

Table R1: Hard encoding of different BCs (e.g., Dirichlet, Neumann, Robin, and Periodic) via padding. Here, the ghost nodes refer to additional nodes to pad outside the domain. In Robin BC, α and β are known.

BC	Continuous Formulation	Discrete Formulation	Padding Nodes	Padding Formulation
Dirichlet	$u(\mathbf{x}) = \bar{u}(\mathbf{x}), \mathbf{x} \in \Gamma_d$	$u_{pj} = \bar{u}_j$	Edge Nodes	$u_{pj} = \bar{u}_j$
Neumann	$\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} = f(\mathbf{x}), \mathbf{x} \in \Gamma_n$	$\frac{u_{(p+1)j} - u_{(p-1)j}}{2\delta_x} = f_j$	Ghost Nodes	$u_{(p+1)j} = u_{(p-1)j} + 2\delta_x f_j$
Robin	$\alpha u(\mathbf{x}) + \beta \frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} = g(\mathbf{x}), \mathbf{x} \in \Gamma_r$	$\alpha u_{pj} + \beta \frac{u_{(p+1)j} - u_{(p-1)j}}{2\delta_x} = g_j$	Ghost Nodes	$u_{(p+1)j} = \frac{2\delta_x}{\beta} (g_j - \alpha u_{pj}) + u_{(p-1)j}$
Periodic	$u(\mathbf{x}_1) = u(\mathbf{x}_2), \mathbf{x}_1 \in \Gamma_1, \mathbf{x}_2 \in \Gamma_2$	$u_{pj} = u_{1j}$	Ghost Nodes	$u_{(p+1)j} = u_{2j}$

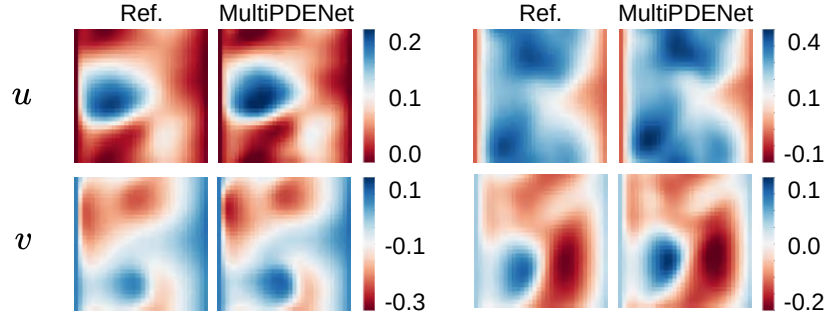


Fig. R1: MultiPDENet generalization over complex BCs (left Dirichlet, right Neumann, top/bottom Periodic) on the Burgers example for two random ICs. Snapshots at $t = 1.4$ s.

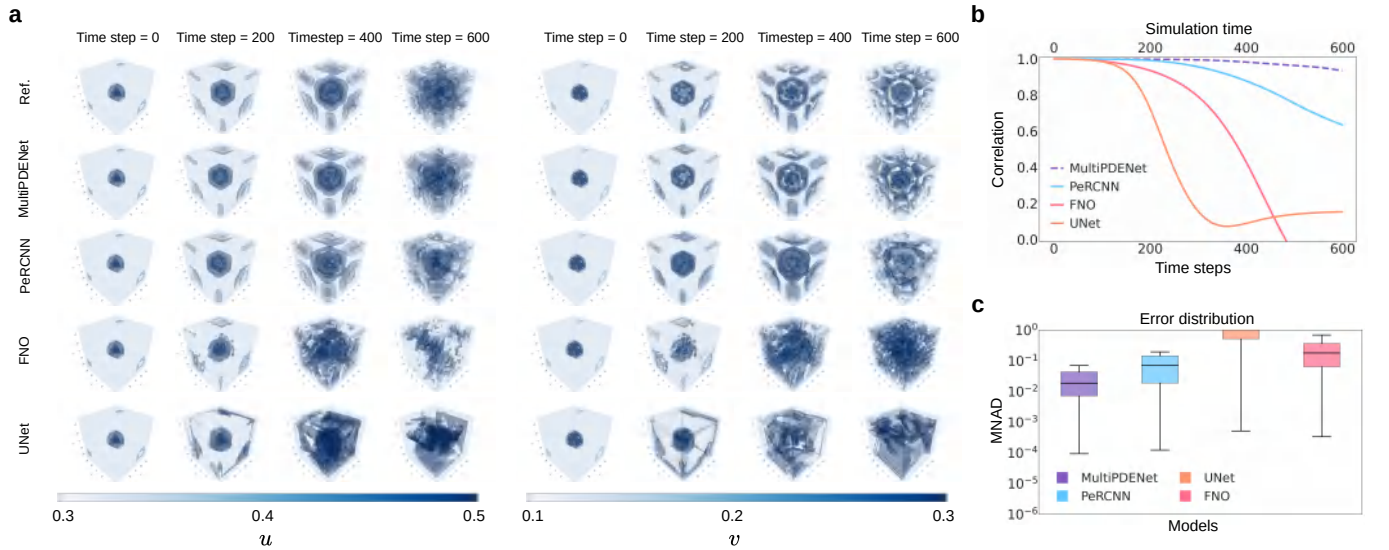


Fig. R2: Qualitative comparison of predicted snapshots for the 3D Gray-Scott between MultiPDENet and baseline models, including (a) predicted solutions, (b) correlation curve, and (c) error distributions.

Table R2: Results of MultiPDENet and baselines. For 3DGS, we inferred upper time limits of 600 s, for the test set as the system dynamics stabilized within these trajectories. These time limits were used to calculate HCT.

Case	Model	RMSE (\downarrow)	MAE (\downarrow)	MNAD (\downarrow)	HCT (s)
3DGS	FNO	0.4381	0.2297	0.2274	297.5
	UNet	NaN	NaN	NaN	119.5
	PeRCNN	<u>0.1558</u>	<u>0.0821</u>	<u>0.0813</u>	<u>468</u>
	MultiPDENet	0.0586	0.0245	0.0242	600.0
	Improvement (\uparrow)	62.4%	70.2%	70.2%	28.2%

Table R3: Results of MultiPDENet and baselines. For KdV, Burgers, and GS, we inferred upper time limits of 50 s, 1.4 s, and 1200 s for the test set as the system dynamics stabilized within these trajectories. These time limits were used to calculate HCT.

Case	Model	RMSE (\downarrow)	MAE (\downarrow)	MNAD (\downarrow)	HCT (s)
KdV	FNO	0.9541	0.4607	0.3469	10.0833
	PhyFNO	<u>0.4120</u>	<u>0.3022</u>	<u>0.2139</u>	<u>13.90</u>
	UNet	1.9887	1.5722	1.6158	3.1250
	DeepONet	NaN	NaN	NaN	0.1500
	MultiPDENet	0.1536	0.1110	0.0833	39.8
	Improvement (\uparrow)	62.7%	63.3%	61.1%	186.3%
Burgers	FNO	0.0980	0.0762	0.0620	0.3000
	PhyFNO	<u>0.0832</u>	<u>0.0749</u>	<u>0.0599</u>	<u>0.5546</u>
	UNet	0.3316	0.2942	0.2556	0.0990
	DeepONet	0.2522	0.2106	0.1692	0.0020
	PeRCNN	0.0967	0.1828	0.1875	0.4492
	MultiPDENet	0.0057	0.0037	0.0031	1.4000
	Improvement (\uparrow)	93.1%	95.1%	94.8%	152.4%
GS	FNO	8774	1303	1303	270
	PhyFNO	0.5721	0.3579	0.3520	510
	UNet	NaN	NaN	NaN	20
	DeepONet	0.4113	0.2961	0.2898	568
	PeRCNN	<u>0.1763</u>	<u>0.1198</u>	<u>0.1198</u>	<u>640</u>
	MultiPDENet	0.0573	0.0294	0.0298	1400.0
	Improvement (\uparrow)	67.5%	75.5%	75.1%	118.8%
NSE	FNO	1.0100	0.7319	0.0887	2.5749
	UNet	<u>0.8224</u>	<u>0.5209</u>	<u>0.0627</u>	<u>3.9627</u>
	LI	NaN	NaN	NaN	3.5000
	TSM	NaN	NaN	NaN	3.7531
	DeepONet	2.1849	1.0227	0.1074	0.1126
	MultiPDENet	0.1379	0.0648	0.0077	8.3566
	Improvement (\uparrow)	83.2%	87.6%	87.7%	110.9%