

Democratizing AI: Open-source Scalable LLM Training on GPU-based Supercomputers

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PS PARALLEL SOFTWARE **G** AND SYSTEMS GROUP





ACM Gordon Bell Prize '24 Finalist

MARYLAND



ACM Gordon Bell Prize

• Awarded annually by ACM to recognize major achievements in HPC

- Focus on innovations in scalability and potential real-world impact

 - Scientific impact Contributions to a scientific domain

Six Finalists at Supercomputing 24 - two of which focused on large scale LLM training.





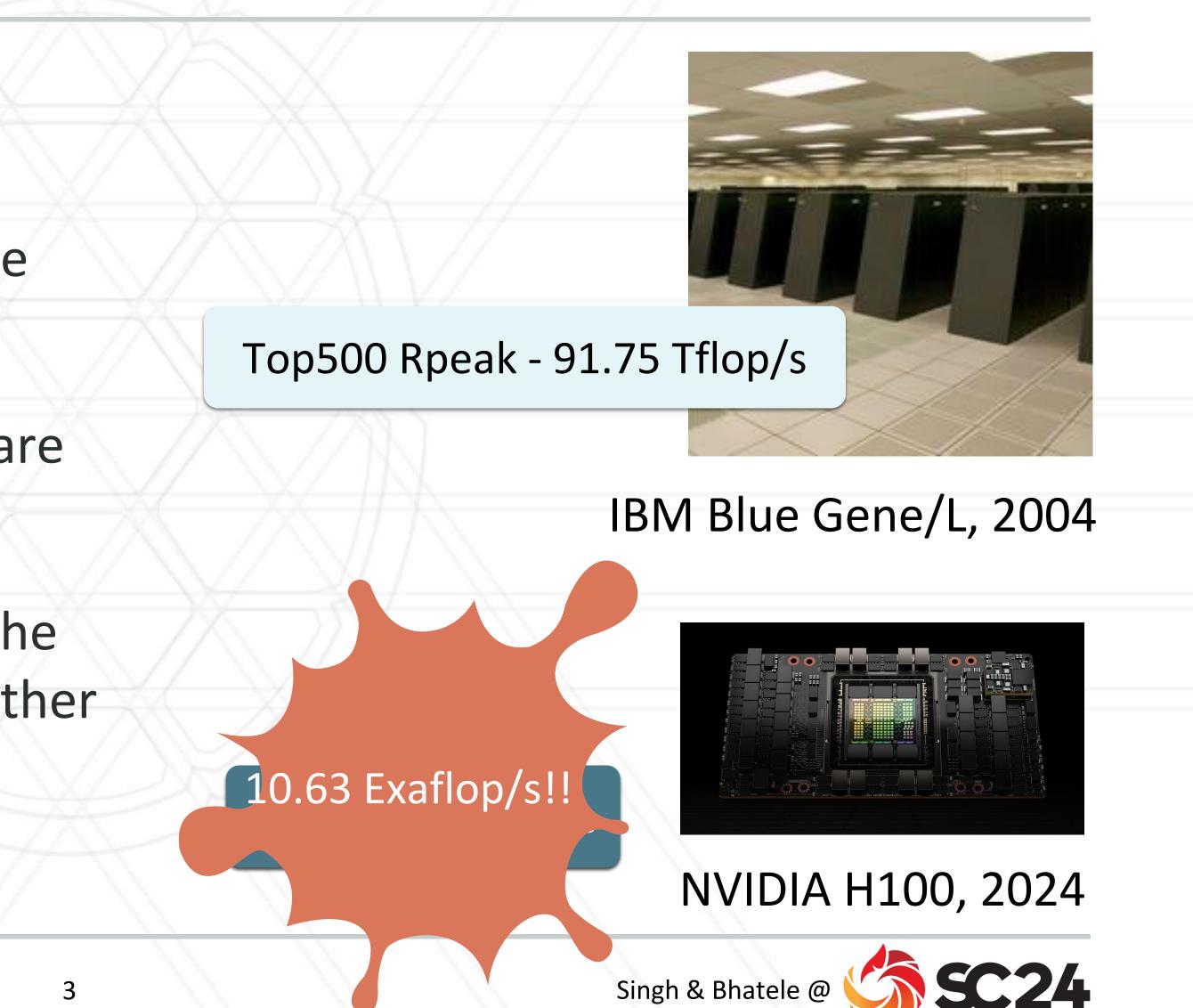
• Scalability – Use as many compute resources (GPUs/CPUs) as efficiently as possible [aka FLOPs-Maxxing]



The evolution of HPC systems and rise of a new revolution in Al

- In the last two decades, an enormous amount of compute power has become available
- Large datasets and open source software such as PyTorch have also emerged
- Led to a frenzy in the world of AI and the effects are being felt in almost every other domain





A few things that are unique about this Gordon Bell submission

- An all CS team only composed of students and academics
- Our "science" problem is not from a traditional computational science domain but from computer science — AI / machine learning
- We report bfloat16 (half-precision) flop/s on tensor cores (of GPUs)
 - 2024 is the first year when AI papers reporting fp16/bf16 flop/s are Gordon Bell finalists

Industs			
		FP64 Exaflop/s	FP16 Exaflop/s
	El Capitan	2.746	43.67
	Frontier	2.056	14.42
	Alps	0.575	10.63





Memorization in Large Language Models A @DocSparse

LLMs can be made to output training data verbatim and this "memorization" increases with model size, and repetitions in training data

The Times Sues OpenAI and Microsoft **Over A.I. Use of Copyrighted Work**

Millions of articles from The New York Times were used to train chatbots that now compete with it, the lawsuit said.

https://x.com/DocSparse/status/1581461734665367554 https://spectrum.ieee.org/midjourney-copyright https://www.nytimes.com/2023/12/27/business/media/new-york-times-open-ai-microsoft-lawsuit.html



@github copilot, with "public code" blocked, emits large chunks of my copyrighted code, with no attribution, no LGPL license. For example, the simple prompt "sparse matrix transpose, cs_" produces my cs_transpose in CSparse. My code on left, github on right. Not OK.

	GitHub Copilot - Javastuff - Visual Studio Code	
	liew Go Run Terminal Help	
,	C Unstitled-T.cpp S C visit counter to the counter to th	C Gibbub Copilot X d 1 Synthesizing 10/10 solutions 2 3 annual Accept Solution
1	File Edit View Search Terminal Help	<pre>5 cs_transpose (const cs *A, int values)</pre>
	<pre>#include "cs.h" /* C = A' */ cs *cs_transpose (const cs *A, csi values) { csi p, q, j, *Cp, *Ci, n, m, *Ap, *Ai, *w ; double *Cx, *Ax ; cs *C ; if (!CS_CSC (A)) return (NULL) ; /* check inputs */ m = A->m ; n = A->n ; Ap = A->p ; Ai = A->i ; Ax = A->x ; C = cs_spalloc (n, m, Ap [n], values && Ax, 0) ; /* allocate result */ w = cs_calloc (m, sizeof (csi)) ; /* get workspace */ if (!C !w) return (cs_done (C, w, NULL, 0)) ; /* out of memory */ Cp = C->p ; Ci = C->i ; Cx = C->x ; for (p = 0 ; p < Ap [n] ; p++) w [Ai [p]]++ ; /* row counts */</pre>	<pre> (int p, q, j, +Cp, *Ci, *w, *Ti, *Tj ; double *Cx, *Tx ; cs *T; if (ICS_CSC (A) ICS_TRIPLET (A)) return (NULL) ; // check inputs T = cs_spalloc (A->n, A->m, A->nzmax, values && A->x, 0) ; w = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); w = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); w = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); w = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); w = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); w = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); v = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); v = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); v = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); v = cs_calloc (A->n, A->m, A->nzmax, values && A->x, 0); for (p = T->p; Ci = T->i; Cx = T->x; Ti = A->i; Tj = A->j; for (p = 0; p < A->nzmax; p++) w [Ti [p]]++; // column counts cs_cumsum (Cp, w, A->m); // column pointers for (j = 0; j < A->n; j++) { for (j = 0; j < A->n; j++) { for (p = A->p [j]; p < A->p [j+1]; p++) {</pre>
	<pre>tor (p = 0 ; p < Ap [n] ; p++) w [At [p]]++ ; /* row counts */ cs_cumsum (Cp, w, m) ; for (j = 0 ; j < n ; j++) { for (p = Ap [j] ; p < Ap [j+1] ; p++) { Ci [q = w [Ai [p]]++] = j ; /* place A(i,j) as entry C(j,i) */ if (Cx) Cx [q] = Ax [p] ; } } return (cs_done (C, w, NULL, 1)) ; /* success; free w and return C */</pre>	<pre>25</pre>

Generative AI Has a Visual Plagiarism Problem >Experiments with Midjourney and DALL-E 3 show a copyright minefield

BY GARY MARCUS REID SOUTHEN 06 JAN 2024 20 MIN READ

ICLR 2023. https://arxiv.org/abs/2202.07646





Catastrophic memorization at scale

- Ability to memorize large documents appears only in large models
- Catastrophic memorization: even a single pass is sufficient

Case 1:23-cv-11195 Document 1-68 Filed 12/27/23 Page 107 of 127

ONE HUNDRED EXAMPLES OF GPT-4 MEMORIZING CONTENT FROM THE NEW YORK TIMES 106

EXAMPLE 88: SCIENTISTS FIND HINTS OF LIFE IN CLOUDS OF VENUS

https://www.nytimes.com/2020/09/14/science/venus-life-clouds.html Copyright number: TX 8 919-710 Effective Date: 2020-11-04

Prompt (taken from article): High in the toxic atmosphere of the planet

Output from GPT-4:

Venus, astronomers on Earth have discovered signs Venus, astronomers on Earth have discovered signs of what might be life.

If the discovery is confirmed by additional telescope If the discovery is confirmed by additional telescope observations and future space missions, it could turn the gaze of scientists to one of the brightest objects in the night sky. Venus, named after the Roman goddess of beauty, roasts at temperatures of hundreds of degrees and is cloaked by clouds that contain droplets of corrosive sulfuric acid. Few have focused on the rocky planet as a habitat for something living.

Instead, for decades, scientists have sought signs of Instead, for decades, scientists have sought signs of life elsewhere, usually peering outward to Mars and life elsewhere, usually peering outward to Mars and more recently at Europa, Enceladus and other icy more recently at Europa, Enceladus and other icy moons of the giant planets.

The astronomers who reported the finding on Moncrobes, nor have they snapped any pictures of them. But with powerful telescopes, they have detected any pictures of them. But with powerful telescopes,

Actual text from NYTimes:

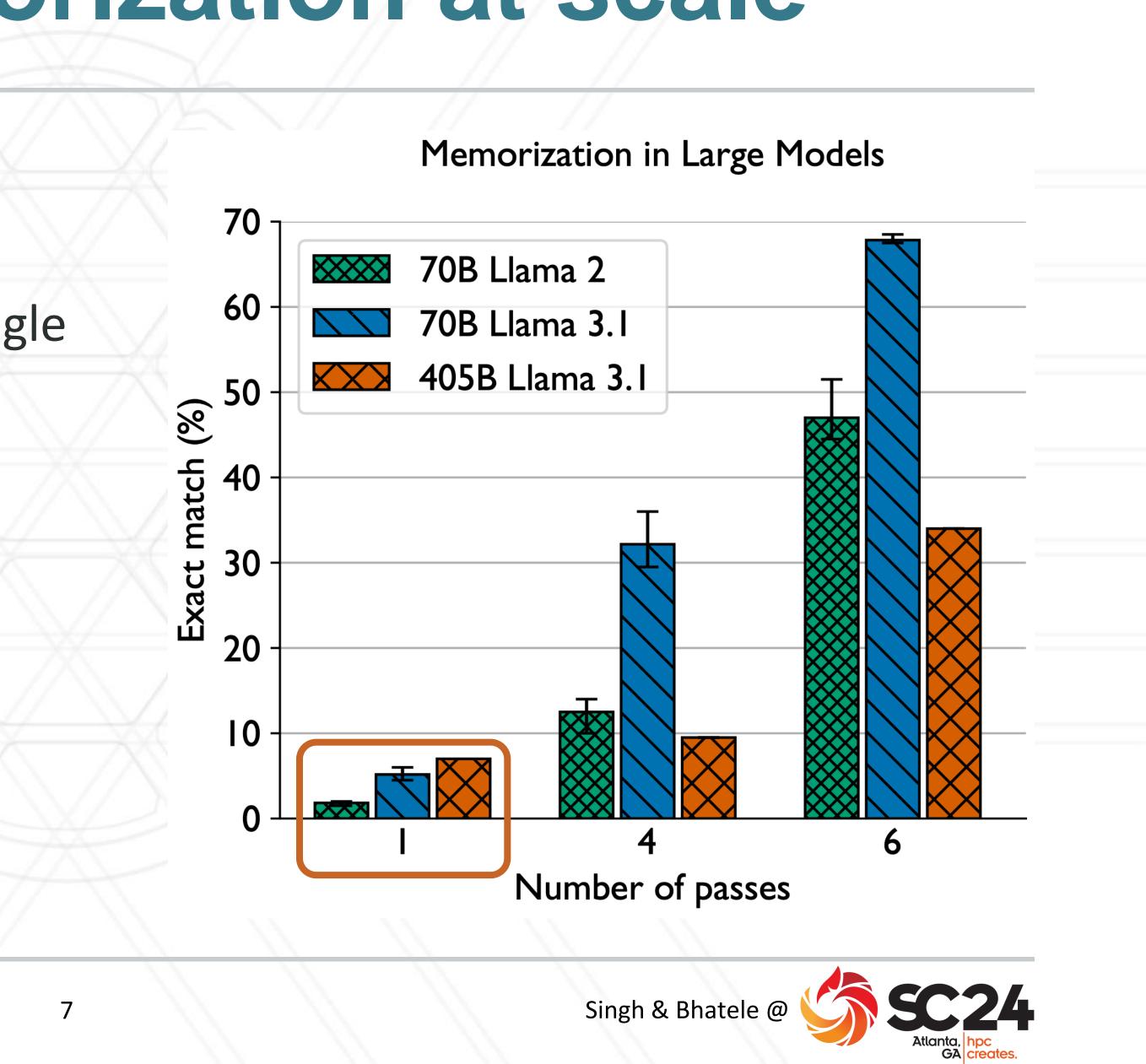
of what might be life.

observations and future space missions, it could turn the gaze of scientists toward one of the brightest objects in the night sky. Venus, named after the Roman goddess of beauty, roasts at temperatures of hundreds of degrees and is cloaked by clouds that contain droplets of corrosive sulfuric acid. Few have focused on the rocky planet as a habitat for something living.

moons of the giant planets.

The astronomers, who reported the finding on Monday have not collected specimens of Venusian mi- day in a pair of papers, have not collected specimens of Venusian microbes, nor have they snapped

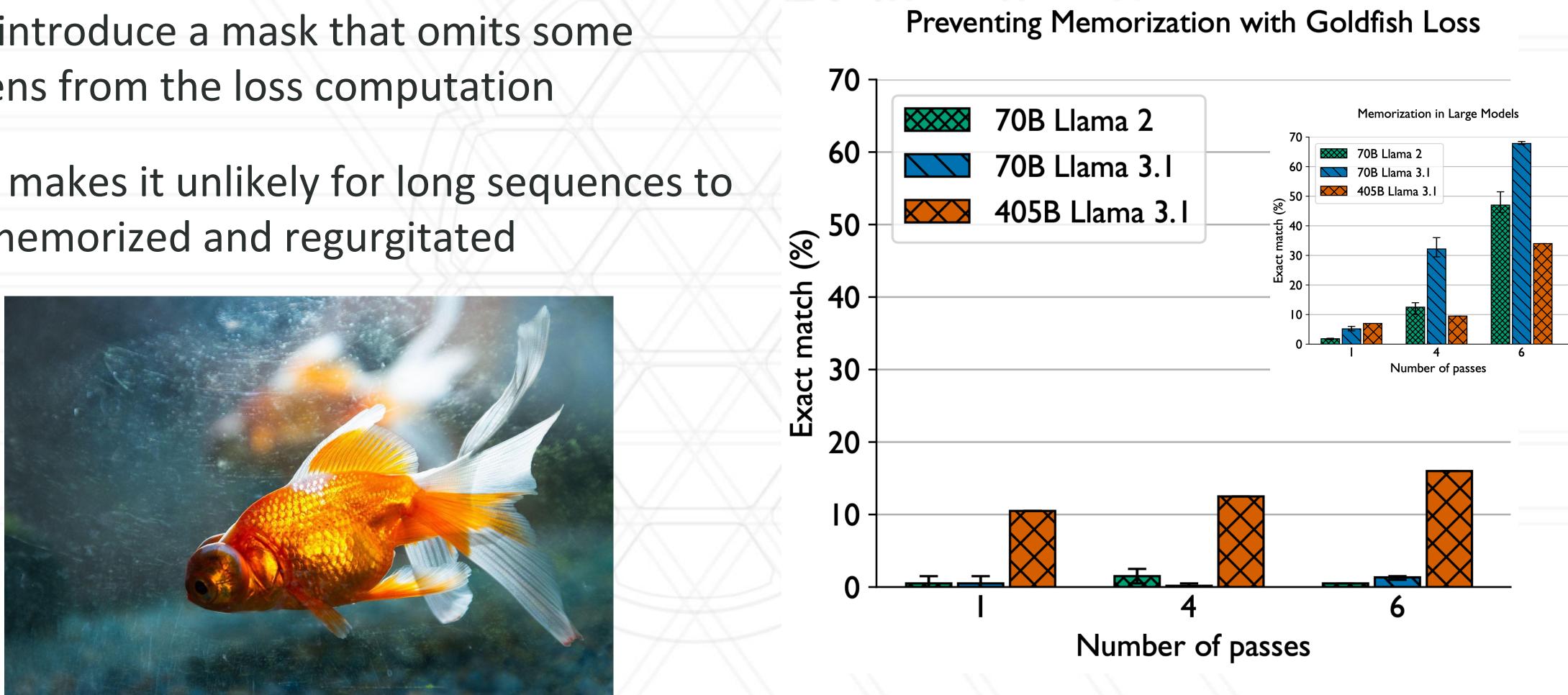






Solution: "Goldfish loss" to prevent memorization

- We introduce a mask that omits some tokens from the loss computation
- This makes it unlikely for long sequences to be memorized and regurgitated











- The largest model you can run on an H100 96 GB GPU is around 3.5-4 billion parameters
- On a single node (with four H100 GPUs): around ~16 billion parameters model
- Training a 16B parameter would take 33 years!
- OpenAl's GPT 4.0 is estimated to have 1.8 trillion parameters
- Meta's Llama-3.1-405B has more than 400 billion parameters



Do we really need parallel resources?



n Sequential LLM training W k k 0 m while (remaining batches) {

Read a single batch

Forward pass: perform matrix multiplies to compute output activations, and a loss on the batch

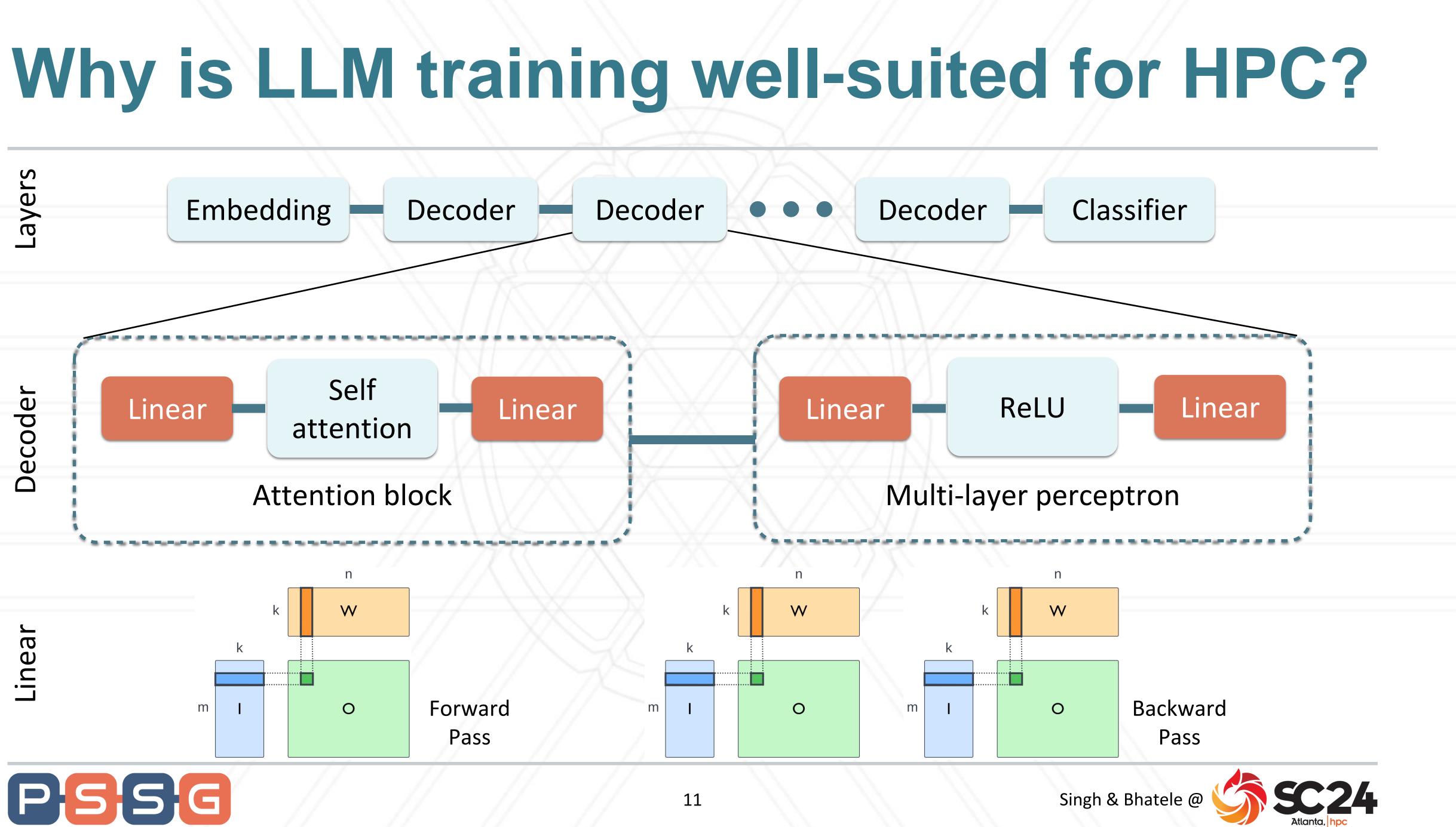
Backward pass: matrix multiplies to compute gradients of the loss w.r.t. parameters via backpropagation

Optimizer step: use gradients to update the weights or parameters such that loss is gradually reduced









How to scale training to 1000s of GPUs?

Step 1: Choose a performant parallel algorithm

- Step 2: Minimize communication overheads

 - Step 2b: Overlapping Computation with Communication

Step 3: Other optimizations



Step 2a: Strategy for communication-optimal work decomposition to GPUs (via heuristics or modelling)



Systems/HPC Innovations in AxoNN_

- 3D parallelization of tensor computations
- Aggressive overlap of computation with communication
- Tuning how we call BLAS routines
- An easy-to-use API for parallelizing serial deep learning models



1. Choose a performant algorithm

• A communication performance model to choose the best decomposition of GPUs

approach to parallel matrix

multiplication

3. Overlap of computation with communication A IIIeedimensional

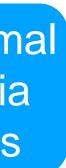
2. Communication-optimal work decomposition via modelling or heuristics

> by R. C. Agarwal S. M. Balle F. G. Gustavson M. Joshi P. Palkar

IBM J. Res. Dev., 1995











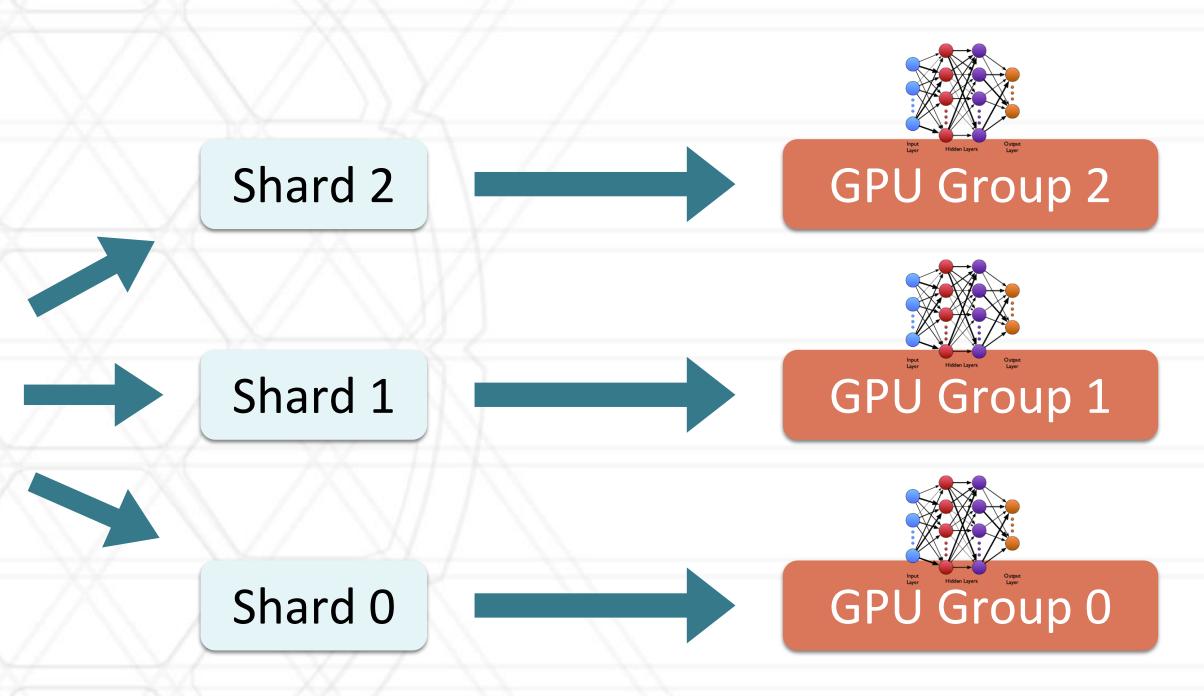
1 A four-dimensional hybrid parallel approach

A hybrid parallelism approach

Batch

Combines data parallelism with 3-dimensional parallel matrix multiplication (PMM)





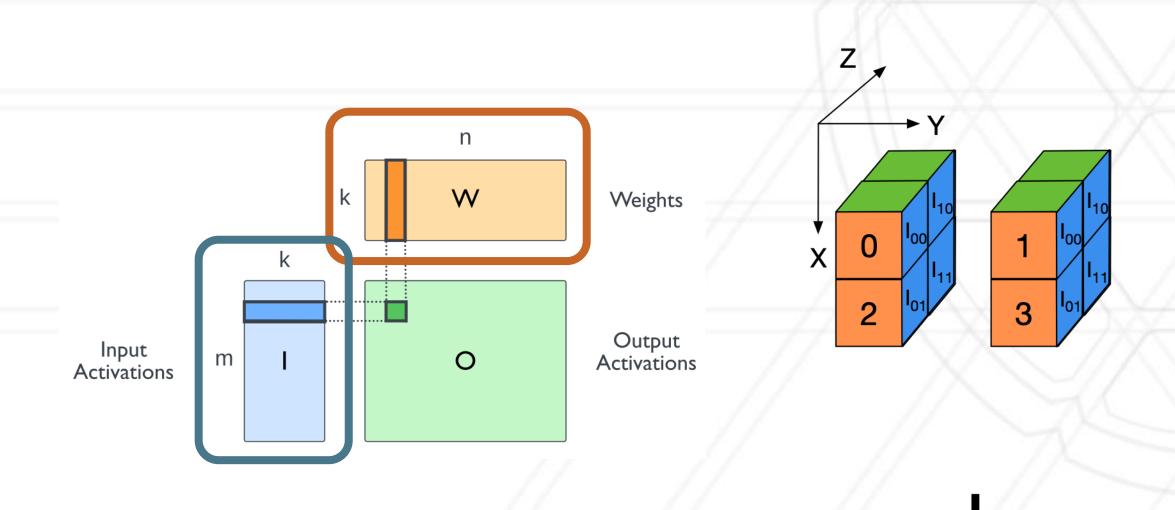
Data Parallelism



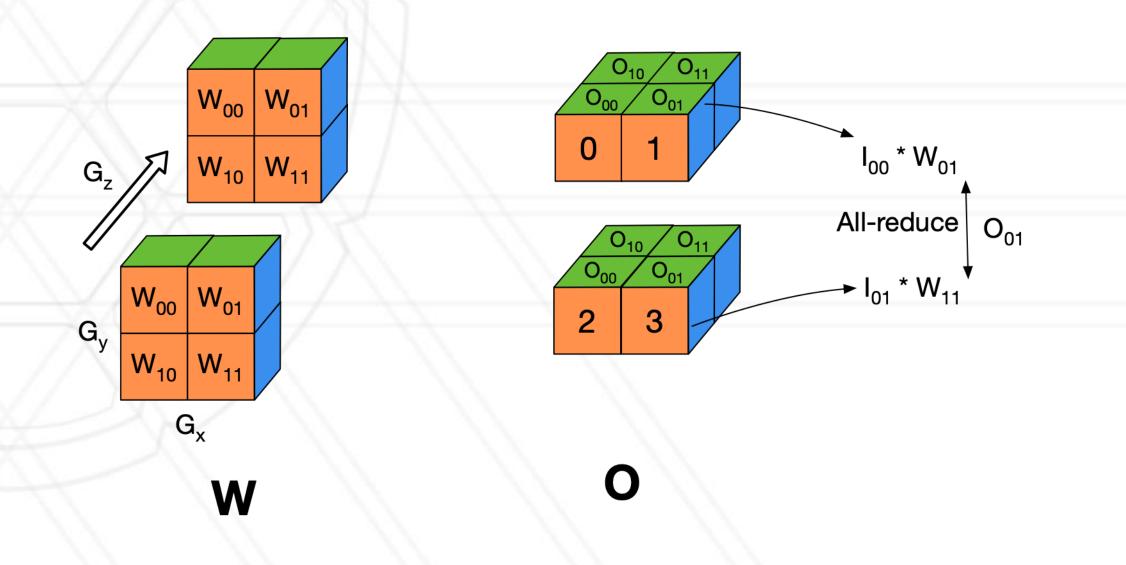


Enabling 3D parallel matrix multiplication in AxoNN

- Each layer is multiplying input activations with weights to produce output activations
- Distribute I and W across a 3D grid of GPUs Compute partial output activations, O on each GPU









2 A Network-aware Communication Model for Work Decomposition

- We have to decompose the GPU allocation (G GPUs) into a 4-dimensional virtual grid, G_{data} * G_x * G_y * G_z = G
 - Problem: what is the optimal number of GPUs in each dimension (G_{data}, G_x, G_y, G_z) w.r.t. performance
- Challenge: the search space of configurations grows with the number of GPUs
 - For example, for 32K GPUs, there are >800 unique configurations
- Solution: A communication model to prune the search space
 - Takes message sizes, collective algorithms, and bandwidths into account
 - The model ranks the configurations in order of decreasing expected performance



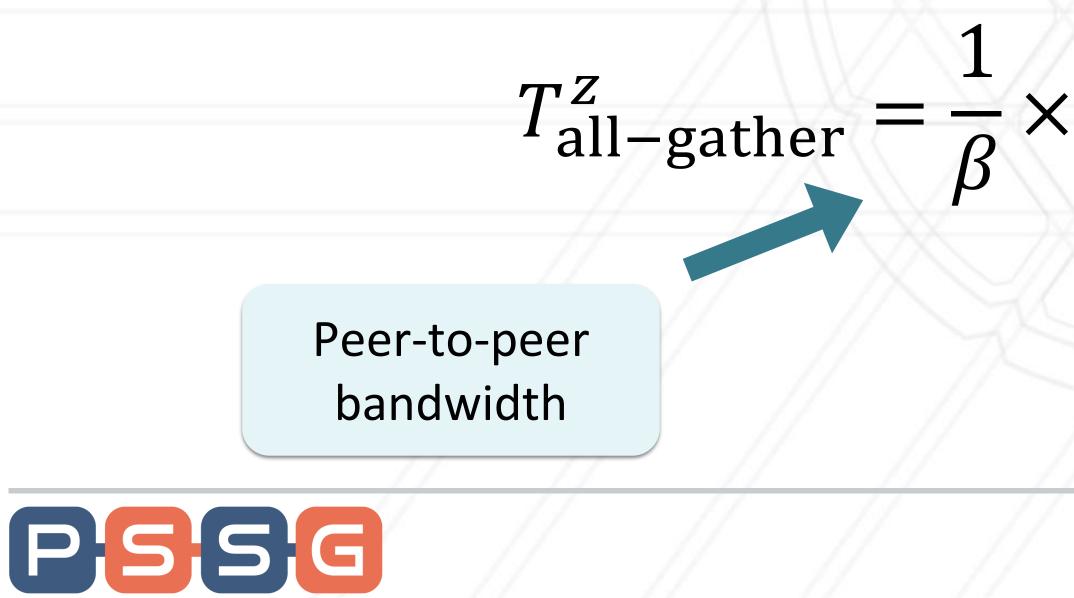


2 Inner workings of the communication model

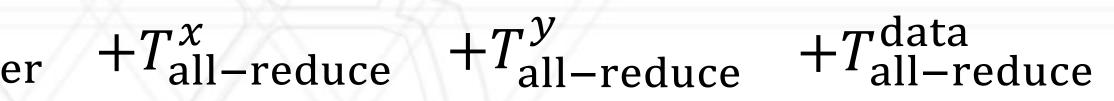
Predict total time spent in communication

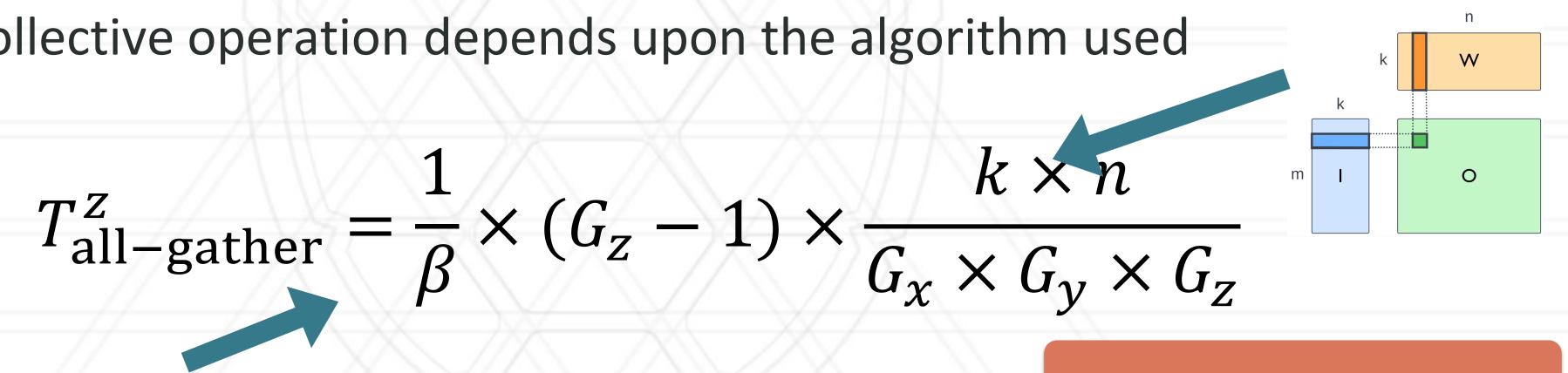
$$T_{\rm comm} = T_{\rm all-gather}^{z} + T_{\rm reduce-scatter}^{z}$$

• Time of each collective operation depends upon the algorithm used





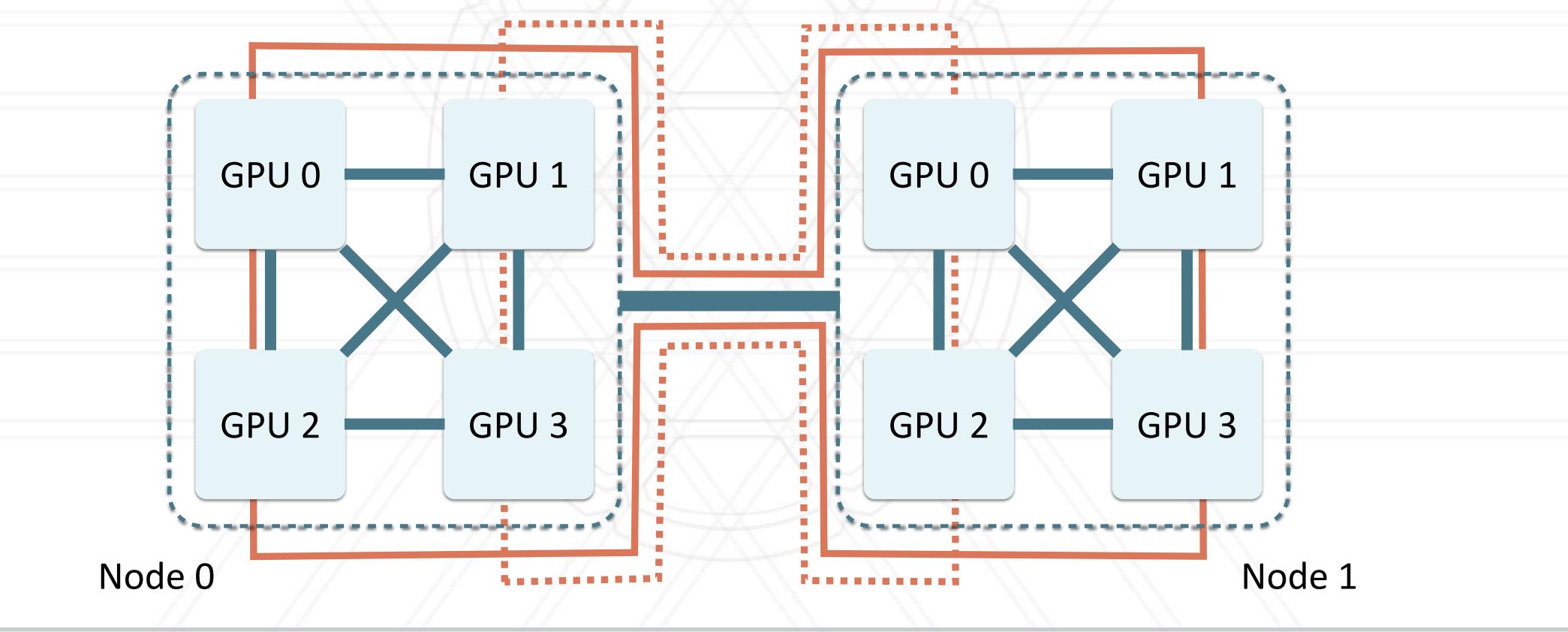




Find near-optimal values of G_{data}, G_x, G_y, G_z



Modeling bandwidth available to each collective operation





• Expected bandwidths are calculated based on number of collectives using a link



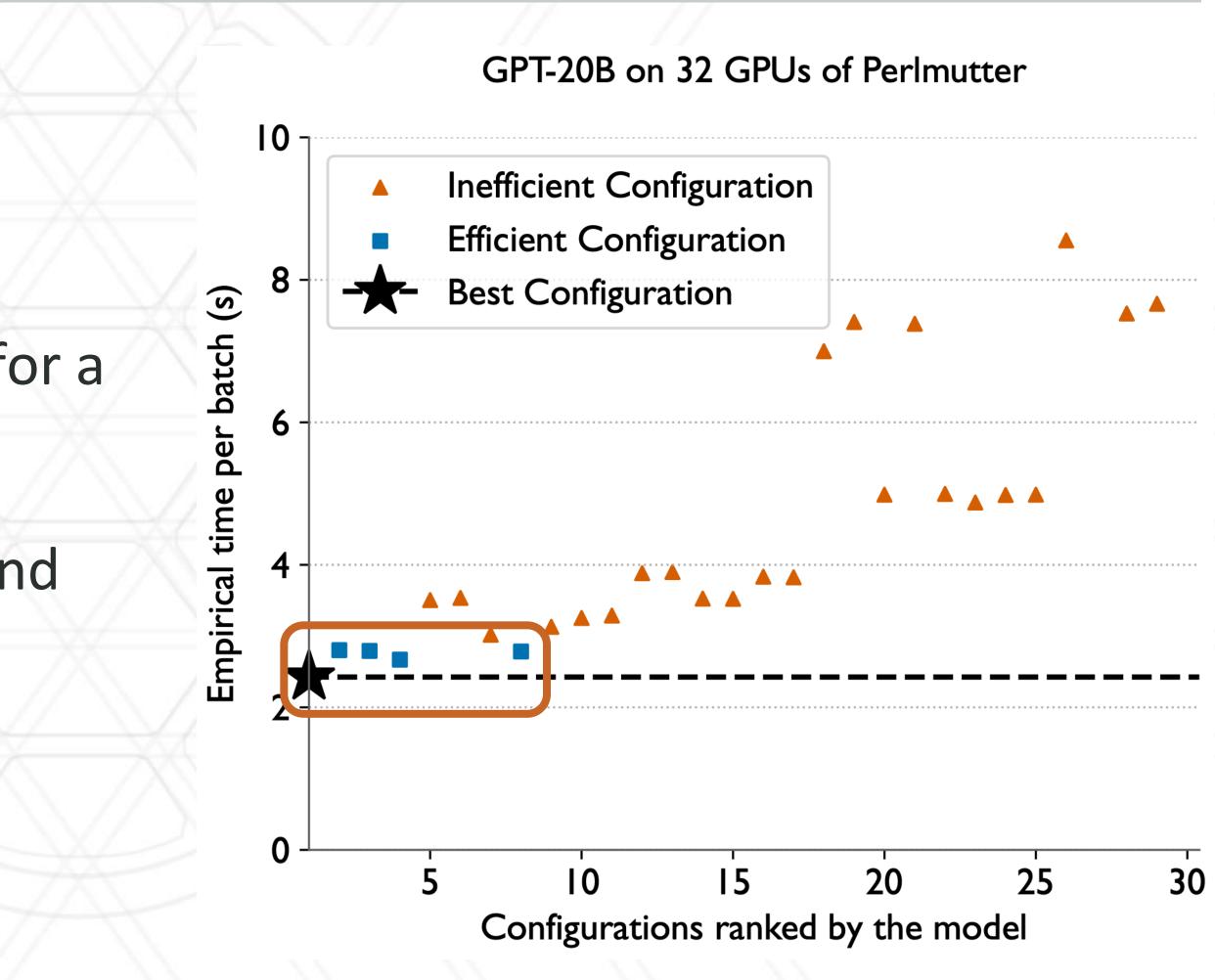


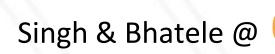


2 Validating the model

- We ran all possible 4D configurations for a "small" model on 32 GPUs
- Compare model predictions with ground truth



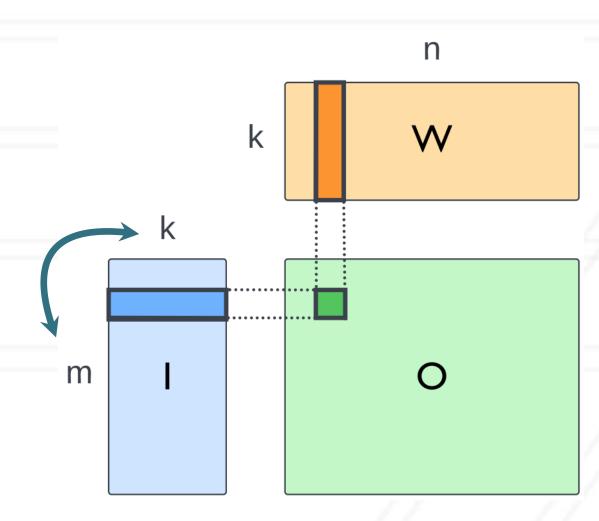




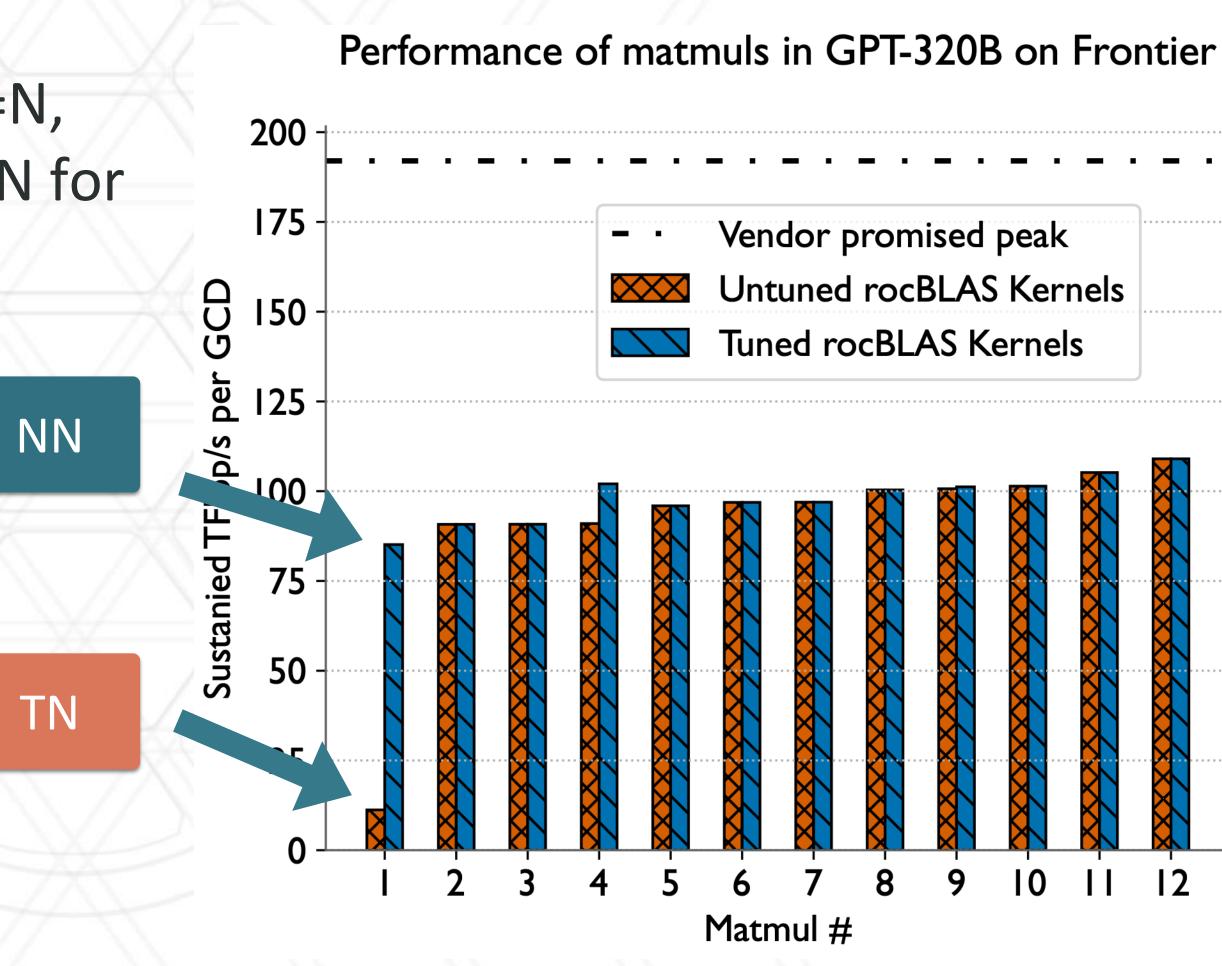


3 Tuning BLAS kernels

 Calling rocblas_gemm_ex with transA=N, transB=N is significantly faster than T, N for some matrix multiplies







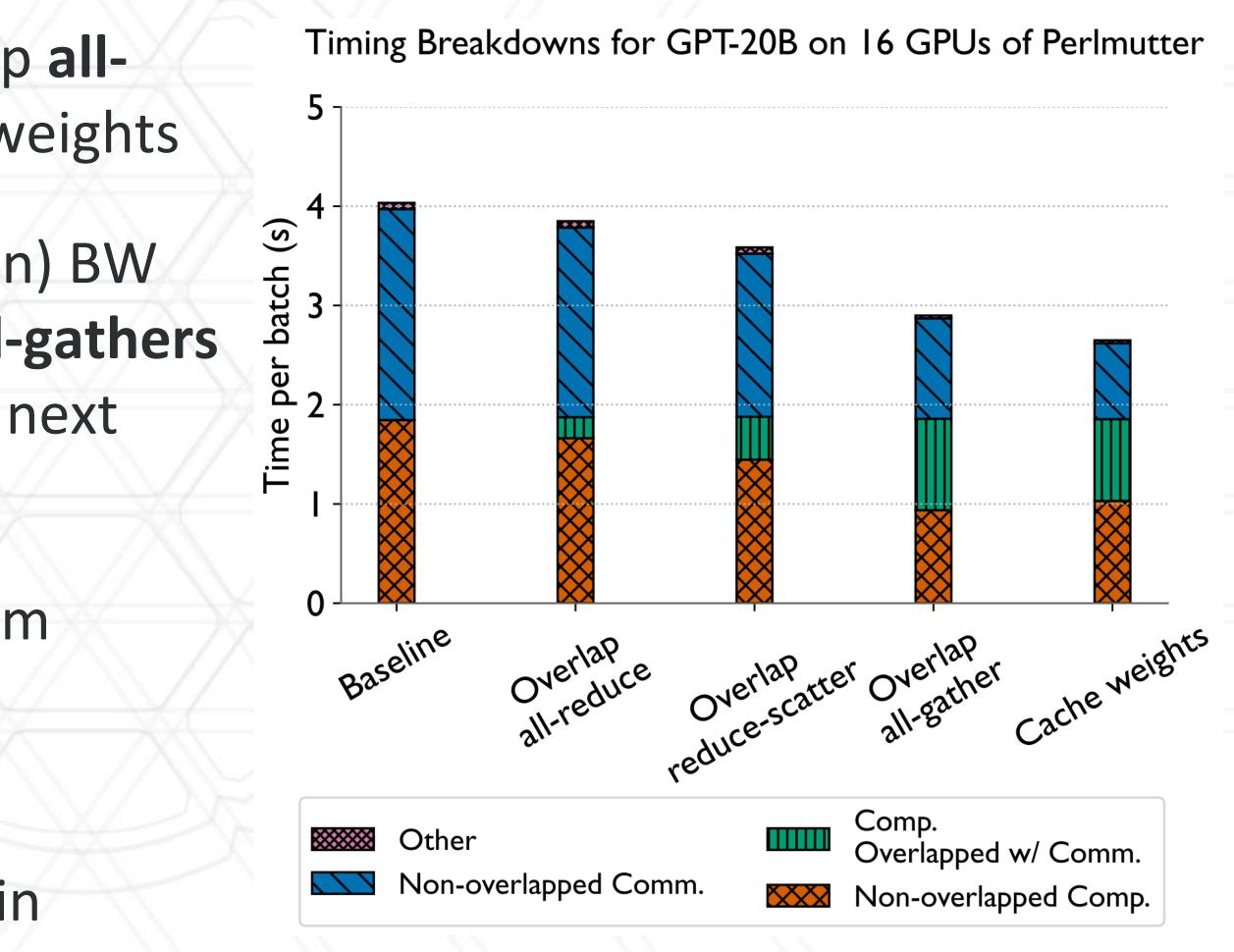




4 Overlap non-blocking collectives with computation

- BW pass, tensor parallel phase: overlap allreduces with calculating gradients of weights
- FW pass and (necessary FW pass within) BW pass, tensor parallel phase: overlap all-gathers of previous layer with computation of next layer
- BW pass, tensor parallel phase: perform reduce-scatters of the gradients asynchronously for the entire model
- Cache all-gathers that are needed again









5 Easy parallelization using AxoNN

- Requires minimal code changes to model architecture (code):

 - with auto parallelize():
- Our ML collaborators used this mode for the memorization experiments
- We also have backends for lightning and accelerate

PSSG

from axonn.intra layer import auto parallelize

net = # declare your sequential model here

• AxoNN intercepts all declarations of torch.nn.Linear, and parallelizes them



Experimental Setup



• You can either keep the model size fixed and keep increasing the batch size — embarrassingly parallel.

• Keep the batch sized fixed and increase the model size — a significantly more challenging problem!

Strong scaling







Friends don't let friends use batch sizes larger than **16M** Yann LeCun 📀 🙉 @ylecun

Well-established in the ML community: batch sizes cannot be increased arbitrarily — leads to convergence issues

Study	Framework	Model Size	Ba	
SUPER	LBANN	3B*		
KARMA	KARMA	17B		
FORGE	GPT-NeoX	1.44B		
Dash et al. [1]	Megatron-DeepSpeed	1000B		
MT-NLG	Megatron-DeepSpeed	530B		
Narayanan et al. [2]	Megatron-LM	1000B		
MegaScale	MegaScale	175B		
Google	Cloud TPU Training	32B		
		40B		
This Work	AxoNN [3]	320B		
		60B		





Training with large minibatches is bad for your health. More importantly, it's bad for your test error.

Friends dont let friends use minibatches larger than 32.



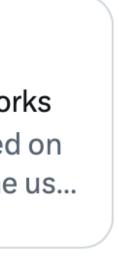
arxiv.org

Revisiting Small Batch Training for Deep Neural Networks Modern deep neural network training is typically based on mini-batch stochastic gradient optimization. While the us...

atch Size

0.5M*	5:00 PM · Apr 26, 2018					
2.0M* 16.8M 19.7M	Q 26	ቲጊ 553	💙 1.5K	167		
4.0M 6.3M						
12.5M 417M						
16.8M 16.8M						
16.8M			https://x.com/ylecun/	status/9896102084973608	8	

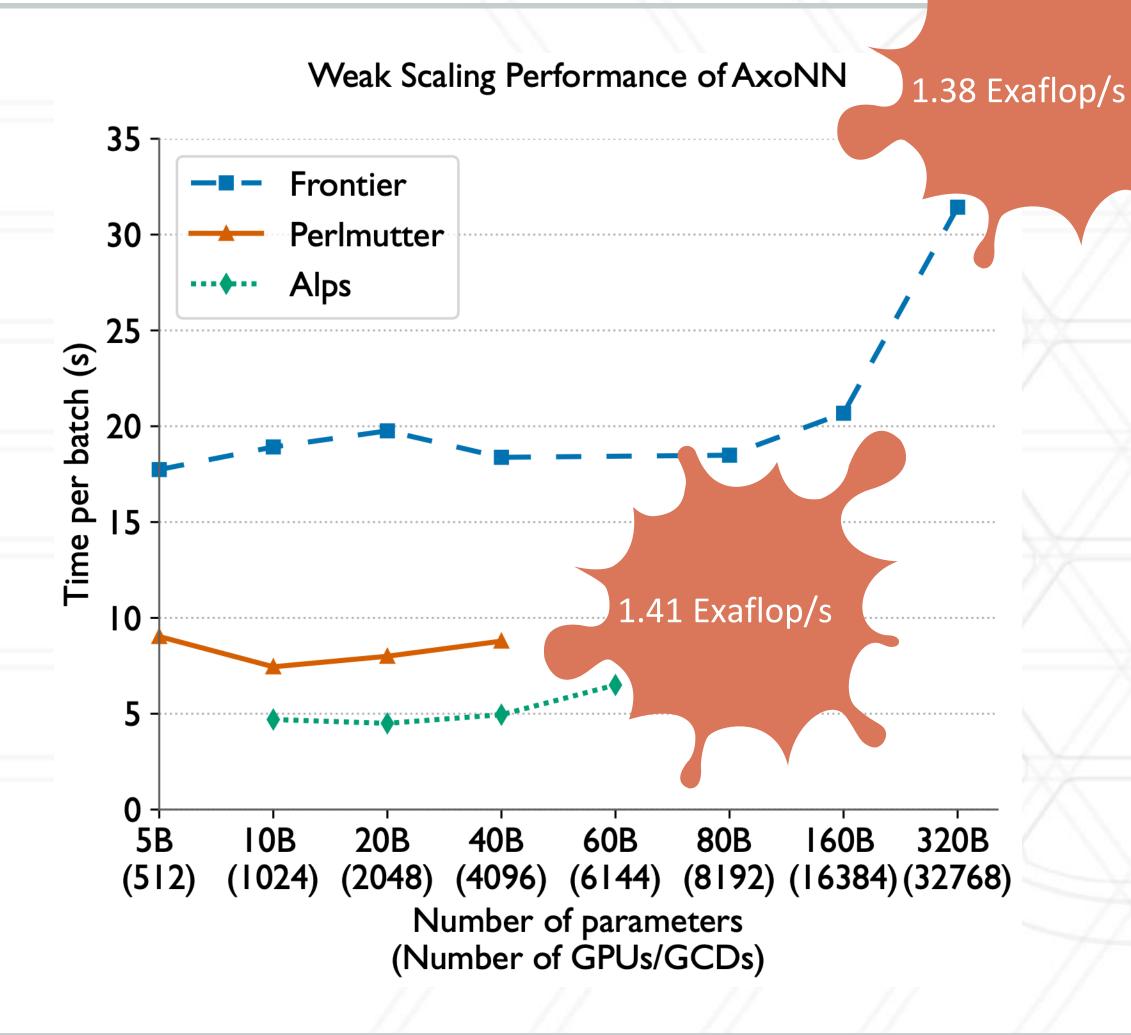




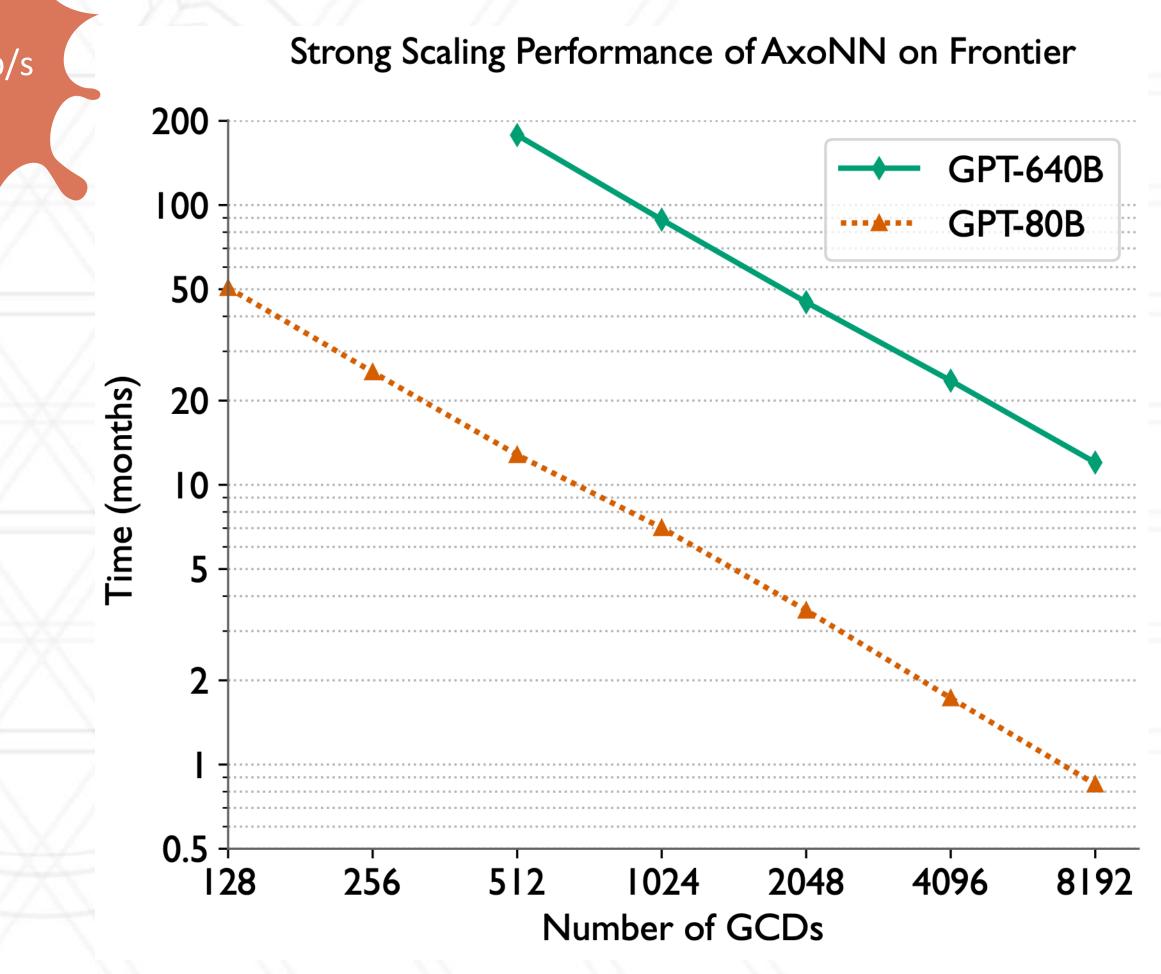




Weak scaling performance











Summary

- LLMs
- Several innovations in AxoNN have enabled us to scale the challenging tensor 16,000 GPUs
- Achieved flop/s of >1.4 BF16 Exaflop/s
- AxoNN: an open-source highly scalable framework for pre-training/finetuning/inference



• Parallel fine-tuning using AxoNN has enabled large-scale memorization studies in

parallelism mode with production (<=16M) batch sizes and very large models to >









Acknowledgments

- Richard Gerber, Rebecca Hartman-Baker, Kevin Gott and Peter Harrington
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- Nicholas Malaya and Alessandro Fanfarillo A M D
- Mark Stock and Mengshiou Wu
- DOE INCITE allocation, 2024

PSSG



Bronson Messer, Phil Roth, Jens Glaser and Michael Sandoval OAK RIDGE LEADERSHIP COMPUTING National Laboratory FACILITY

Maria-Grazia Giuffreda, Fabian Bosch, Theofilos Manitaras, Henrique Mendonica and

NVIDIA

Hewlett Packard Enterprise













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- Siddharth Singh and Abhinav Bhatele
- Parallel Software and Systems Group
- University of Maryland, College Park

