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End-to-end Learning in Hybrid Modeling Systems: How to Deal with Backpropagation Through Numerical Solvers

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Artificial intelligence and deep learning are currently reshaping numerical simulation frameworks by introducing new modeling capabilities. These frameworks are extensively investigated in the context of model correction and parameterization where they demonstrate great potential and often outperform traditional physical models. Most of these efforts in defining hybrid dynamical systems follow offline learning strategies in which the neural parameterization (called here sub-model) is trained to output an ideal correction. Yet, these hybrid models can face hard limitations when defining what should be a relevant sub-model response that would translate into a good forecasting performance. End-to-end learning schemes, also referred to as online learning, could address such a shortcoming by allowing the deep learning sub-models to train on historical data. However, defining end-to-end training schemes for the calibration of neural sub-models in hybrid systems requires working with an optimization problem that involves the solver of the physical equations. Online learning methodologies thus require the numerical model to be differentiable, which is not the case for most modeling systems. To overcome this difficulty and bypass the differentiability challenge of physical models, we present an efficient and practical online learning approach for hybrid systems. The method, called EGA for Euler Gradient Approximation, assumes an additive neural correction to the physical model, and an explicit Euler approximation of the gradients. We demonstrate that the EGA converges to the exact gradients in the limit of infinitely small time steps. Numerical experiments are performed on various case studies, including prototypical ocean-atmosphere dynamics. Results show significant improvements over offline learning, highlighting the potential of end-to-end online learning for hybrid modeling.