Learning and Learning to Learn at Scale

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Progress in deep learning is anchored on a tripod: increased computational power, more sophisticated neural network architectures, and growing datasets. Tremendous advances have been made, but we are yet to maximize what is possible. Training of neural networks for vision and language model applications are inhibited by the prohibitive cost of model exploration and model training. Scientific applications of interest to the US Department of Energy and US national laboratories face additional challenges: (1) scientific data are often hard to label and require domain expertise, (2) the measure of uncertainty required by predictive models, and (3) satisfying scientific constraints. Given these requirements and others, neural network architectures must be frequently tuned for specific scientific applications requiring extensive architecture search and hyperparameter tuning. In this talk, I will present our on-going work in large-scale training and architecture search of deep neural networks. I will discuss different parallelization techniques in an HPC-centric deep learning toolkit- Livermore Big Artificial Neural Networks (LBANN)- and its extension for fast, robust, and scalable neural architecture search. Experimental results from different application domains including small molecule antiviral drug design for CoVID-19 will be presented.

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Zoom Link to Register for Remote Access:
us06web.zoom.us/meeting/register/tZwkcumrqzMuHdZPiZg7dbEhMURWvn5Zjws4

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