Pacific Northwest
NATIONAL LABORATORY

SEA-CROGS
Scalable, Efficient & Accelerated Causal Reasoning Operators, Graphs & Spikes for Earth & Embedded Systems

Multifidelity Deep Operator Networks

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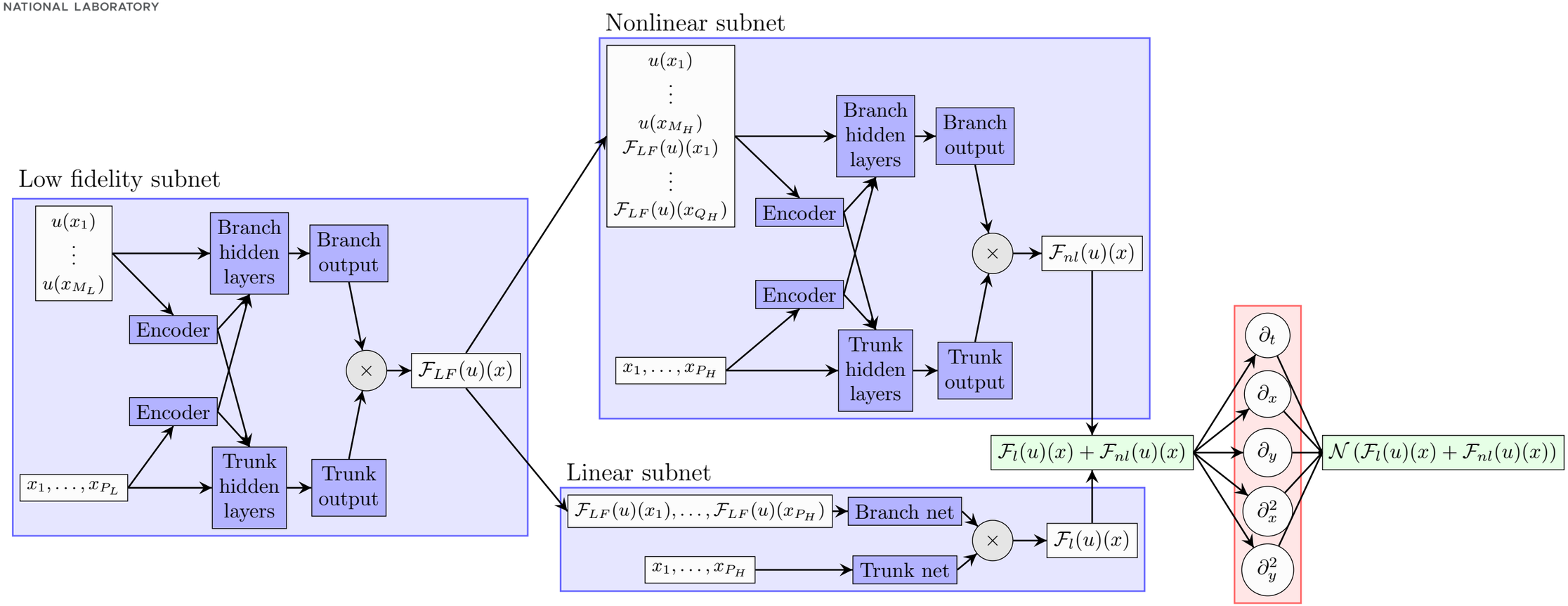
U.S. DEPARTMENT OF ENERGY BATTELLE

PNNL is operated by Battelle for the U.S. Department of Energy

General framework



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

Modified DeepONet: https://arxiv.org/abs/2110.01654

One-dimensional jump function

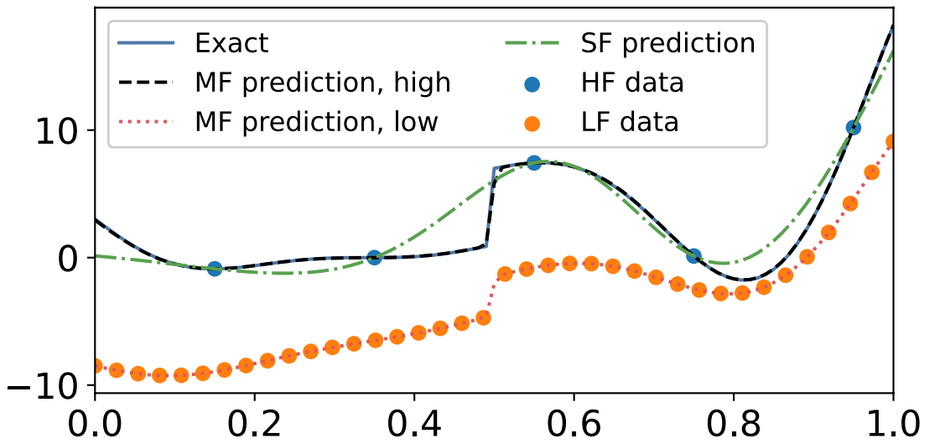
$$y_L(u)(x) = \begin{cases} 0.5(6x-2)^2\sin(u) + 10(x-0.5) - 5 & x \le 0.5 \\ 0.5(6x-2)^2\sin(u) + 10(x-0.5) - 2 & x > 0.5 \end{cases}$$

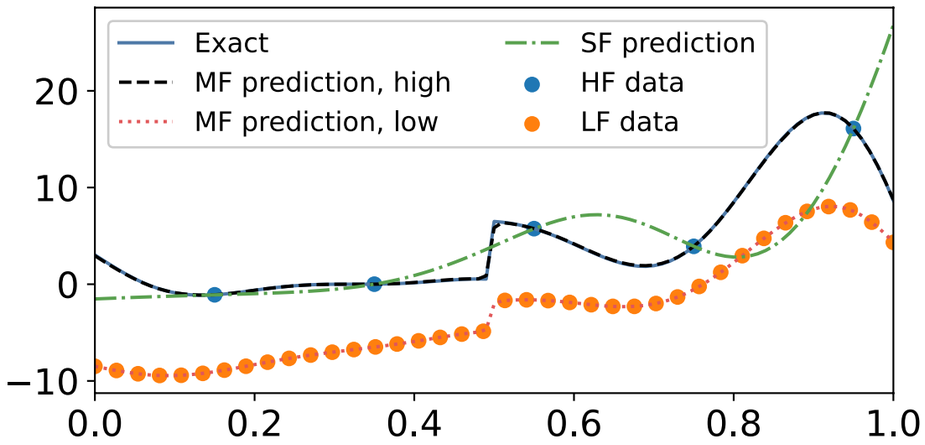
$$y_H(u)(x) = 2y_L(u)(x) - 20x + 20$$

$$u = ax - 4$$

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

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



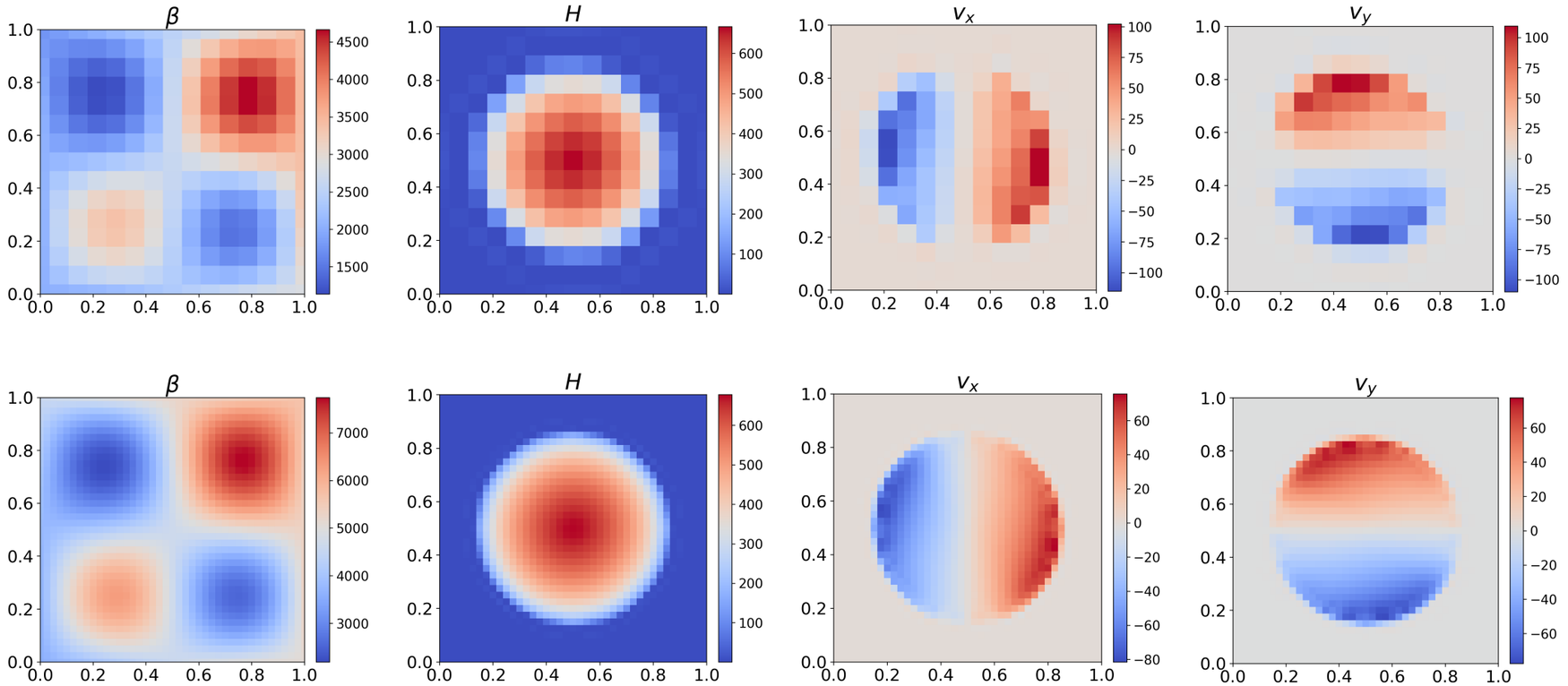


Ice sheets: multiresolution

Mono-layer higher-order (MOLHO) FEM code
Halfar dome ice sheet

P_L = 15x15

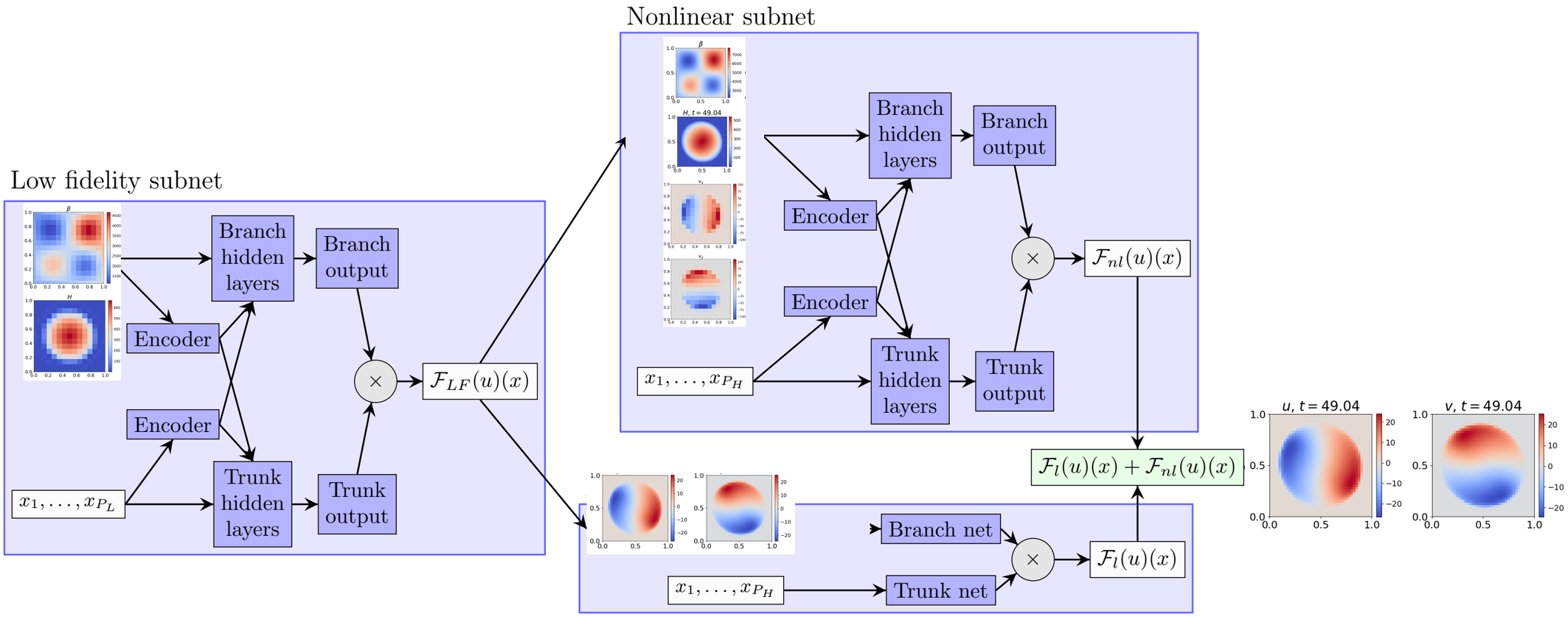
P_H = 41x41



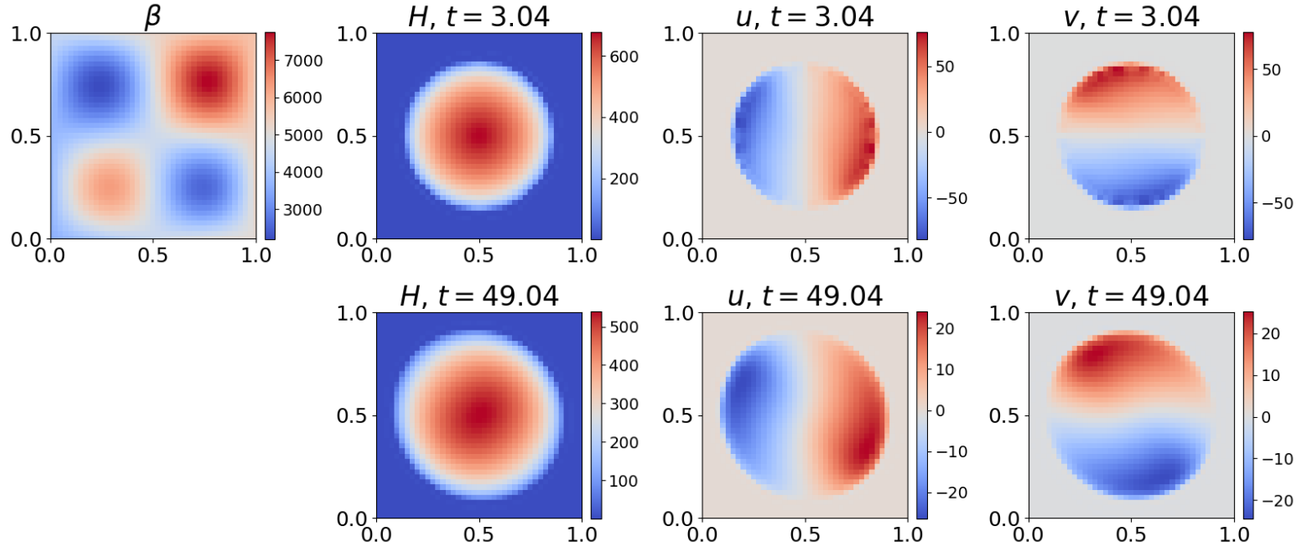
$$\beta = \exp(\gamma)$$

$$\gamma \sim \mathcal{G}\left(\log(\beta_{\text{opt}}), k_l\right), \quad \text{and} \quad k_l(\mathbf{x}_1, \mathbf{x}_2) = a \exp\left(-\frac{|\mathbf{x}_1 - \mathbf{x}_2|^2}{2l^2}\right)$$

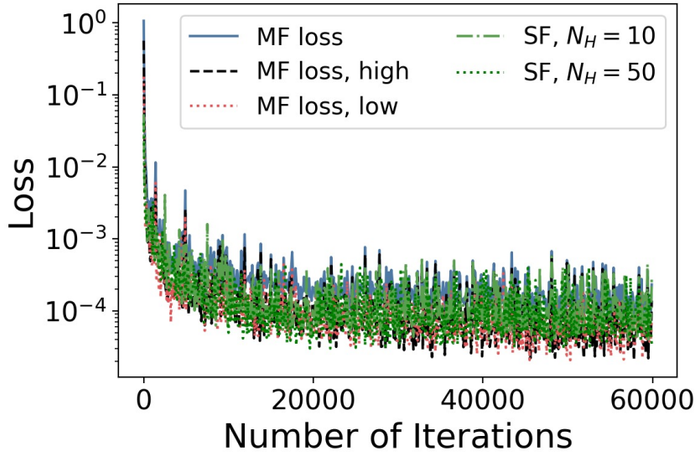
QiZhi He, Mauro Perego, AAH, George Em Karniadakis, Panos Stinis, “A Hybrid Deep Neural Operator/Finite Element Method for Ice-Sheet Modeling” (2023) https://arxiv.org/pdf/2301.11402.pdf


Nonlinear subnet
Low fidelity subnet
Branch hidden layers
Branch output
Encoder
Encoder
Trunk hidden layers
Trunk output
$x_1, \ldots, x_{P_L}$
$\mathcal{F}_{LF}(u)(x)$
Branch hidden layers
Branch output
Encoder
Encoder
Trunk hidden layers
Trunk output
$x_1, \ldots, x_{P_H}$
$\mathcal{F}_{nl}(u)(x)$
$\mathcal{F}_l(u)(x) + \mathcal{F}_{nl}(u)(x)$
Branch net
Trunk net
$x_1, \ldots, x_{P_H}$
$\mathcal{F}_l(u)(x)$
$u, t = 49.04$
$v, t = 49.04$

Ice sheets: multiresolution



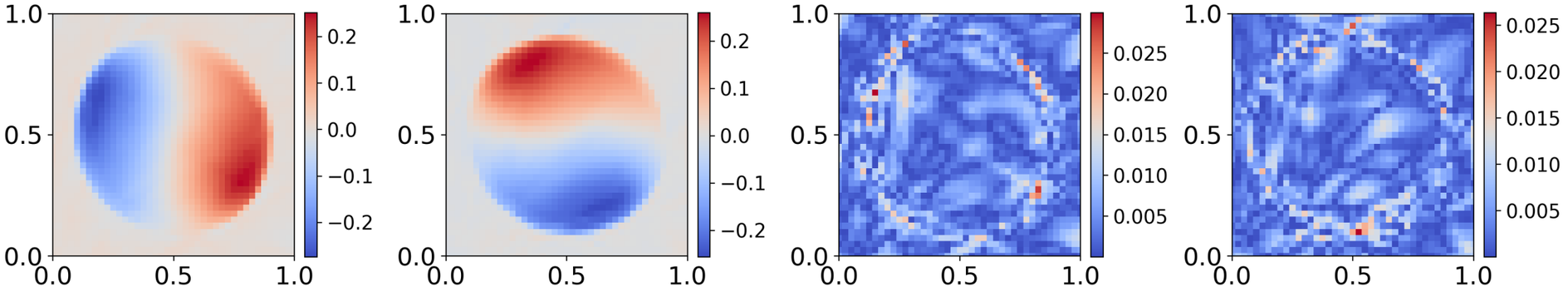
SF $N_H = 10$ or 50
MF $N_L = 100$
MF $N_H = 10$
$M_L = P_L = 2\text{x}15^2$
$M_H = P_H = 2\text{x}41^2$



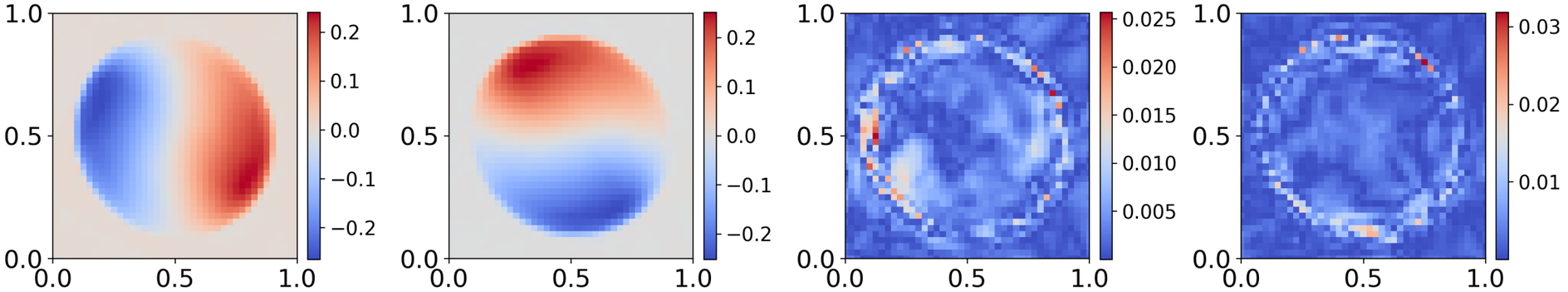
Method	Mean MSE	Mean relative L2 error
Single fidelity, $N_H = 10$	0.15814	0.66923
Single fidelity, $N_H = 50$	0.00012	0.05074
Multifidelity	8.8973×10^{-5}	0.04442

Ice sheets: multiresolution

$N_H = 50$



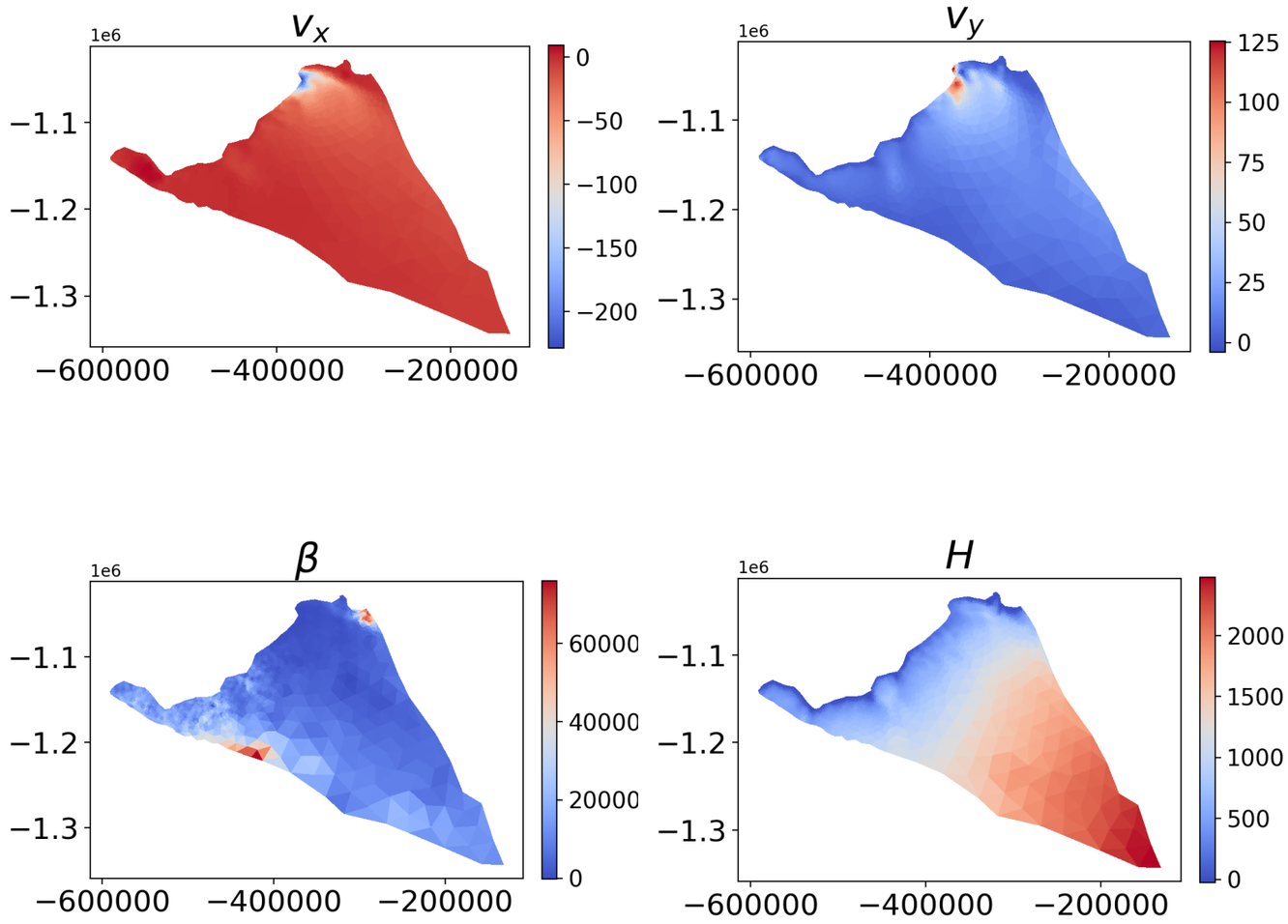
Multifidelity, $N_H = 10$



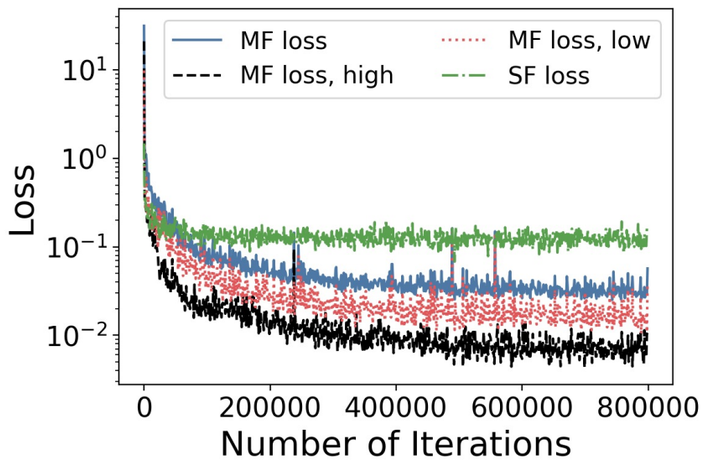
Ice sheets: multiorder

Two numerical models
MOLHO – low fidelity
Shallow Shelf Approximation–high fidelity

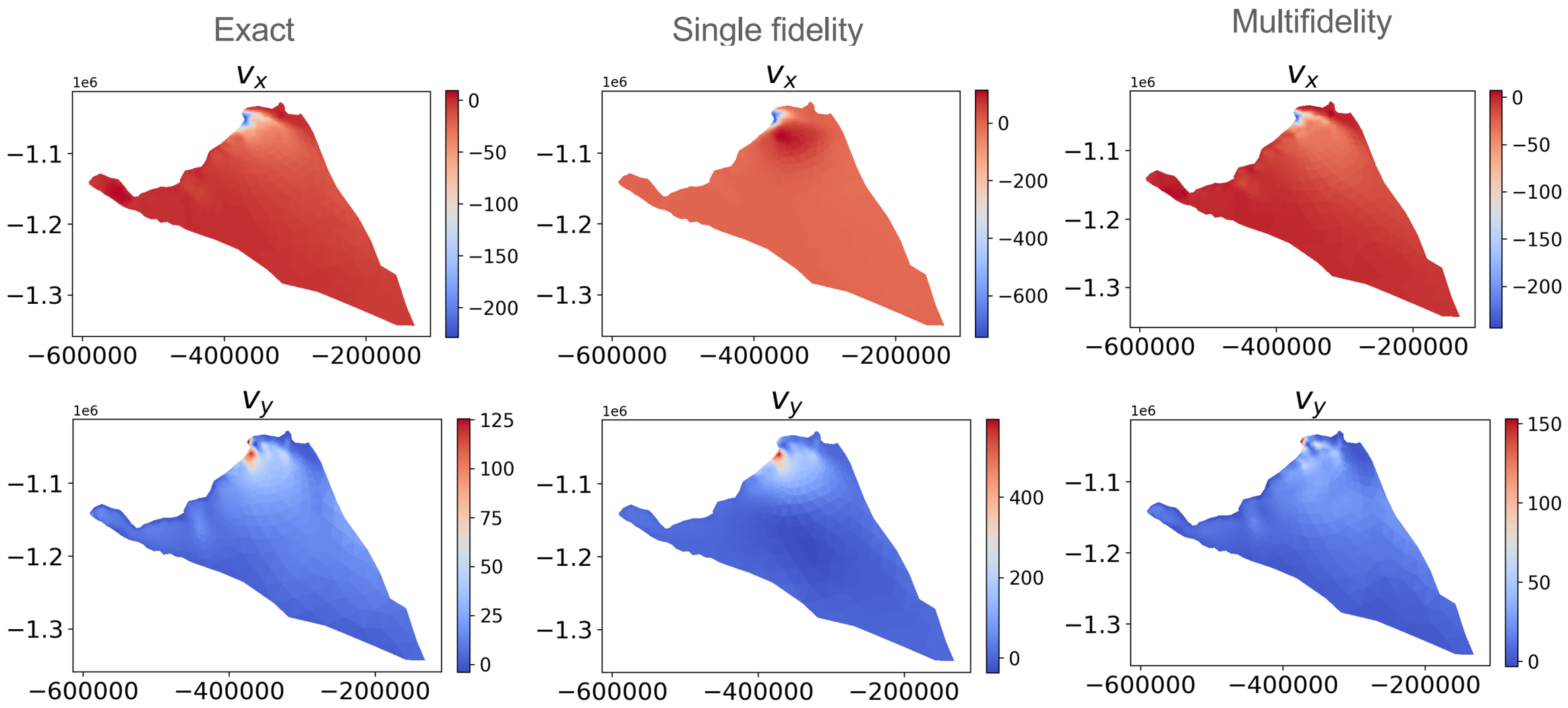
Humboldt glacier, Greenland



SF $N_H = 20$
MF $N_L = 80$
MF $N_H = 20$



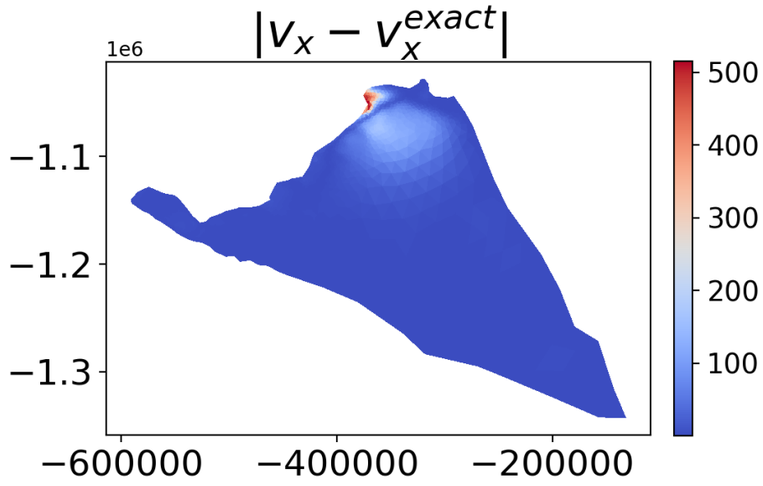
Ice sheets: multiorder

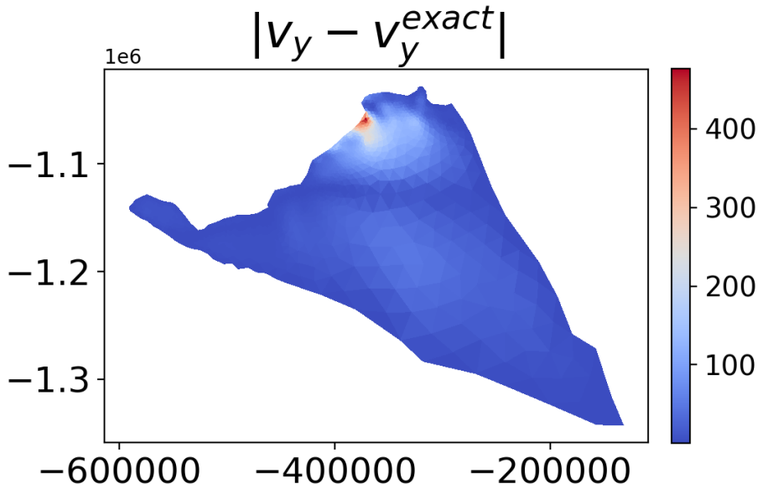


Ice sheets: multiorder

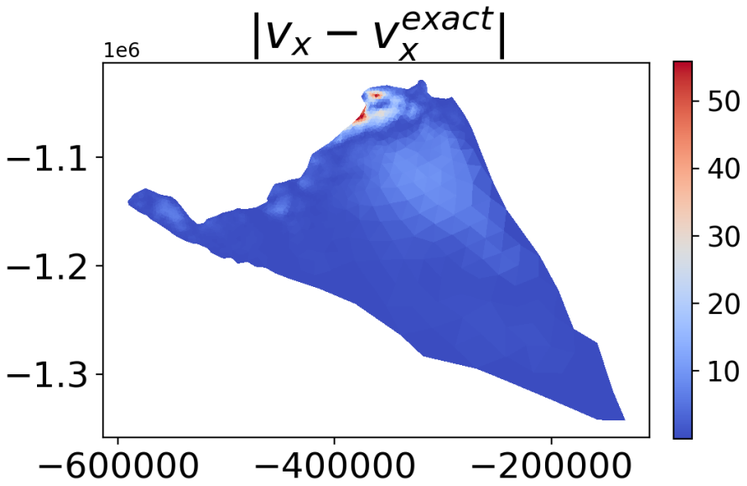
Method	Mean relative L2 error
Single fidelity	1.1005
Multifidelity	0.3676

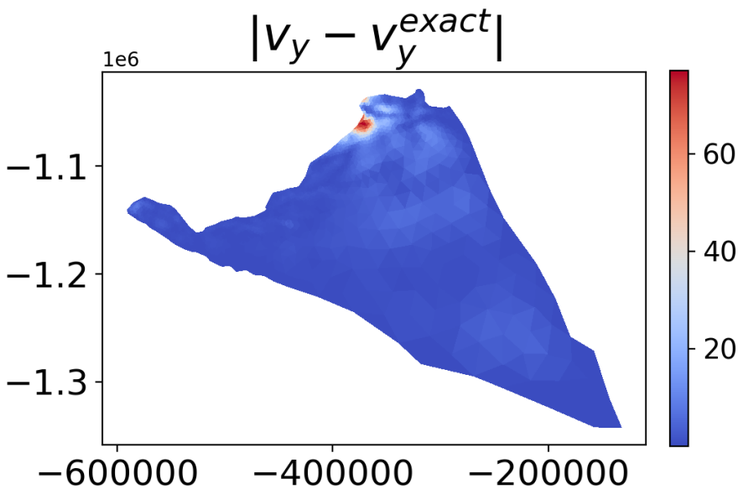
Single fidelity



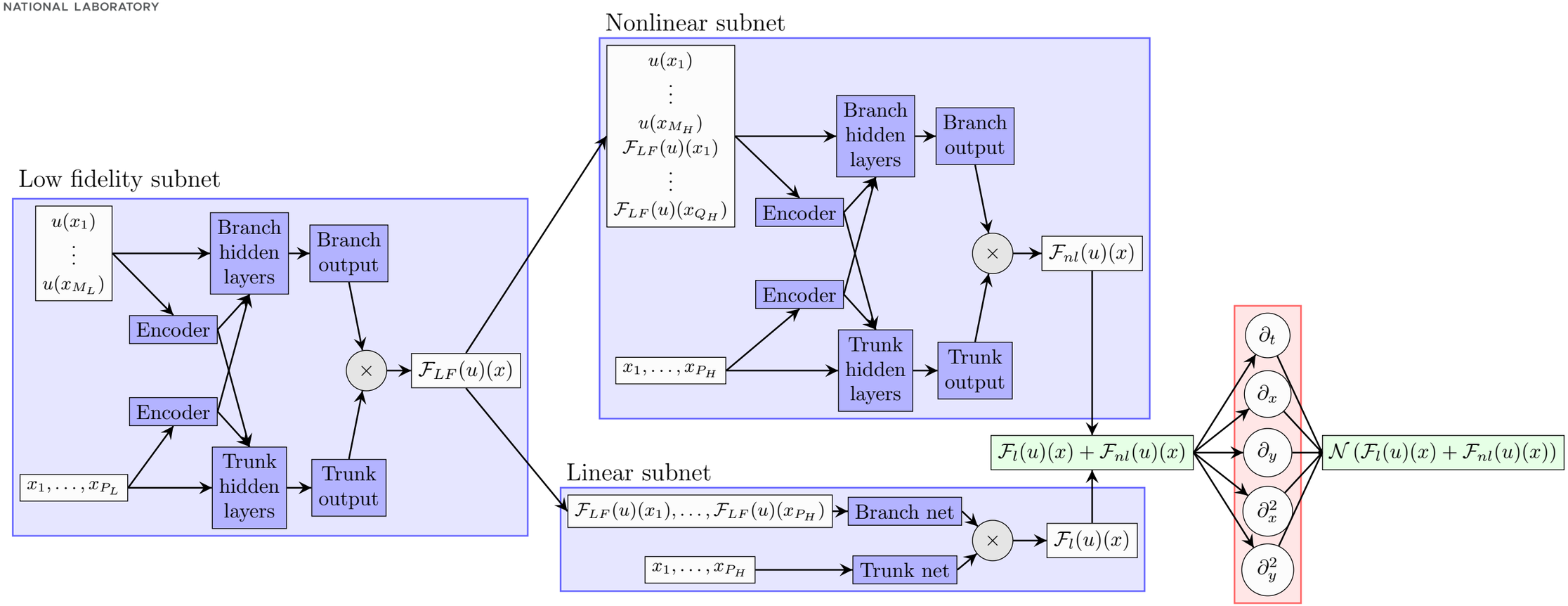


Multifidelity





General framework



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

Modified DeepONet: https://arxiv.org/abs/2110.01654

Burgers equation

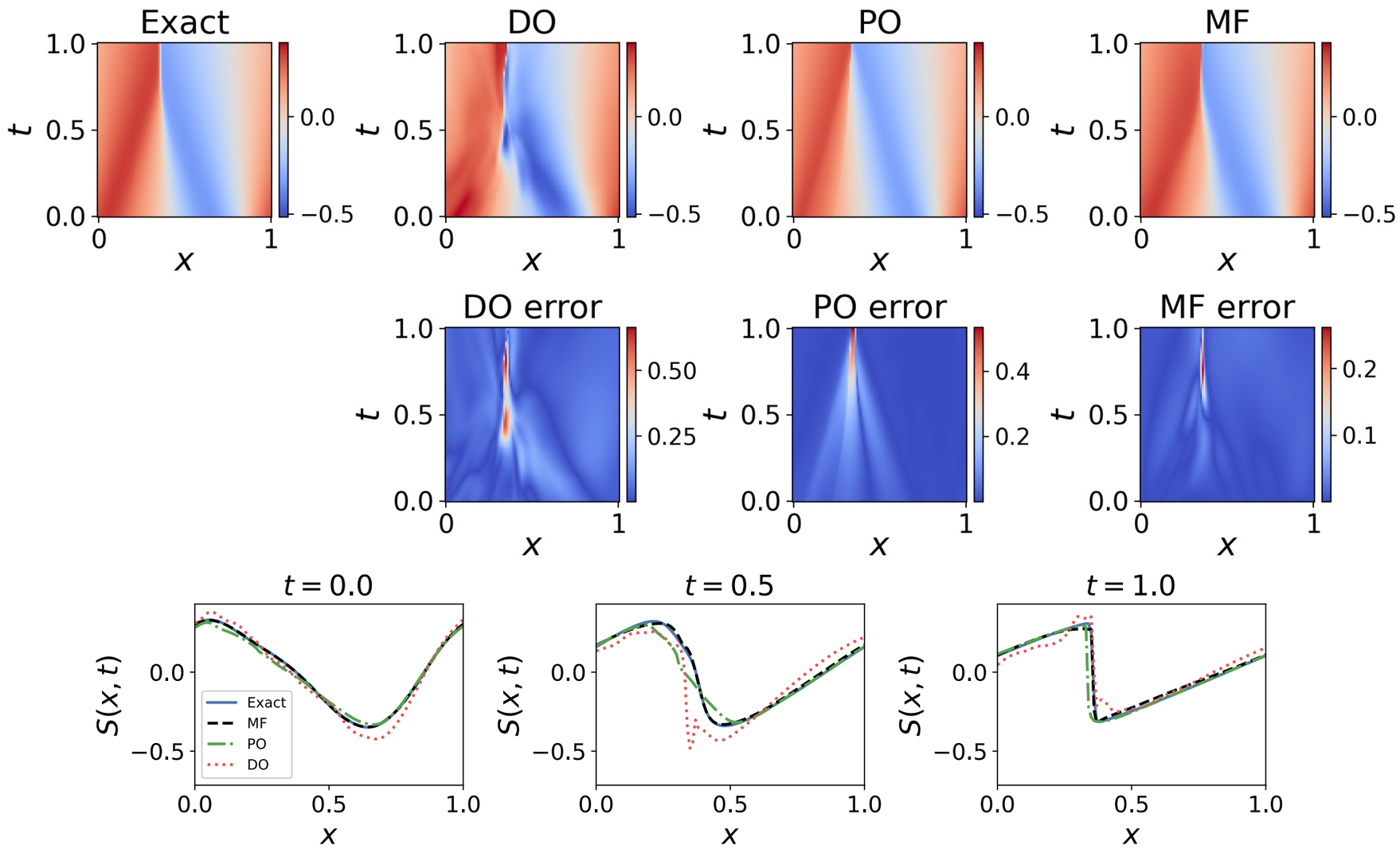
- Low fidelity simulations
- Physics enforced as high fidelity model

$$\frac{ds}{dt} + s\frac{ds}{dx} - \nu\frac{d^2s}{dx^2} = 0,\ (x,t) \in (0,1) \times (0,1]$$
$$s(x,0) = u(x),\ x \in (0,1),$$
$$s(0,t) = s(1,t),\ t \in (0,1),$$
$$\frac{ds}{dx}(0,t) = \frac{ds}{dx}(1,t),\ t \in (0,1)$$

Parameters	$\nu = 10^{-2}$ $N_L = 1000$	$\nu = 10^{-3}$ $N_L = 1000$	$\nu = 10^{-4}$ $N_L = 1000$	$\nu = 10^{-4}$ $N_L = 200$
Data-only	$1.02\% \pm 0.81\%$	$2.46\% \pm 1.67\%$	$7.64\% \pm 2.66\%$	$13.57\% \pm 7.40\%$
Data-only with noise	$4.44\% \pm 3.48\%$	$6.50\% \pm 3.45\%$	$10.63\% \pm 5.54\%$	$26.11\% \pm 15.38\%$
Physics-only	$3.97\% \pm 5.71\%$	$8.66\% \pm 6.47\%$	$23.63\% \pm 10.22\%$	–
Multifidelity	$2.81\% \pm 1.81\%$	$6.25\% \pm 2.20\%$	$7.05\% \pm 3.01\%$	$9.70\% \pm 4.60\%$
Multifidelity with noise	$2.89\% \pm 1.70\%$	$6.65\% \pm 2.48\%$	$7.03\% \pm 3.10\%$	$10.16\% \pm 5.55\%$

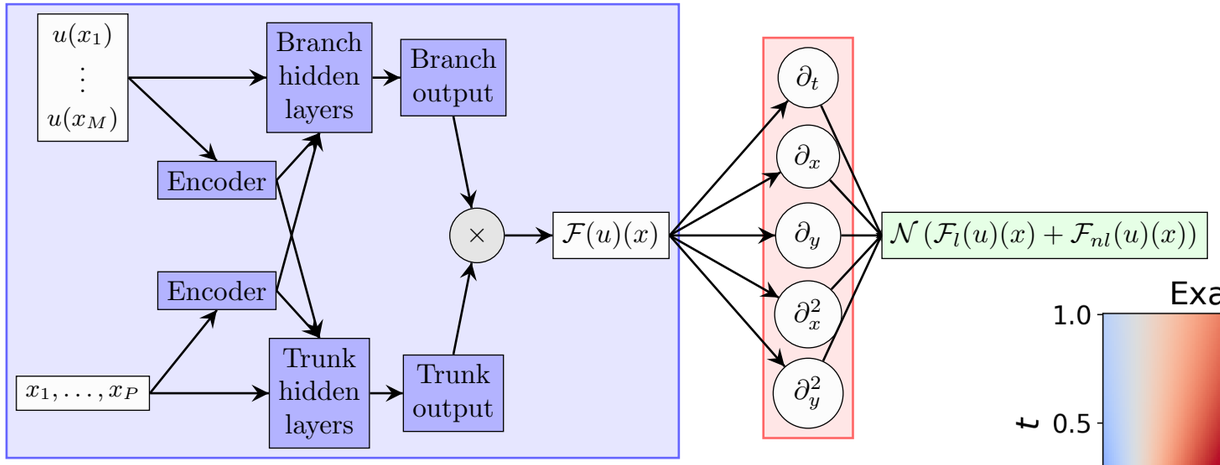
Table 2: Physics-informed multifidelity: viscous Burgers equation mean relative L_2 errors. The physics-only and multifidelity cases all use $N_H = 1000$. Note that the physics-only case does not use any low-fidelity data.

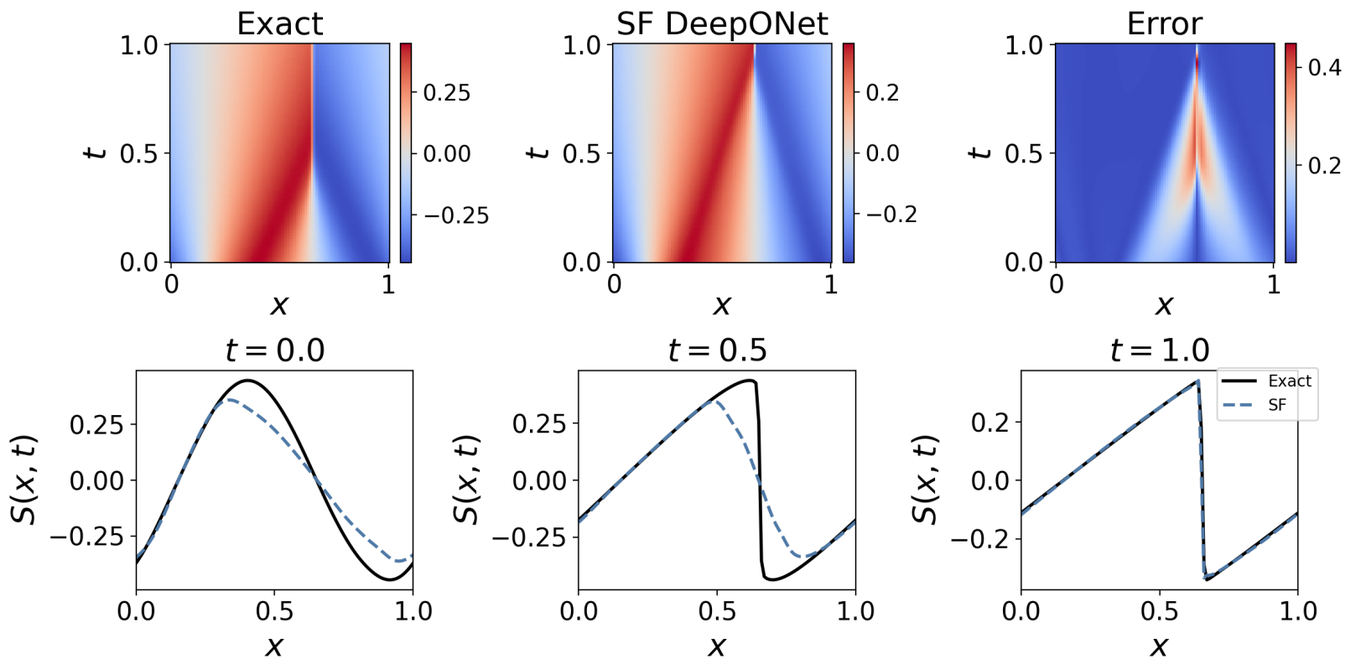
$\nu = 10^{-4}, N_L = 200$ with noise



Bootstrapping DeepONets

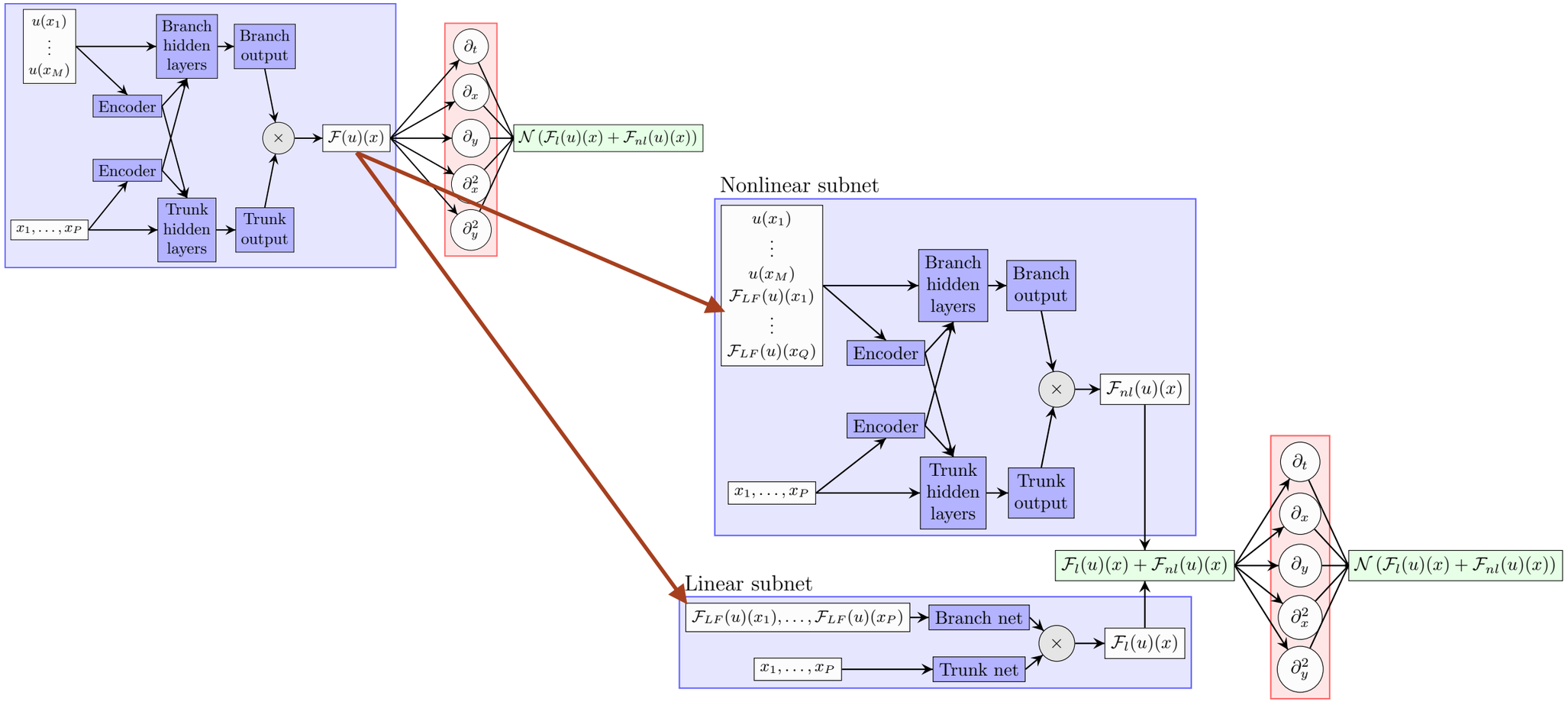
1) Train a single fidelity physics-informed DeepONet





Bootstrapping DeepONets

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



Bootstrapping DeepONets

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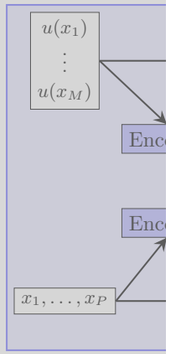
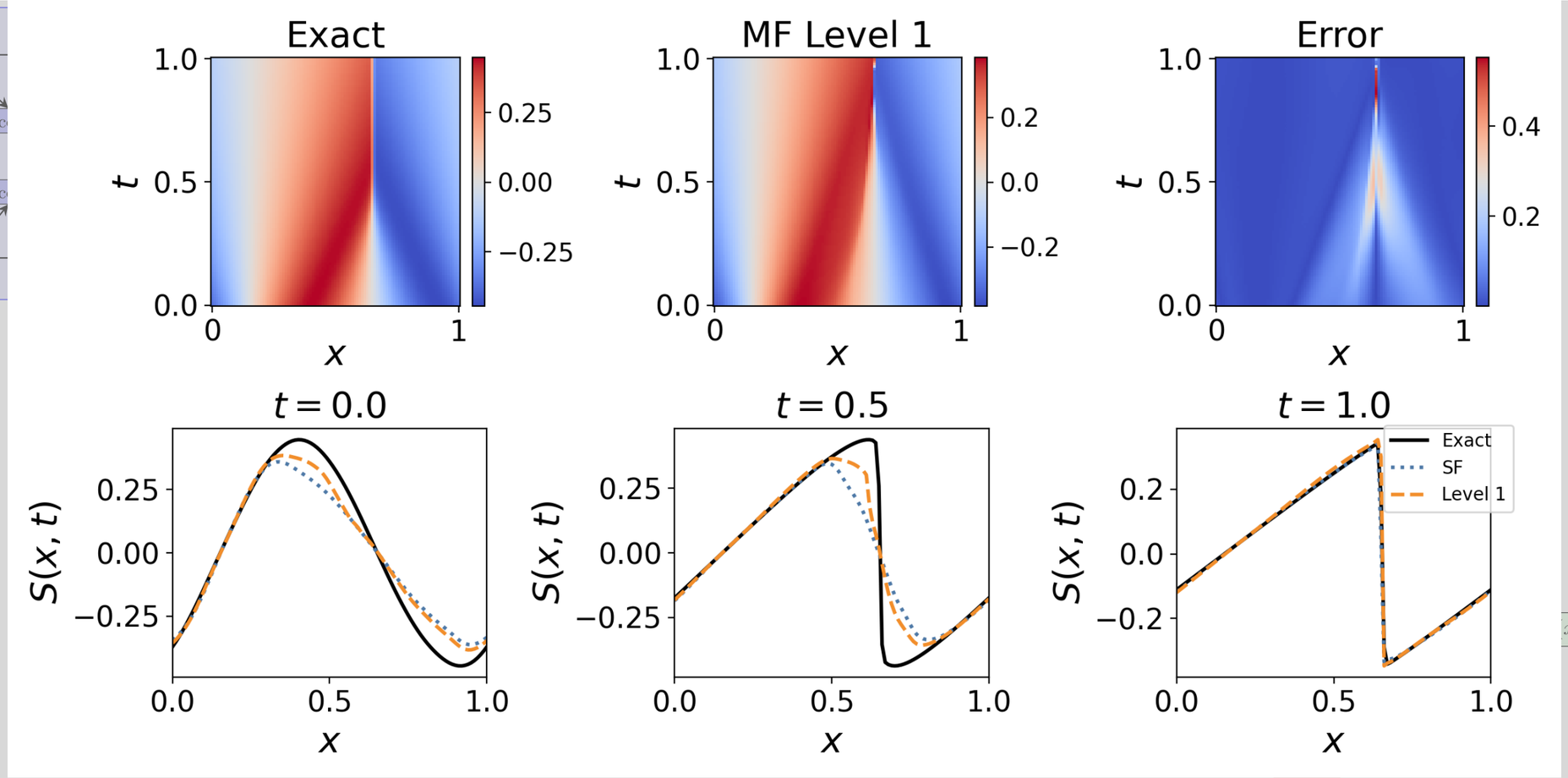
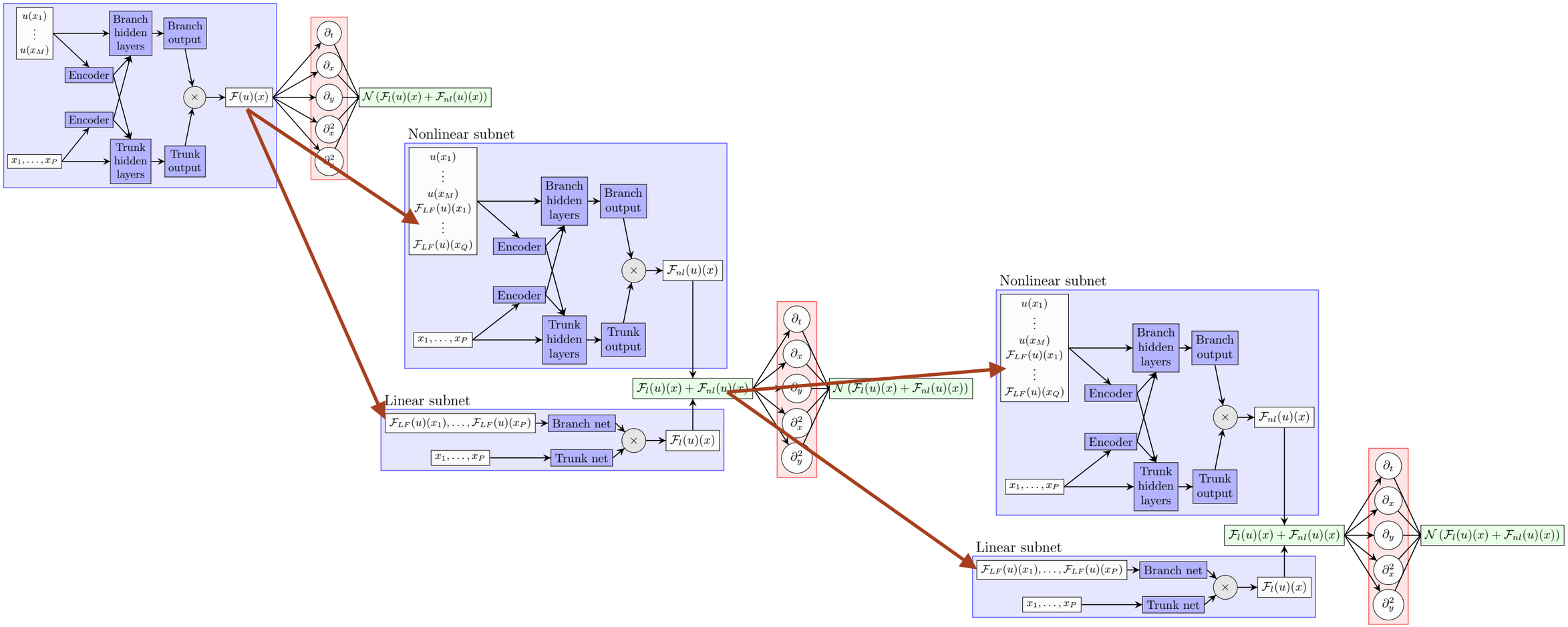




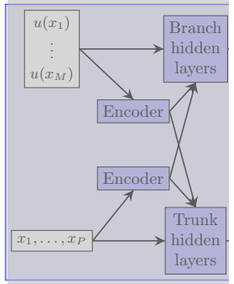
Bootstrapping DeepONets

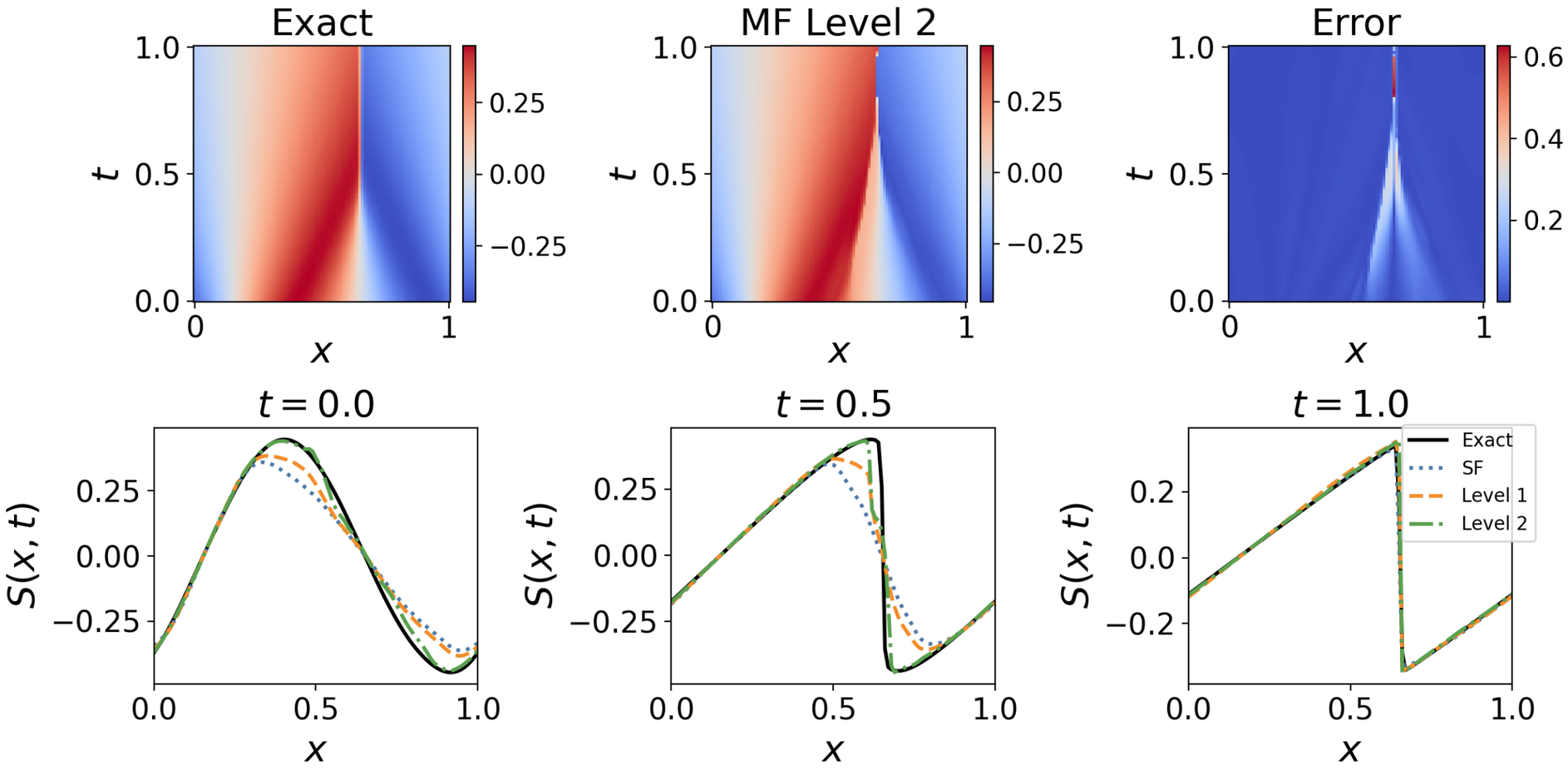
3) Train another non-composite multifidelity physics-informed DeepONet



Bootstrapping DeepONets

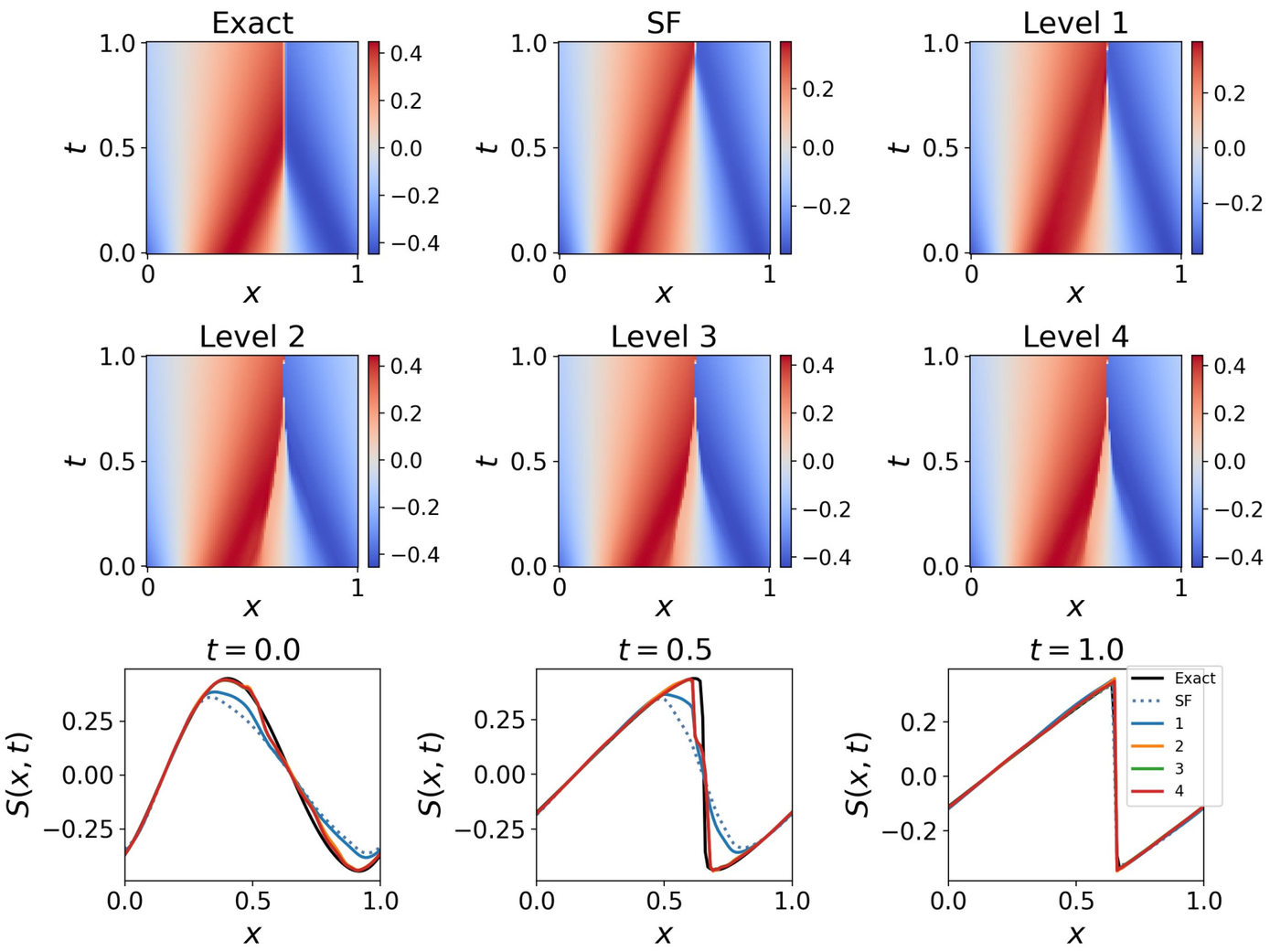
3) Train another non-composite multifidelity physics-informed DeepONet





$(\mathcal{F}_l(u)(x) + \mathcal{F}_{nl}(u)(x))$

Bootstrapping DeepONet



Thank You

https://arxiv.org/pdf/2204.09157.pdf

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