GNN Scaling – next steps

Steve Farrell
NERSC, LBNL

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Why should we use distributed training?

- We said we'd use HPC + distributed training in our proposal ;)
- It allows to more quickly train large models on large, complex datasets
- We have large, complex graphs; a lot of potential intra-event parallelism
- We can have large simulated datasets in HEP
- Publishing research on large scale GNN training will be valuable to the community

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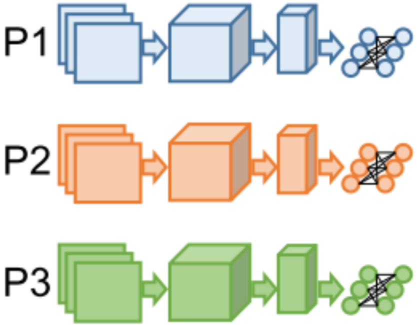
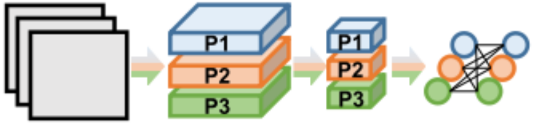
Parallelism strategies



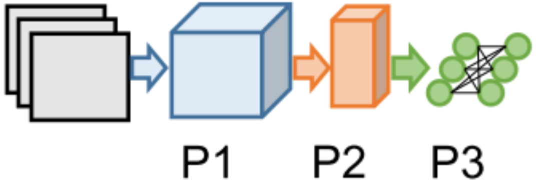
Data Parallelism

Distribute input samples.



Model Parallelism

Distribute network structure (layers).



Layer Pipelining

Partition by layer.

Fig. credit: Ben-Nun and Hoefler arXiv:1802.09941

Data parallelism, synchronous Updates

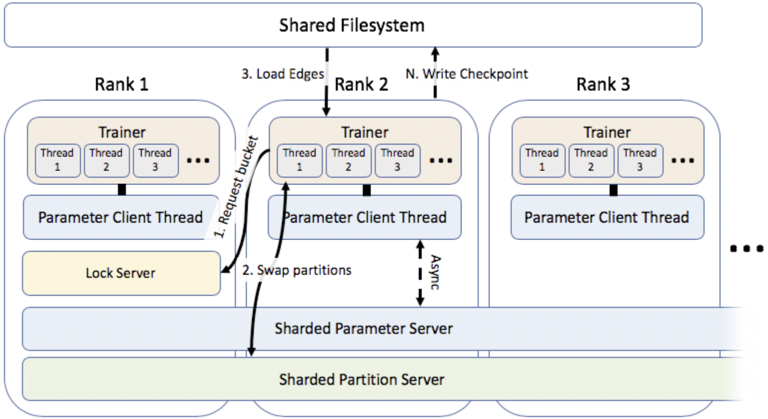
Gradients are computed locally and summed across nodes. Updates are propagated to all nodes

- stable convergence
- scaling is not optimal because all nodes have to wait for reduction to complete
- global (effective) batch size grows with number of nodes

Synchronous SGD, decentralized

Parallelizing Graph Neural Networks

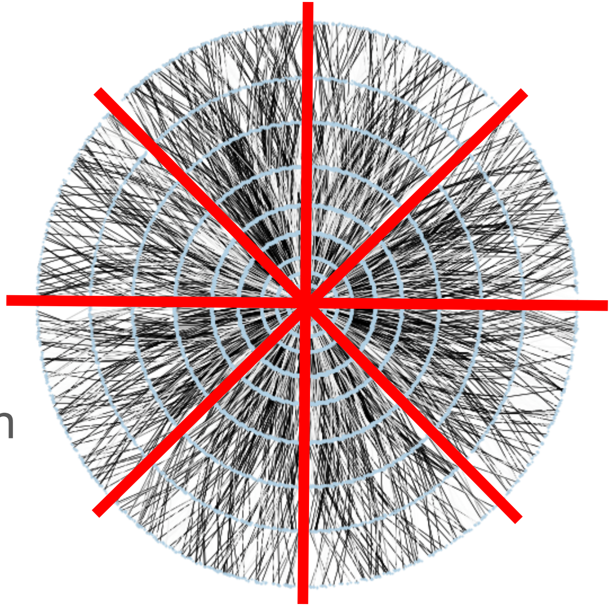
- Most deep learning literature on scaling training is on *computer vision applications*
- Graph deep learning is much newer, so methods for scaling are much less established
- Also, graph deep learning is a *diverse* set of applications, not all of which are applicable to us
  - E.g., FaceBook has (probably) the largest social network graph, but it's essentially just one enormous graph



PyTorch-BigGraph: https://arxiv.org/abs/1903.12287
"scale to graphs with billions of nodes and trillions of edges"

Our GNN parallelism

- Naïve domain parallelism
  - Split into sectors, train on them independently
  - You don't need the whole detector context to find tracks in a region
  - (Minor) technical challenges in doing inference on a whole event
  - Small batch sizes are good for generalization
- Proper domain parallelism
  - Break graph into sectors/partitions, but handle the boundaries with communication
  - Definitely more difficult to implement



Other approaches also under consideration

HPC scaling work with Cray BDC

- **Through the Cray Big Data Center collaboration, we’re engaging with folks from Cray and LBNL’s CRD to push on HPC scaling of GNNs (for tracking)**
  - Strong interest in scaling GNNs in PyTorch
  - The basic plan is to do large scale training of GNNs in a larger Population Based Training run
- **Computational challenges**
  - Graphs with sparse connectivity => need sparse op support
  - Variable sized graphs => need to handle load imbalance at scale
  - Large scale training of GNNs => not much experience/intuition
- **Using my PyTorch implementation of message-passing and “attention” networks here:** https://github.com/sparticlesteve/heptrkx-gnn-tracking

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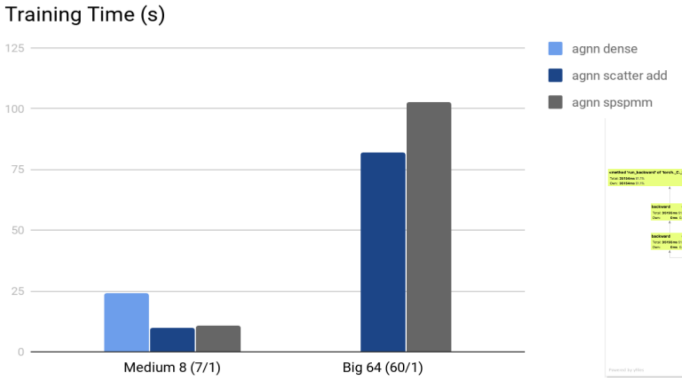
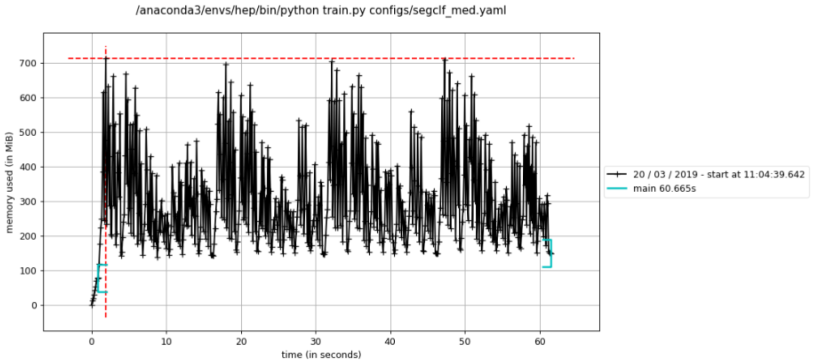
Single node performance [Saliya Ekanayake, LBNL]

- Compared speed and memory of dense and multiple sparse representations

	Training Time (s)		
Dataset N (tr/val)	**agnn dense**	**agnn scatter add**	**agnn spspmm**
Med 8 (7/1)	24.0416	9.63175	10.6389
Big 64 (60/4)		81.9128	102.74

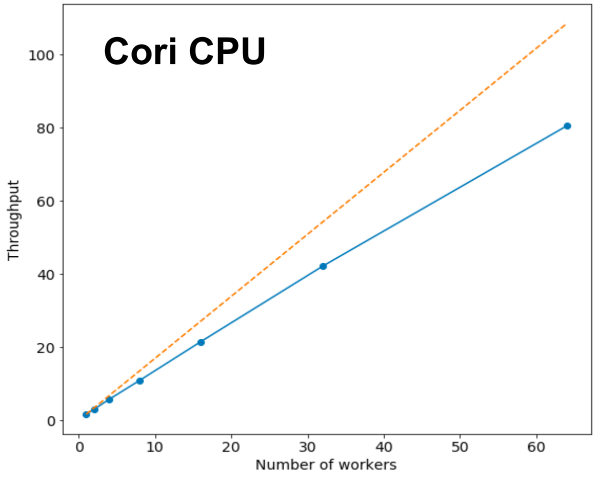


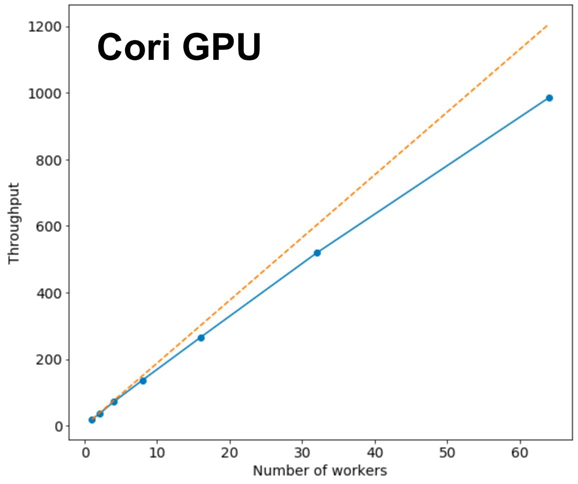
- **PyTorch-Geometric was the best of what we tested in terms of speed and memory**

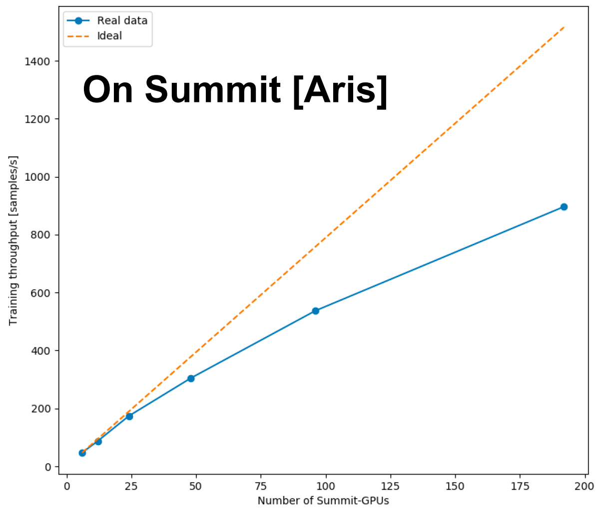


Scaling

- Distributed training scaling on OLCF and NERSC machines
- Scaling efficiency is not bad, actually, considering that it's expected to be adversely affected by load imbalance

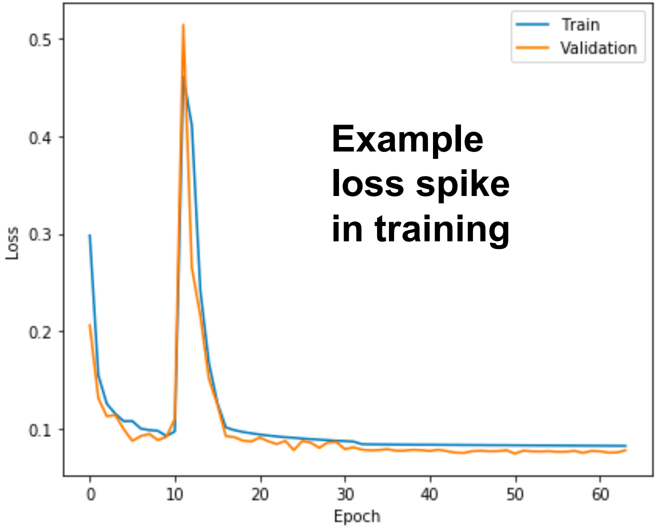






Training instabilities

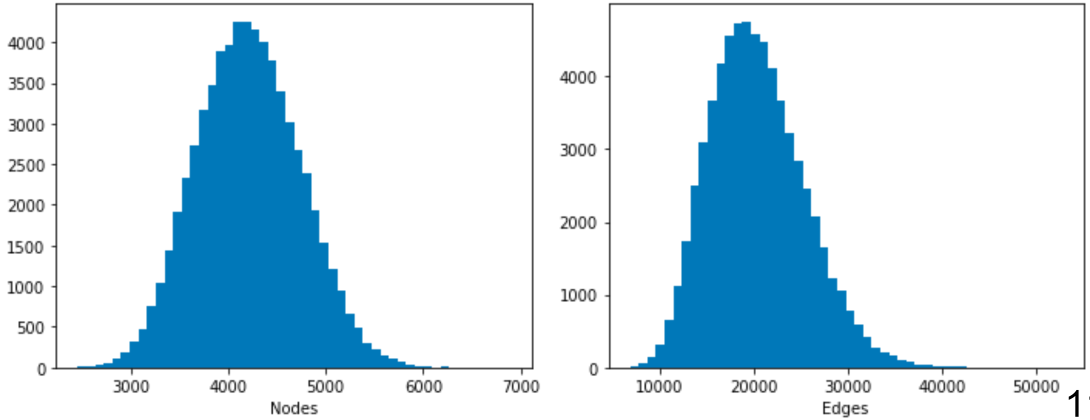
- Occasionally suffering from spikey/unstable behavior in the training loss when training distributed
- I've spent a bit of time digging into this
  - Tracking gradient norms, weight norms
  - Reducing graph size variance
  - Gets worse with larger models
  - Improved somewhat with layer norm, weight decay
- It was not fully solved, but I expect it's related to the interactions between, class weights (real vs. fake edges), variable sample sizes and purities, optimizer momentum, and gradient reductions as averages of averages.
- Other things expected to help
  - Stabilize training with auxiliary targets (e.g. predicting p_T)
  - Balance data sampling



Balanced data sampling

- Distribution of graph sizes leads to load imbalance
- Solution in development, inspired by the work done in Etalumis project: https://arxiv.org/abs/1907.03382
  - Bin dataset into buckets of similar "size"
  - Sample batches from these buckets
- There can be effects on convergence, which we'll need to study
  - It worked for Etalumis, though

Graph size variability



Outlook and next steps

- This work stalled because of lack of time, but is now being picked back up
- Our original plan was to use Cori KNL for a large scale study (and submit to something like SC, IPDPS), but this has been abandoned
  - KNL speed was factor ~8 slower than Haswell, would require considerable effort with Intel to improve; decided not worth it
  - Haswell system could still be useful, though it is in high demand nowadays
- Current plan is to target a smaller system with GPUs (e.g. Cori-GPU) to wrap up the work with Cray, and submit to a workshop
- After that, there are more fun things to do
  - Push further on scaling, run on Summit and upcoming Perlmutter
  - Smarter graph partitioning/parallelization
  - Scale the newer methods explored by Nick and Daniel (and others)

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