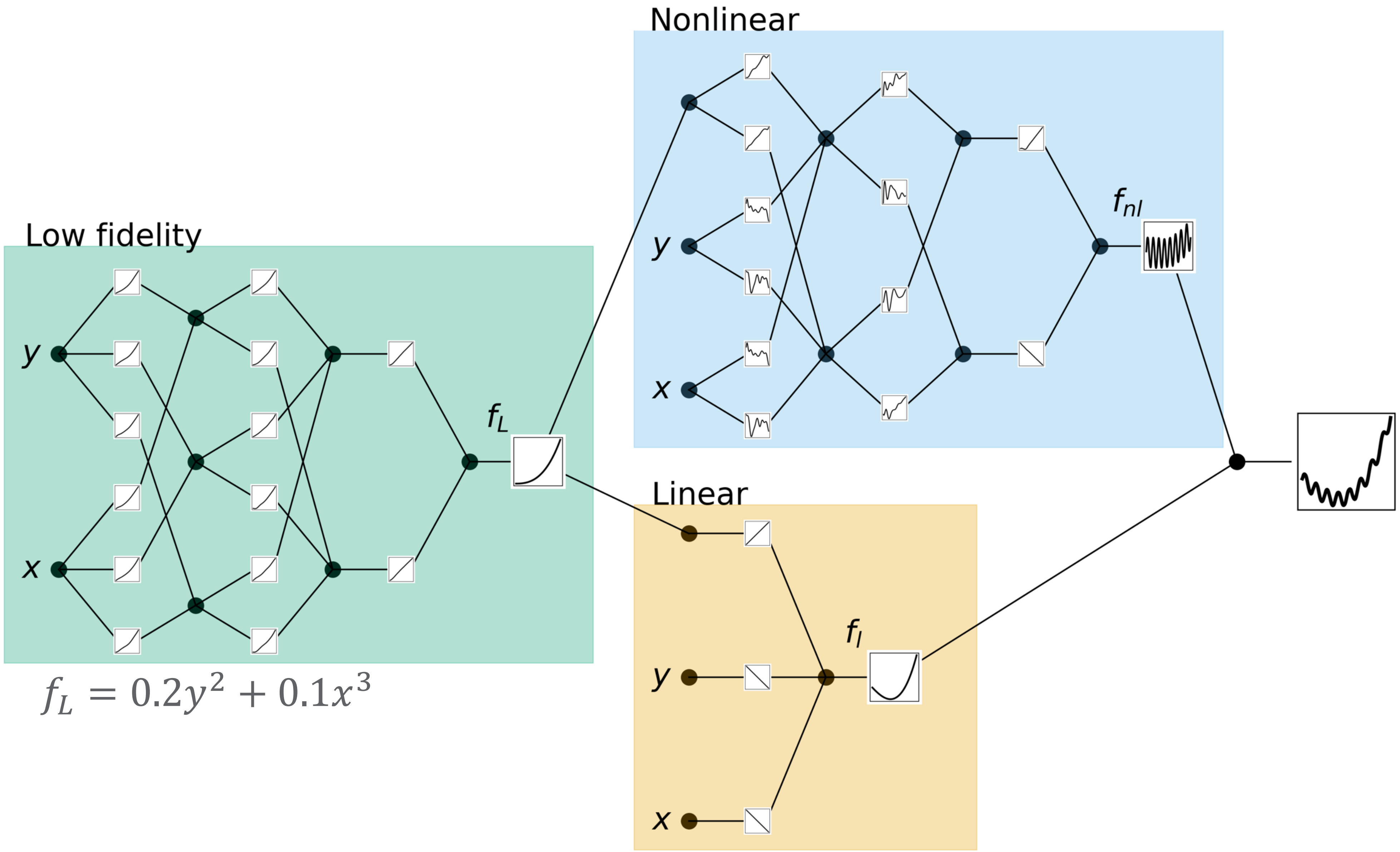
FBKANs





https://arxiv.org/abs/2406.19662

Multifidelity KANs

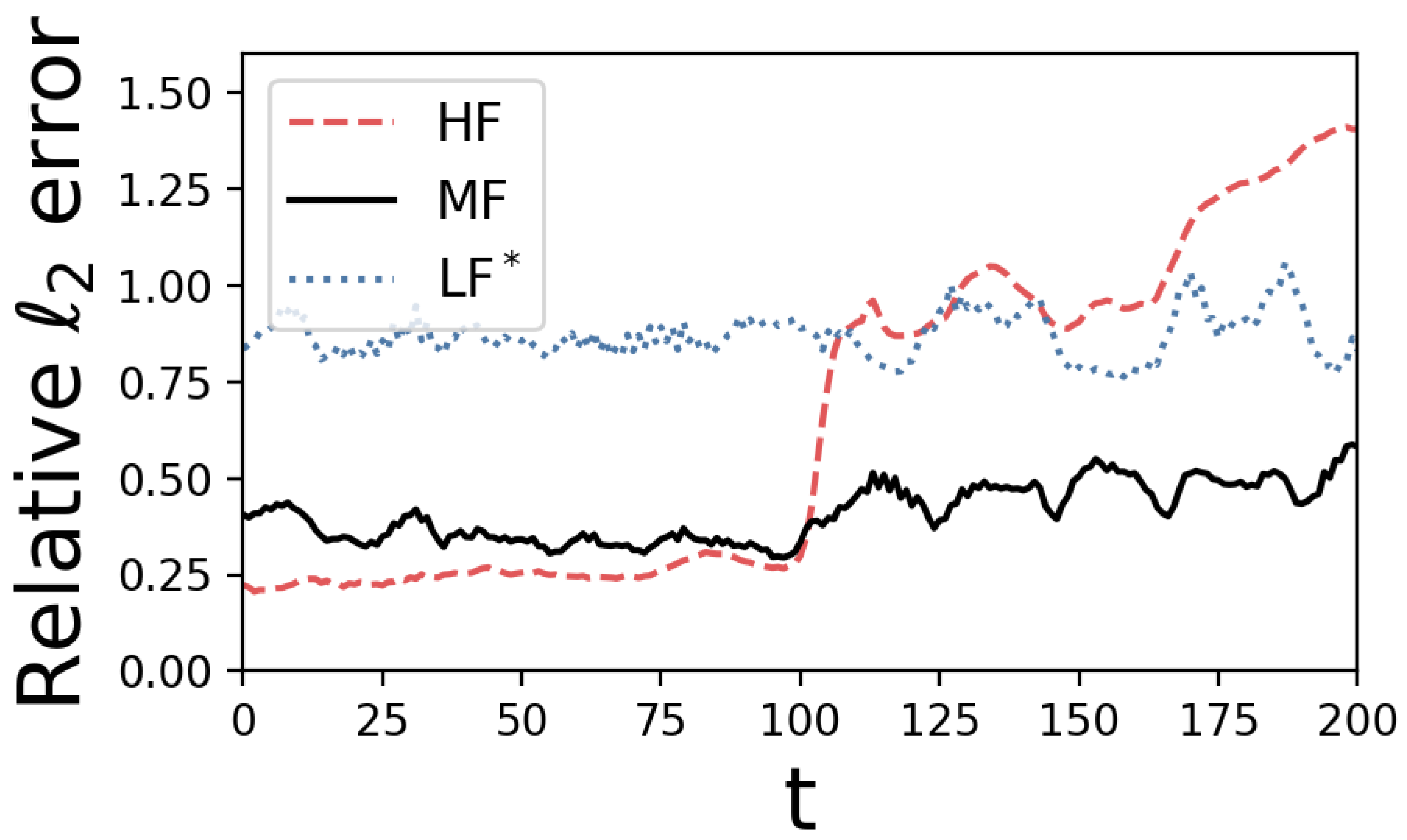


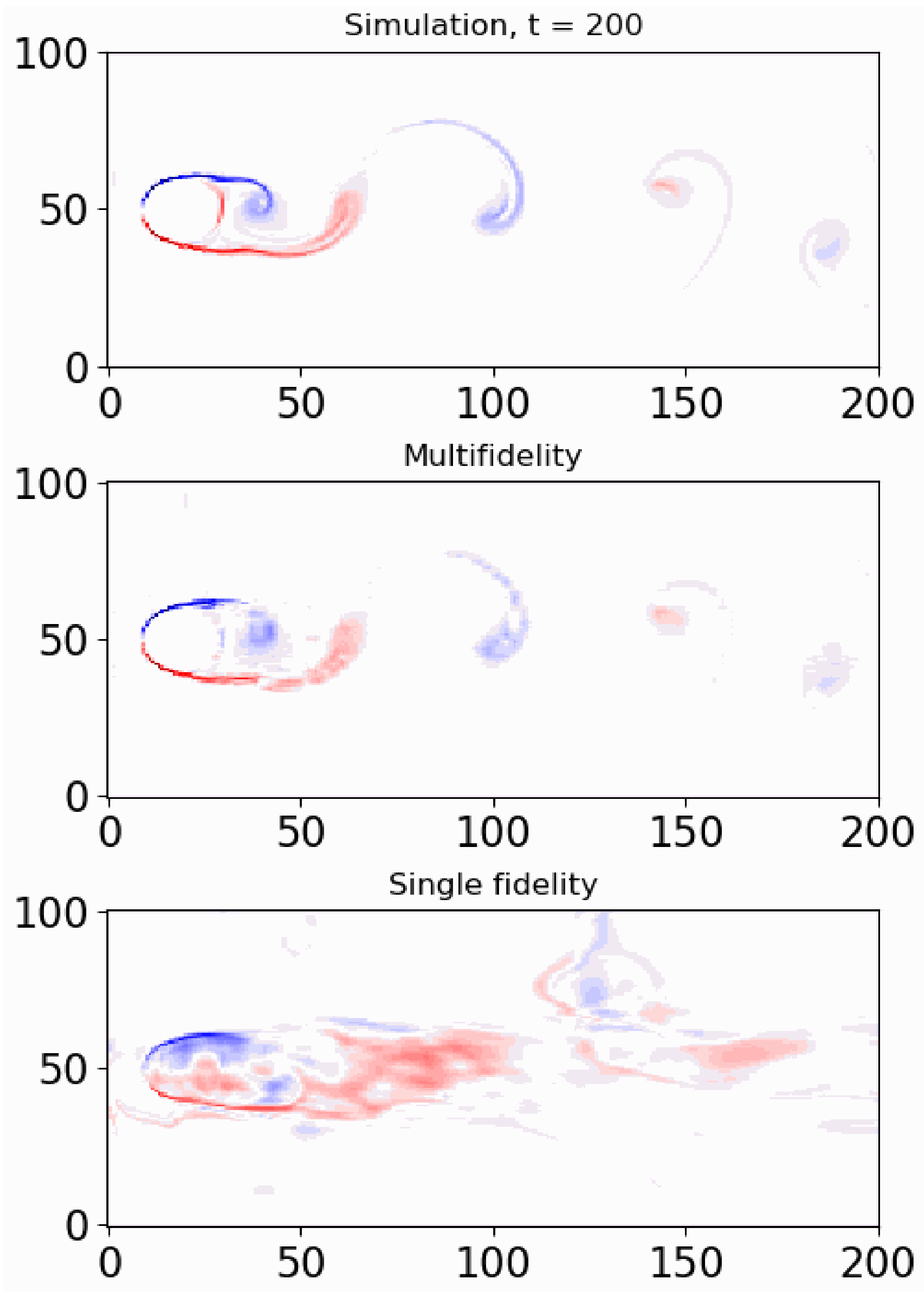
$f_L = 0.2y^2 + 0.1x^3$

$f_H = f_L - x - y + \sin(10x)$

Fluid flow

- Low fidelity data on t=[0, 200]
- High fidelity data only on t=[0, 100]
- Use low fidelity solver directly as a surrogate





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Thank you

SEA-CROGS

Papers & code

https://multy.me/p1KTst

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