DATA SCIENCE INSTITUTE

Scaling Deep Learning for Cancer Drug Discovery on HPC Systems

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MOTIVATION

- Along with sources like PubChem, Genomics of Drug Sensitivity in Cancer (GDSC), and Genomics Data Common, the recently released NCI-ALMANAC database provides access to millions more cancer data samples than were previously available
- This exponential growth in size of cancer dataset makes parallel processing for large-scale deep learning an attractive tool for cancer research
- We present preliminary scaling studies of a deep learning algorithm for predicting tumor cell line response to drug pairs

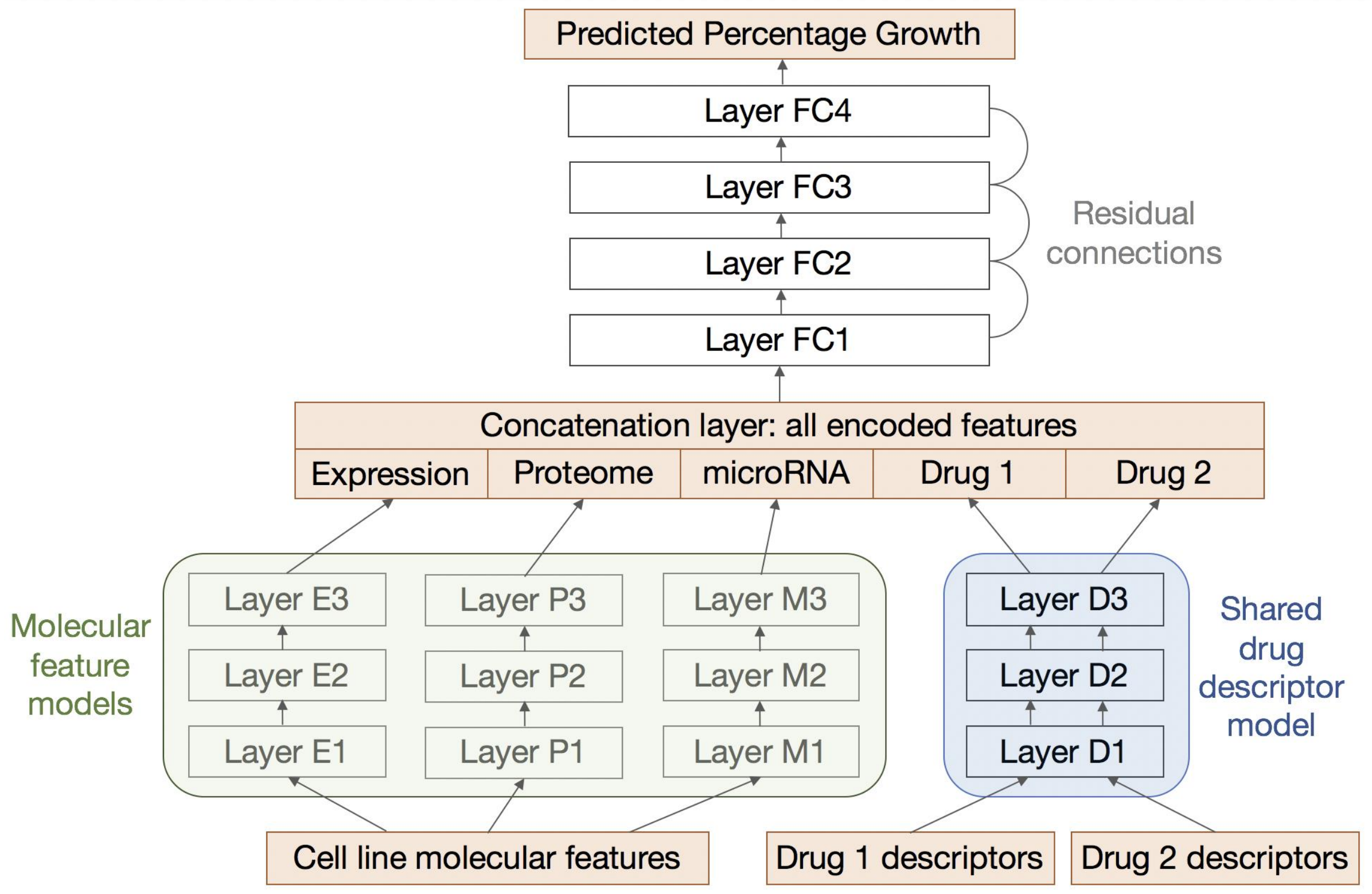
NEURAL NETWORK MODEL FOR PREDICTING TUMOR CELL LINE RESPONSE TO DRUG PAIRS

Regression Problem

- Given drug features D; descriptors, fingerprints, structure, dose etc
- And a combination of genomic cell feature τ; gene expression levels, protein abundance, microRNA expression, DNA etc
- Predictive (neural network) models quantify the response $R = f(\tau , D)$ of a given cell line τ to drug(s) D

Network Architecture

- Input is a combination of genomics features and drug descriptors
- Hidden (latent space) layers are multi-level multi-headed fully connected layers with lower level two paths consisting of drug and gene feature encoding submodels. These paths are later concatenated to feed the upper level “growth prediction” submodel
- Output is regression value typically measured with IC50 regression, G150, percentage tumor growth, or Z-score

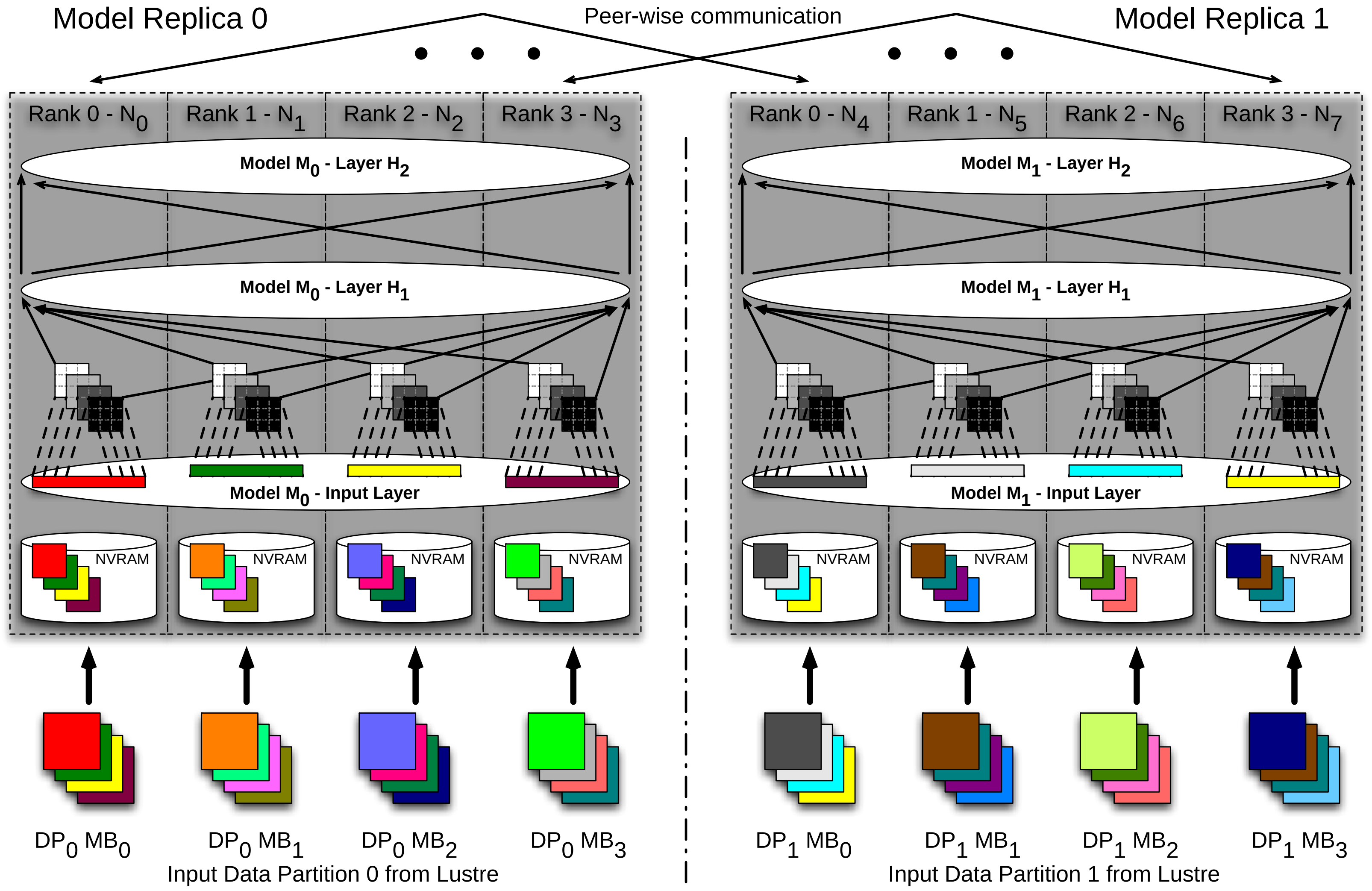


Combo model for predicting tumor cell line response to drug pairs [1]

PARALLELIZATION IN LBANN

Livermore Big Artificial Neural Network (LBANN) [2]

- HPC-centric deep learning toolkit
- Optimized distributed memory algorithm
- Optimized asynchronous all-reduce communication library
- Supports basic and advanced neural networks: MLP, CNN, RNN, GAN
- Exports to TensorFlow for finetuning, inference etc



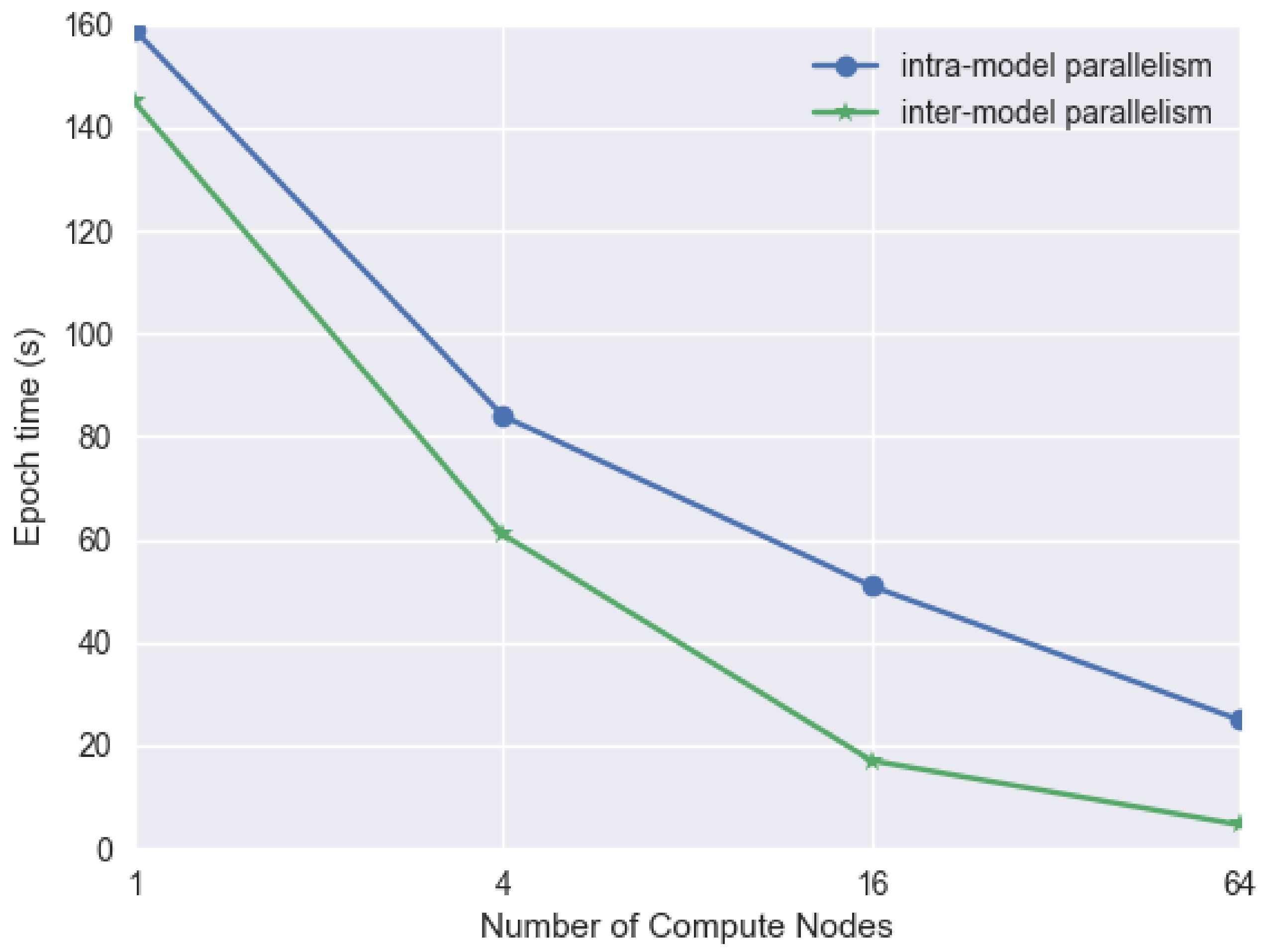
LBANN parallelism modes (distributing data samples and model parameters across processes)

Multiple Levels of Parallelism in LBANN

- Parallelism within one model instance (intra-model parallelism)
  - Model Parallel – distributed linear algebra
  - Data Parallel – distributed training data
- Parallelism across multiple model instances (inter-model parallelism)
  - Tightly coupled inter-trainer-peer-to-peer reduction trees
- Data parallelism across multiple models
  - Loosely-coupled inter-trainer data parallel tournament voting (LTFB[3])

EXPERIMENTAL RESULTS

- Dataset from NCI-ALMANAC database preprocessed for ingestion into LBANN. The preprocessed dataset consist of 244501 and 61125 training and test (validation) samples of cell-drugs combination respectively. Each sample consist of 8579 features
- Trained the Combo model on Catalyst HPC cluster at LLNL[4] with the following network architectures and hyper parameters: FC layers each of 1000 neurons, ReLU activations, dropout, Adam optimizer, 0.001 learning rate, 256 minibatch, and MSE loss



Strong scaling studies of Combo model

CONCLUSIONS

- Data-intensive scientific applications such as genomics present challenges and opportunities for exploring deep learning at scale
- We demonstrate LBANN as a toolkit for addressing problems of large data, large models training with promising results for further exploration (e.g., extension to complex models that predict the effect of multiple drugs on a tumor)

REFERENCES

1. Fangfang X. et.al., Predicting Tumor Cell Line Response to Drug Pairs with Deep Learning, CAFCW17
2. https://github.com/llnl/lbann
3. Jacobs S.A., Dryden N., Pearce R., Van Essen B., Towards Scalable Parallel Training of Deep Learning, MLHPC17
4. https://hpc.llnl.gov/hardware/platforms/catalyst

Towards Scalable Machine Learning for Scientific Discovery in HPC Environments

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