A. Appendix

A.1. Choice of NN architecture

We experimented with ResNet and UNet architectures for the neural network part of the purely data driven and hybrid NN-PDE approach discussed in section 3.3 of the main paper. Table A.1 provides details of the convolutional blocks, layers of the network, and activation function. The *UNet32* architecture with 2 layers is used for 32×32 cases and the *UNet100* architecture with 3 layers is used for 100×100 case discussed in the paper. Table A.2 shows the comparison between MAPE achieved by ResNet and UNet architectures for the purely data-driven and the hybrid NN-PDE approach for different cases considered in the paper. For the hybrid NN-PDE approach with 32×32 resolution cases, the ResNet and UNet achieve comparable performance with the UNet yielding the lowest error. The main difference arises in the 100×100 resolution case. The ResNet fails to converge during training, leading to high test error. On the contrary, the UNet achieves low training and testing errors. The main advantage of UNet comes from transforming high resolution input to low resolution representation and reconstructing it back to the high resolution output. Therefore, we choose the UNet architecture for the hybrid NN-PDE approach. For the purely data-driven approach the ResNet was found to be better for 2 out of 3 cases. Specifically for the nonUniform-Bunsen32 case, UNet performs very poorly for the PDD approach. Therefore, we report ResNet errors for the PDD approach throughout the paper.

A.2. Additional Experiments

We additionally compare against the variant of the purely data-driven model described in section 3.2. It employs a neural network model to learn the complete flow states $\mathcal{P}_c(\phi)$ given an input flow state ϕ^S where $\phi^S = [T, Y_f, Y_o, u, p]$. Keeping all hyperparameters the same, the ResNet is trained to predict all quantities of flow state for nonUniform-Bunsen32 case. As the PDD approach does not enforce any physical laws, the inclusion of additional quantities results in a more difficult learning task, which

Hyper-parameters	ResNet	UNet32	UNet100
Kernel size	5	5	5
Latent size	32		
Activation	LeakyReLu	LeakyReLu	ReLu
Loss	MSE	MSE	MSE
# ResBlocks	5		
# UNet layers		2	3
CNN stack depth	2	3	2
Base latent size		16	16
Spatial down-sample by layer		2	2
latent sizes		(32)	(32,64)
# trainable parameters	261,953	136,227	362,371

Table A.1. Details of various neural network architectures used in this paper.

Table A.2. Mean and standard deviation of errors over different architectures for purely data-driven and hybrid NN-PDE approaches.

		PDD ResNet	PDD UNet	Hybrid NN-PDE ResNet	Hybrid NN-PDE UNet
MAPE	Planar-v0 uniform-Bunsen nonUniform-Bunsen32 nonUniform-Bunsen100	$6.33 \pm 3.05\%$ 7.58 ± 3.73% 12.48 ± 11.31%	$7.09 \pm 4.40\%$ $2.87 \pm 1.53\%$ $19.19 \pm 14.92\%$	$\begin{array}{c} 1.62 \pm 0.44\% \\ 2.01 \pm 0.99\% \\ 3.25 \pm 2.35\% \\ 15.68 \pm 10.44\% \end{array}$	$1.40 \pm 0.65\% \\ 0.72 \pm 0.37\% \\ 2.04 \pm 1.39\% \\ 3.23 \pm 3.76\%$



Figure A.1. Bar plot of MAPE of temperature field predictions by a purely data-driven model trained to predict 5 quantities of flow state (PDD-5), PDD model trained to predict 3 quantities of flow state (PDD), and hybrid NN-PDE model (Hybrid).

given the same number of learnable parameters naturally results in a deteriorated quality of the inferred results. Figure A.1 shows the MAPE of the temperature field predicted by this new variant (referred to as PDD-5) with the PDD approach described in section 3.3 and hybrid NN-PDE approach for the nonUniform-Bunsen32 case. Across all test cases, PDD-5 performs worse with an overall MAPE of $23.45 \pm 18.07\%$ than the PDD approach ($12.48 \pm 11.31\%$) as problem complexity has increased.