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Towards Building Robust Neural Network Models for Fluid Simulations¹ PEETAK MITRA, MAJID HAGHSHENAS, University of Massachusetts Amherst, NICCOLO DAL SANTO, CONOR DALY, SHOUNAK MI-TRA, MathWorks Inc, DAVID SCHMIDT, University of Massachusetts Amherst — The rise of Machine Learning (ML) for modeling complex problems in fluid physics has brought with it challenges in developing tools that are robust and explainable. Scientific data being high-dimensional, multimodal, and complex makes it difficult to choose the appropriate hyper-parameters for such networks. In this work, we explore the possibility to fully automate the network design process for a data-driven fluid physics emulator - in this case modeling a key turbulence prognostic critical for closure in a Large Eddy Simulation (LES) compressible flow code; including neural architecture search as well as optimizing the hyper-parameters using Bayesian principles. Further we investigate the network learnings by analyzing the gradient flows and conduct variance-based sensitivity analysis to understand the trained network predictions thereby improving explainability of these so called black-box models

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