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	$u_{(p+1)j} = u_{2j}$

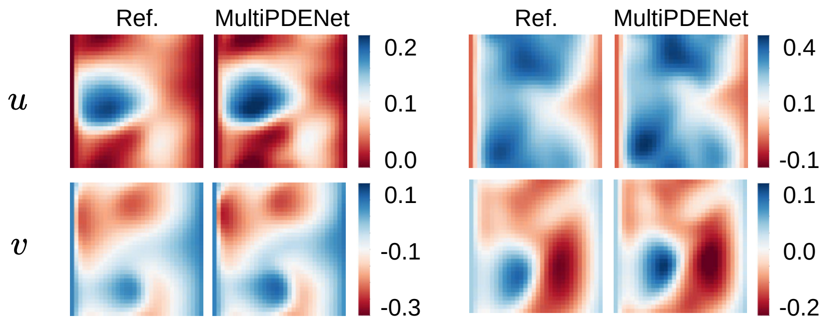

Fig. R1: MultiPDENet generalization over complex BCs (left Dirichlet, right Neumann, top/bottom Periodic) on the Burgers example for two random ICs. Snapshots at $t = 1.4$ s.

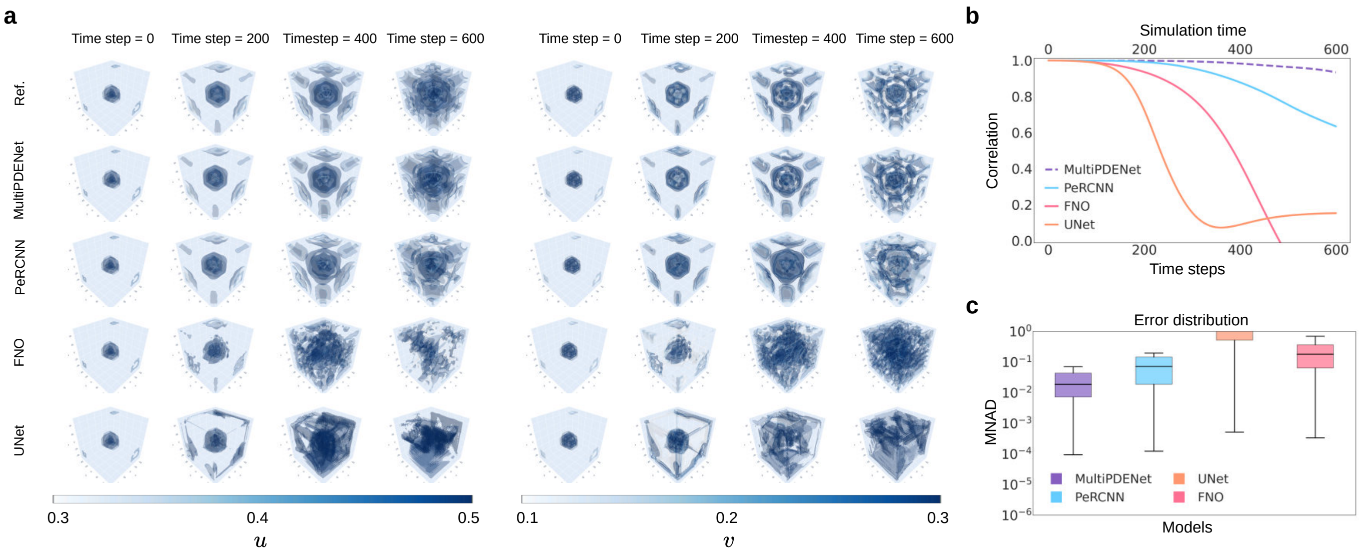

Fig. R2: Qualitative comparison of predicted snapshots for the 3D Gray-Scott between MultiPDENet and baseline models, including (a) predicted solutions, (b) correlation curve, and (c) error distributions.

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 (↓)	MAE (↓)	MNAD (↓)	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 (↑)	62.4%	70.2%	70.2%	28.2%