Distributed Training

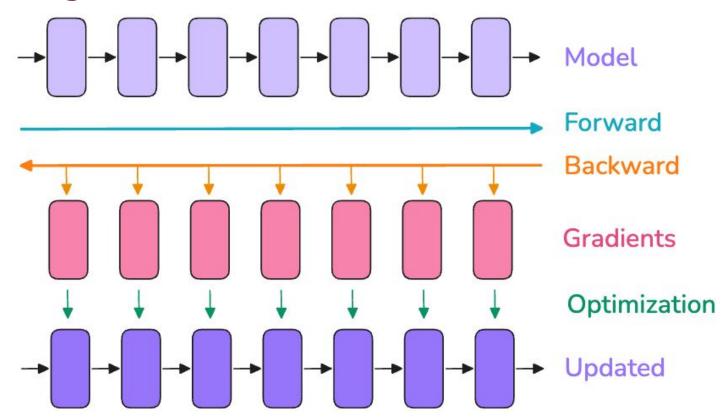
Make training system go brrrrr

Yongye Zhu, Anderson Lee, Ahmed Khaled

Problem Statement

- How to train a 405B model from scratch?
 - o How to train a smaller 1B model?
 - How to scale the model size with multiple GPUs? (e.g. 16k)
 - How to let the training run as fast as possible? Run fast means keep the GPU doing matmul

Training Model



Calculating Memory Usage

Model Parameter: λ·N

Model Gradient: λ·N

Optimizer State: $2\lambda \cdot N$

+ Activation + Data

λ: Bytes per parameter

Peak GPU Memory Usage

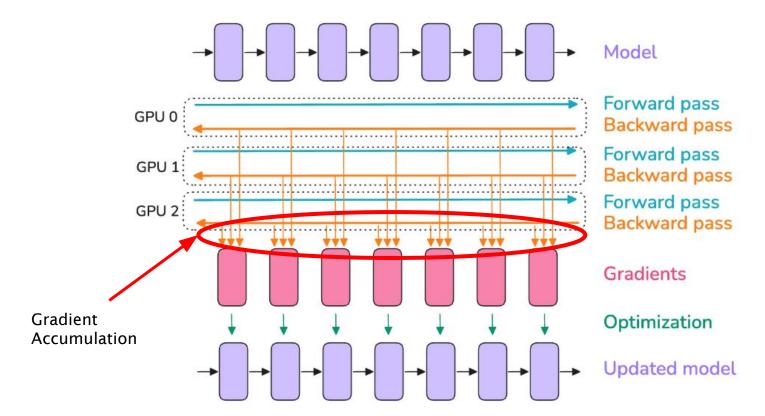
Model parameters	FP32 or BF16 w/o FP32 grad acc
1B	16 GB
7B	112 GB
70B	1120 GB
405B	6480 GB

We can only train 1B on single GPU!!

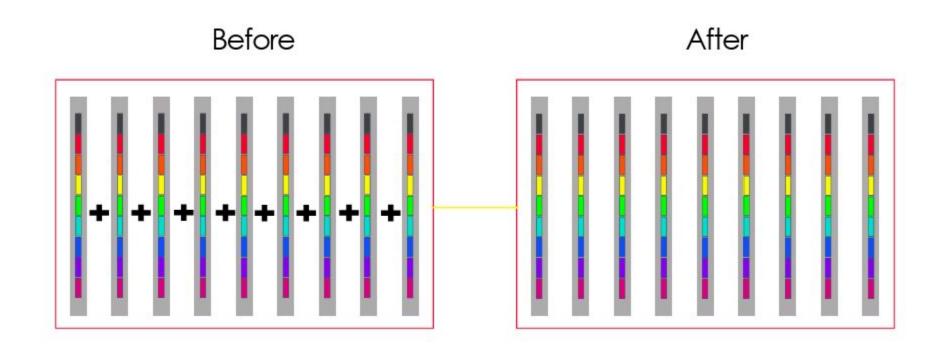
Gradient Accumulation

- We training LLM in batches
 - We will update the parameter every gbs (global batch size)
- During forward pass, we keep activation to calculate gradient.
- We can calculate the mean of gradient to update the parameter. (Parallel-Friendly)

Data Parallel



GPU Communication: All-Reduce

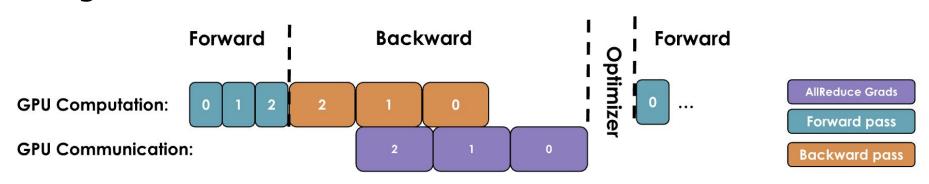


Data Parallel

- Each GPU perform *mbs* = *gbs* // *num_gpus* batches
- Result gradient are all-reduced (averaged). This can be hidden in computations
- Each GPU update parameter independently.
- Training total batches faster with more GPUs.
- Still can't train a 7B model since each GPU has full model parameter.

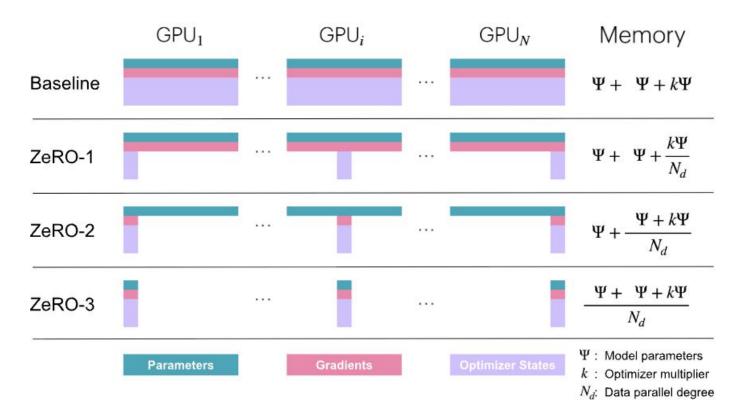
Compute/Communication Overlap

- Gradient accumulation for each layer happens immediately after calculated.
- Communication happens in the next (previous) layer gradient calculation.



Parameter Sharding

Big Picture



Measuring network efficiency

How to Scale Your Model

A Systems View of LLMs on TPUs

Training LLMs often feels like alchemy, but understanding and optimizing the performance of your models doesn't have to. This book aims to demystify the science of scaling language models: how TPUs (and GPUs) work and how they communicate with each other, how LLMs run on real hardware, and how to parallelize your models during training and inference so they run efficiently at massive scale. If you've ever wondered "how expensive should this LLM be to train" or "how much memory do I need to serve this model myself" or "what's an AllGather", we hope this will be useful to you.

AFFILIATION

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Feb. 4, 2025

FLOP utilization

- FLOPs/s of operation ÷ FLOPs/s of accelerator
- Example: If H100 achieves 989 TFLOPS peak for BF16, but your model runs at 400 TFLOPS Utilization = 400/989 ≈ 40%
- For LLM training, Model FLOPs Utilization (MFU) we usually aim for is around 50%-60%

Communication intensity

- Communication bytes ÷ (Memory / Network bandwidth bytes)
- Measures fraction of bandwidth used for inter-device communication
- Example: all-reduce gradient
 - Simplest form of parallelism
 - Must communicate 2×(N-1)/N × gradient_size bytes per iteration

Arithmetic Intensity

- Computation FLOPs ÷ Memory bytes accessed
- Measures compute per byte of memory traffic
- High arithmetic intensity
 - = compute-bound (good!)
- Low arithmetic intensity
 - = memory-bound
- E.g. for H100:
 - Need >240 FLOPs/byte to be compute-bound with BF16

Matrix multiplication example

- Most computations in a transformer are just mat muls
- Consider multiplying two N×N matrices:
 - FLOPs: 2N³ (in reality can be different due to blocking)
 - Memory read/write: 3N² elements
 - \circ Arithmetic intensity (AI) = $2N^3 \div (3N^2 \times bytes per element)$
 - \circ N=1024, BF16: AI = 341 FLOPs/byte
 - Compute-bound for H100.

Sharded matrix multiplication (I)

- What if we sharded the matrices?
- Consider two NxN matrices distributed across M devices
- Device i holds

$$A[iN/M:(i+1)N/M,:]$$
 — N/M rows of A $B[:,iN/M:(i+1)N/M]$ — N/M columns of B

Sharded matrix multiplication (II)

Each device i needs to compute C[iN/M:(i+1)N/M, :]:

- 1. Local compute: $A_{local} \times B_{local} \rightarrow C[i,i]$ block
- 2. Ring communication: Send B_{local}, receive B_{neighbor}
- 3. Repeat M-1 times to compute all blocks of C's rows

Sharded matrix multiplication (III)

- FLOPs per device: 2N³/M (perfectly scaled!)
- Memory per device: 2N²/M (input) + N²/M (output)
- Communication: $(M-1) \times N^2/M$ elements = $N^2(M-1)/M$
- Arithmetic intensity: $2N^3/M \div N^2(M-1) \approx 2N/(M-1)$
 - Decreases with more devices
 - Need larger N to maintain compute-bound operation

Some key numbers

- H100 BF16 Performance: 989 TFLOPS
- Transformer Training FLOPs: $6 \times N \times T$
 - N = number of parameters
 - T = number of tokens per step
- Intranode bandwidth (NVLink): 900 GB/s
- Internode bandwidth:
 - InfiniBand NDR: 400 Gbps = 50 GB/s
 - Ethernet alternatives: 100-400 Gbps typical

Forms of parallelism

Review: Adam

- Parameters: N
- Gradients: N
- Momentum: N
- 2nd order
 - momentum: N
- Total: 4N
 parameters in memory
- + Activations + Data

$$m_t = eta_1 m_{t-1} + (1 - eta_1) g_t$$

 $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$

$$\hat{m}_t = m_t/(1-eta_1^t)$$

$$\hat{v}_t = v_t/(1-\beta_2^t)$$

$$heta_t = heta_{t-1} - lpha \cdot \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon)$$

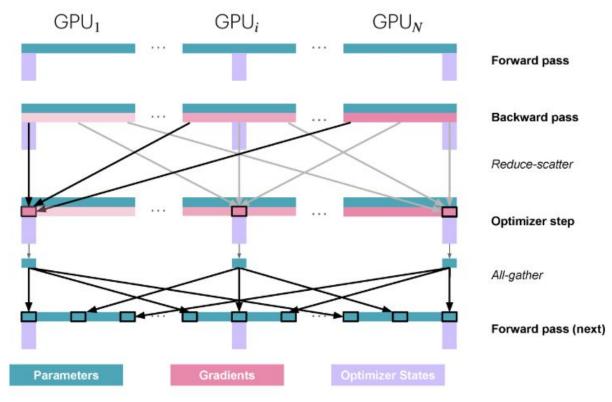
Sharding

- Different slices of a tensor belong to different devices
- Example: Weight matrix $W \in \mathbb{R}^{M \times N}$ with 4 devices
 - Device 0: W[0:M/4, :]
 - Device 1: W[M/4:M/2, :]
 - Device 2: W[M/2:3M/4, :]
 - Device 3: W[3M/4:M, :]
- Key challenge: Managing communication when sharded tensors interact

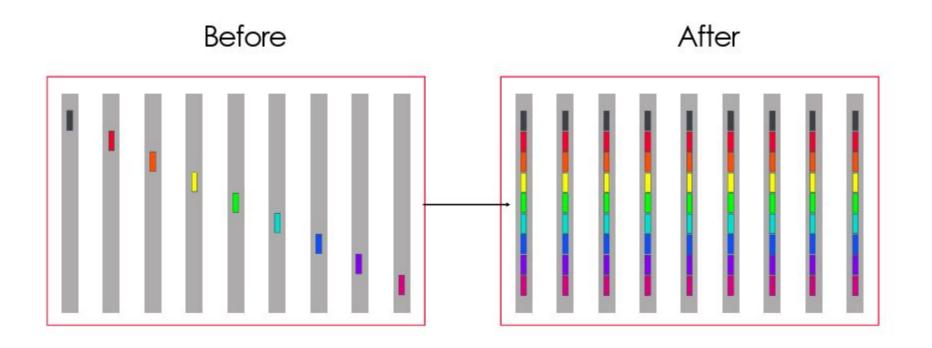
ZeRO-1 Optimizer State Sharding

- Optimizer states (m, v from Adam) divided layerwise among devices
- Each device only maintains optimizer states for its assigned layers
- After computing gradients:
 - Device updates only its owned optimizer states
 - Broadcasts updated parameters to all devices

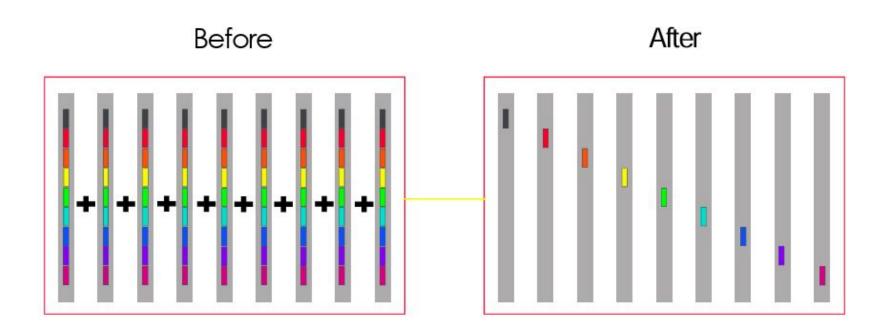
ZeRO-1 Optimizer State Sharding



All-Gather



Reduce-Scatter



ZeRO-1: Memory & Communication

- Memory: kΨ/N+2Ψ parameters per device
- Communication:
 - Same as data parallelism
 - No additional communication overhead (q for class: why?)
 - Again we can hide this overhead in forward and backward computation

Note on ZeRO

- This was a bit confusing to me personally
- We need to differentiate between memory usage for all layers vs transient memory usage (i.e. for a single layer)
- (see whiteboard)

ZeRO-2: Optimizer+Gradient Sharding

- Gradients also sharded with same layout as optimizer states
- During backward:
 - Compute full gradients locally
 - Reduce-scatter to get sharded gradients
 - Each device keeps only gradients for its layers

ZeRO-2: Memory & Communication

- **Memory:** $(k + 1)\Psi/N+\Psi$ parameters per device
- Communication:
 - Same as data parallelism
 - No additional communication overhead
 - We don't need to get the gradients for other layers
 - Still communicate updated params
- Supported by DeepSpeed, Megatron-LM, PyTorch FSDP

ZeRO-3: Full Parameter Sharding

- Parameters also sharded layerwise across devices
- At layer L:
 - Before forward pass: All-gather parameters for this layer -> do forward computation (replicated)
 - After forward: Discard non-owned parameters
 - Before backward: All-gather parameters again -> do backward computation (replicated)
 - After backward: Do optimizer step + discard non-owned parameters

ZeRO-3 Tradeoffs

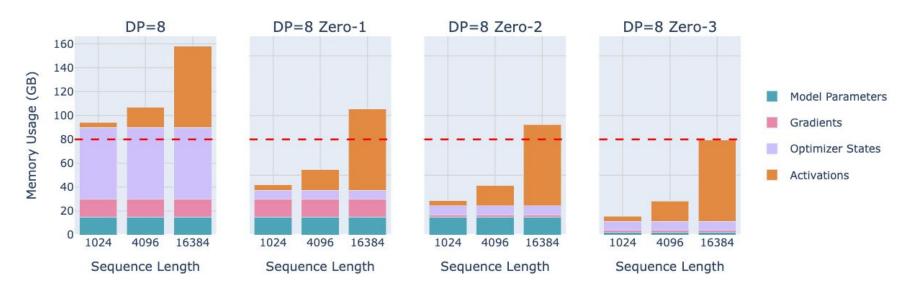
- Memory: (k+2)Ψ/N bytes per device
- Communication: 1.5X of DP
 - Prev: one all-gather in bwd pass
 - Now: one all-gather in fwd, one all-gather in bwd
- "Sharded parameters, replicated computation"

FSDP2

- Like ZeRO-3, but instead of sharding layerwise, shard across dim-0 of every param/grad/optimizer state tensor
- Easier conceptually to implement
- Natively integrated into PyTorch
- Can be integrated with smarter torch.compile.

Where we are now?

Memory Usage for 8B Model



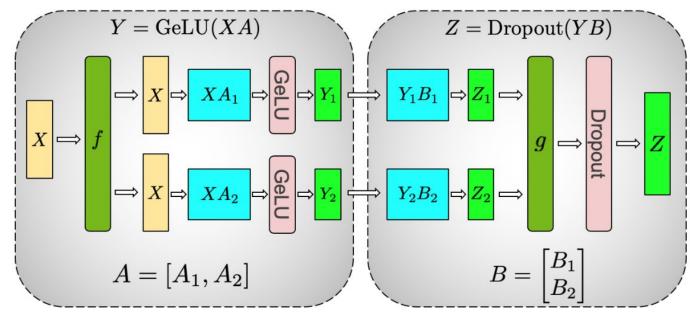
Still bottlenecked by activation memory (especially with long seq len)

Activation Sharding

- Like ZeRO-3, but computation is also sharded
- Parameters stay on assigned devices
- Activations are all-reduced/all-gathered between devices as needed for computation
- How we choose to do the sharding strongly influences the computation/communication

- Consider MLP: Y = GeLU(XA) followed by Z = YB
- Row-wise split of A:
 - Partition: $X = [X_1, X_2], A = [A_1; A_2]$
 - Result: $Y = GeLU(X_1A_1 + X_2A_2)$
 - o Problem: GeLU(X₁A₁ + X₂A₂) ≠ GeLU(X₁A₁) + GeLU(X₂A₂)
 - Requires synchronization before GeLU, beating the point

- Consider MLP: Y = GeLU(XA) followed by Z = YB
- Column-wise split of A:
 - \circ Partition: $A = [A_1, A_2]$
 - Result: $[Y_1, Y_2] = [GeLU(XA_1), GeLU(XA_2)]$
 - GeLU applied independently no sync needed!
 - Second GEMM: Split B row-wise to match
 - Only one all-reduce after second GEMM



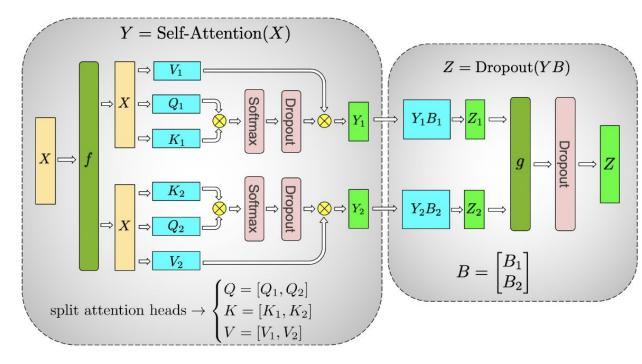
From Megatron-LM paper

(a) MLP

```
class f(torch.autograd.Function):
    def forward(ctx, x):
        return x
    def backward(ctx, gradient):
        all_reduce(gradient)
        return gradient
```

Code 1. Implementation of f operator. g is similar to f with identity in the backward and all-reduce in the forward functions.

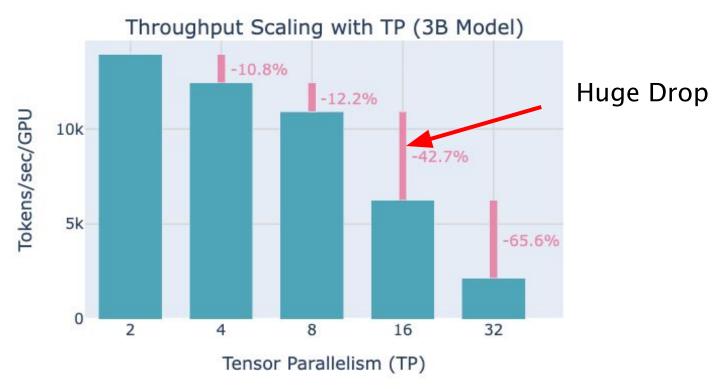
From Megatron-LM paper



From Megatron-LM paper

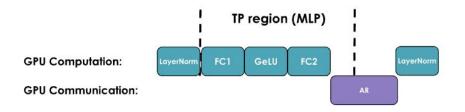
(b) Self-Attention

Tensor Parallel Performance



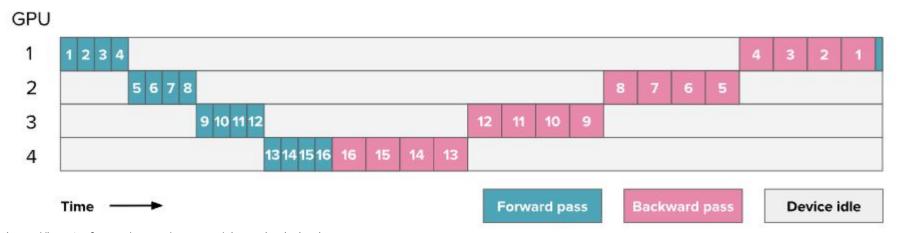
Tensor Parallel Performance

- All-Reduce sits on the critical path during forward.
- One node has 8 GPUs.
- Cross-node comm is much slower than inter-node comm. (NvLink vs InfiniBand)



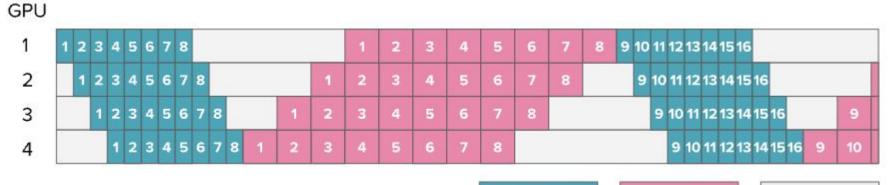
Pipeline parallelism

- Model divided into stages (groups of layers)
- Each device owns one pipeline stage
- Data flows through devices sequentially
- Limitation: Device Idle



Microbatch All Forward All Backward

- Micro-batching to reduce pipeline bubbles
- Reduce total computation time by *m*, number of microbatches
- Problem: Need to store all microbatch activations





1Forward 1Backward (Depth-First Scheduling)

- Prioritize backward pass over forward pass
- Immediate release activation memory after backward pass
- Still same time as AFAB, but more memory efficient



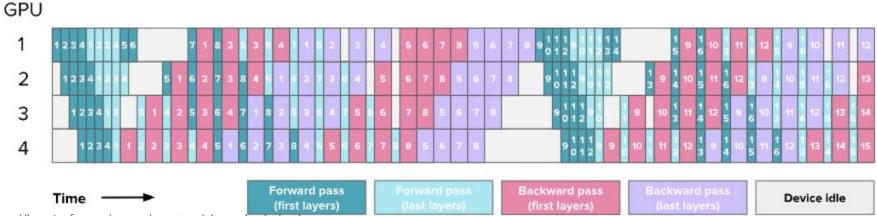


Backward pass

Device idle

Interleaved 1F1B

- Each GPU has more than one layer
- Computation circulating around GPUs
- Further reduce overall training time by **n**, number of layer each GPU has.

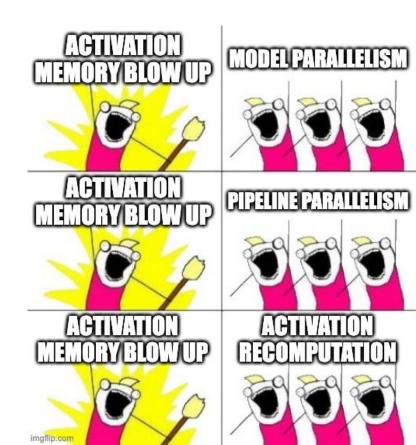


Zero Bubble Pipeline/DualPipe

DeepSeek-V3 Technical Report: <u>arxiv:2412.19437</u>

Memory problem in training models

- Tensor parallelism
 - Help but introduces overhead
- Pipeline Parallelism
 - Doesn't help if maintaining device utility to avoid bubble
- Activation Recomputation



Activation Recomputation

- A.k.a. Gradient Checkpointing
- Select all/some layers' output to save, then re-forward pass from closest "checkpoint"
- Trading off compute for saving memory

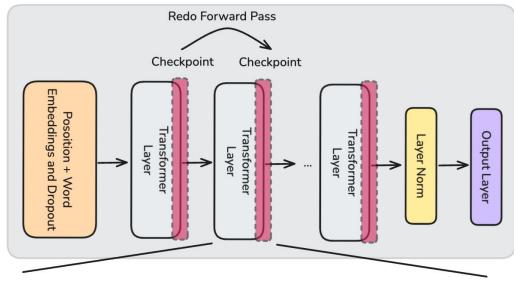
Activation Recomputation

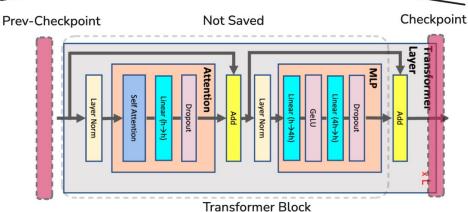
Within-block activation not saved

Redo forward pass from last block's output

Bottom figure from Megatron-LM

Activation Recomputation





Reducing Activation Recomputation

- Three main components
 - Tensor Parallelism (Megatron-LM)
 - Sequence Parallelism
 - Selective Activation Recomputation
- where 2. and 3. Are orthogonal

Computing Activation Memory

Setup/Notation

Table from Korthikanti et. al

```
egin{array}{c|cccc} a & {
m number of attention heads} & p & {
m pipeline parallel size} \ b & {
m microbatch size} & s & {
m sequence length} \ h & {
m hidden dimension size} & t & {
m tensor parallel size} \ L & {
m number of transformer layers} & v & {
m vocabulary size} \ \end{array}
```

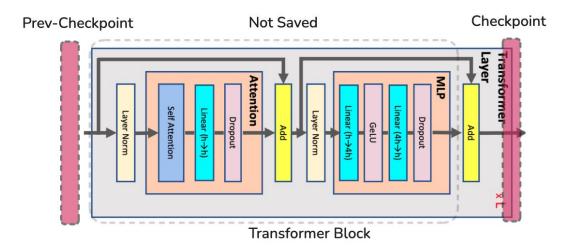
 Fp16 → each element takes 2 bytes, except dropout mask takes 1 byte

Agenda: Computing Activation Memory

- Full Activation Recomputation (Lowest)
- Full Activation (Highest)
- w/ Tensor Parallelism
- w/ Sequence Parallelism
- w/ Selective Activation Recomputation

Full Activation Recomputation

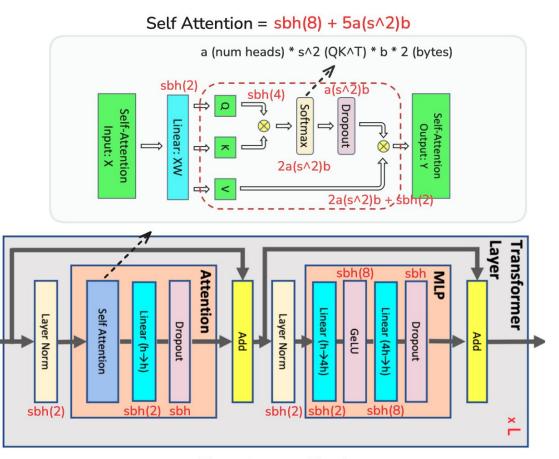
Memory (per layer): sbh(2)



Full Activation

Memory (per layer)

$$sbh\left(34+5\frac{as}{h}\right)$$

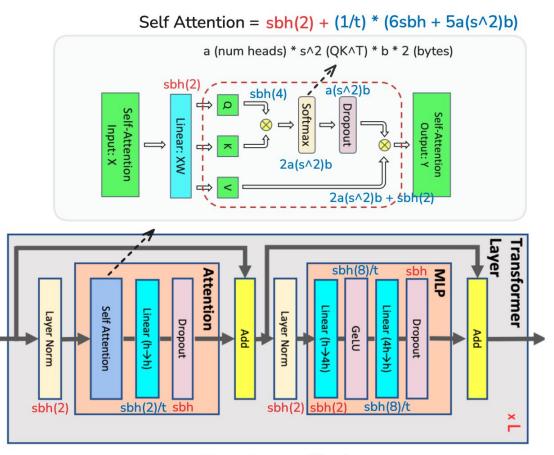


Transformer Block

Memory (per layer)

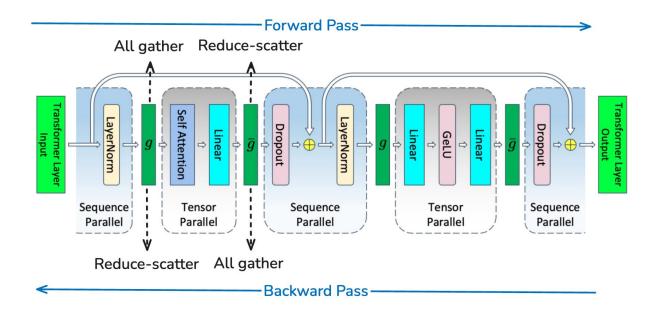
$$sbh\left(10 + \frac{24}{t} + 5\frac{as}{ht}\right)$$

Can we do better?



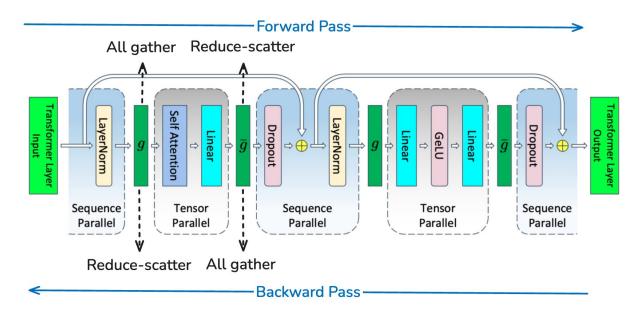
Transformer Block

Main Observation – Those *tensor-parallelism-excluded* components are not *sequence-dependent*



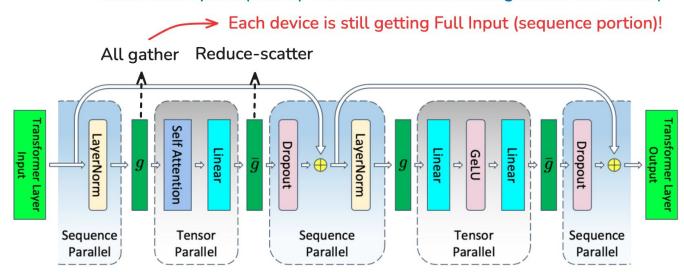
Does it increase extra communication by all-gather + reduce-scatter? No, because ring all reduce = all-gather

+ reduce-scatter



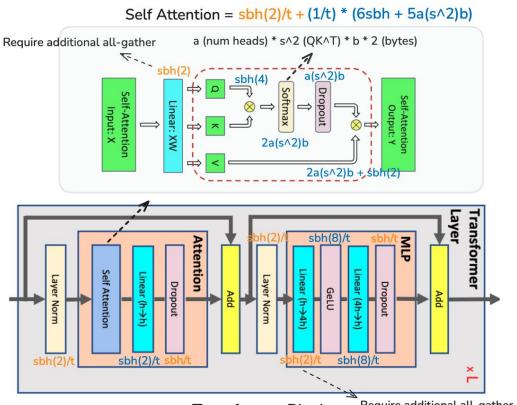
We are not yet achieving 10 / t

Solution: save only the i-th (sequence-wise) proportion on device. Then, introduce an additional all-gather to gather all sequence-wise proportions in backward pass. (overlap the communication with gradient calculation)



Memory (per layer)

$$sbh\left(\frac{10}{t} + \frac{24}{t} + 5\frac{as}{ht}\right) = \frac{sbh}{t}\left(34 + 5\frac{as}{h}\right)$$



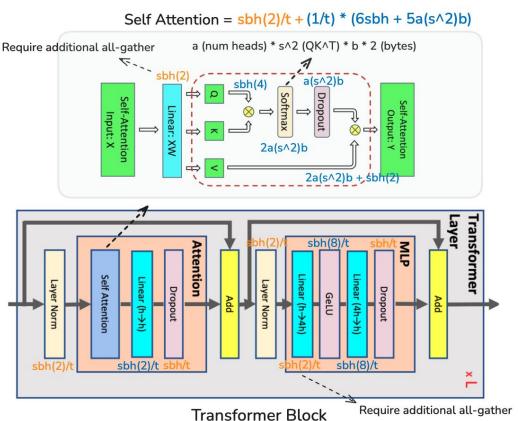
Transformer Block

Require additional all-gather

Memory (per layer)

$$sbh\left(\frac{10}{t} + \frac{24}{t} + 5\frac{as}{ht}\right) = \frac{sbh}{t}\left(34 + 5\frac{as}{h}\right)$$

Can we do **even** better?



+ Selective Activation Recomputation

- Recompute the portion isn't too expensive
- Trade-off those recomputation for better memory saving

Self Attention =
$$sbh(2)/t + (1/t) * (6sbh + 5a(s-2)b)$$

Require additional all-gather a (num heads) * $s imes 2$ (QK^T) * $b imes 2$ (bytes)

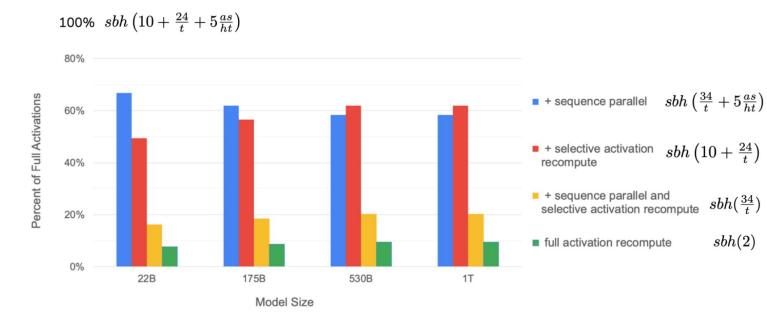
$$sbh(2) \qquad \qquad sbh(4) \qquad shh(4) \qquad shh(4)$$

Summary

- Tensor parallelism saves parallelized parts intuitively
- Sequence parallelism saves the rest (some trade-off)
- Selective Recomputation trades off compute for large memory reduction (s^2)
 - Pointer → FlashAttention solves this problem nowadays!

Evaluation

The terms reduced matter! (linearly reducing the 10 with number of devices)



Evaluation

 Select the right thing to recompute, introducing much less overhead (while saving much more memory)

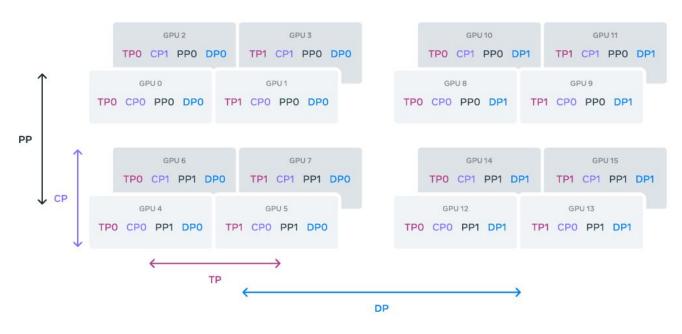
Experiment	Forward (ms)	Backward (ms)	Combined (ms)	Overhead (%)
Baseline no recompute	7.7	11.9	19.6	j-1
Sequence Parallelism	7.2	11.8	19.0	-3%
Baseline with recompute	7.7	19.5	27.2	39%
Selective Recompute	7.7	13.2	20.9	7%
Selective + Sequence	7.2	13.1	20.3	4%

Table 4: Time to complete the forward and backward pass of a single transformer layer of the 22B model.

Question

- Can we do even even better? What components discussed were not optimized yet?
- Can we do an analysis on overhead of recomputation (over components) and memory reduction to fit even smaller device?

Combined Parallelism in real world training



Training LLama3 in 16k GPUs

Context Parallel

- In Data Parallelism, we shard activation (for attention and FFN) in alone batch dimension, how about long context training?
 Where we are unable to shard efficiently since batch size is small
- In Sequence Parallel, only the non-attention parts are sharded across devices. The attention part still remains the full sequence
- What about extremely long context (1M tokens) -> Context
 Parallel!!! Next Lecture!!

Expert Parallelism

- MoE layer contains multiple expert networks
- Example: 32 experts distributed across 8 GPUs (4 experts/GPU)
- Tokens routed to different GPUs based on expert selection
- Each token typically activates k experts (e.g., k=2)

Expert Parallelism

- Conceptually still a form of model parallelism
- Differences
 - Requires specialized routing implementation
 - Dynamic load balancing challenges
 - Token dropping and auxiliary losses
 - Different communication patterns (all-to-all vs all-reduce)

Reference

[1] Ultra-Scale Playbook:

https://huggingface.co/spaces/nanotron/ultrascale-playbook

[2] UCSD CSE 234: https://hao-ai-lab.github.io/cse234-w25/

[3] The Llama 3 Herd of Models, arXiv:2407.21783