October 10 – 12, 2023

ALCF Hands-on HPC Workshop

Sam Foreman

- I'm currently an associate computational scientist in the Data Science Group at ALCF[1].
  - Personal Website: samforeman.me
  - Background: `{HEP, Lattice QCD, ML + Generative Modeling, Large Scale Training, LLMs, MCMC, ...}`

Ongoing / recent work:

- AI + Science
  - Building better sampling methods for Lattice QCD
  - GenSLMs: Genome-scale language models reveal SARS-CoV-2 evolutionary dynamics
  - Foundation models for long term climate forecasting
- Scaling Large Language Models
- Optimizing distibuted training across thousands of GPUs
- Building new parallelism techniques for efficient scaling
- Generative modeling (esp. for physical systems)

1. Mostly getting supercomputers to stop yelling at each other

Status of Large Language Models[1]

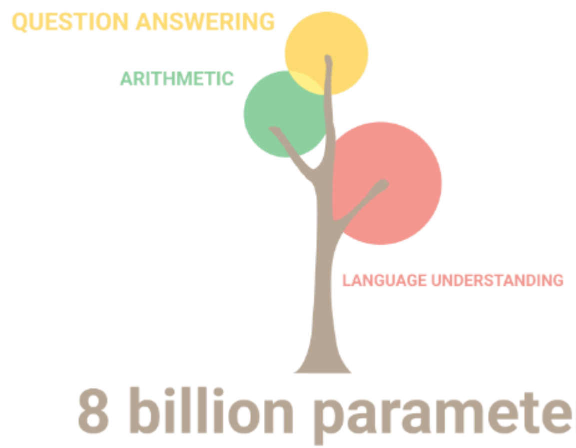
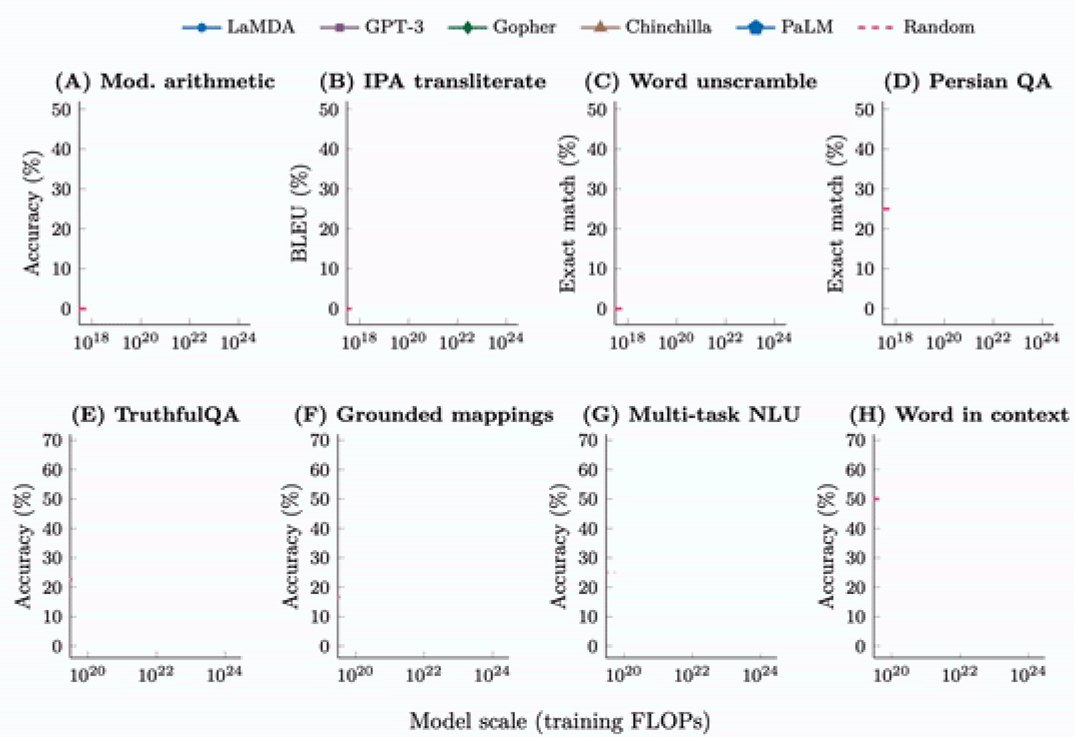


Figure 1: Large Language Models have (LLM)s have taken the ~~NLP community~~ **world** by storm[2]

1. saforem2/llm-lunch-talk (slides)
2. Hannibal046/Awesome-LLM

Emergent Abilities



Emergent abilities of Large Language Models Yao et al. (2023)

Training LLMs

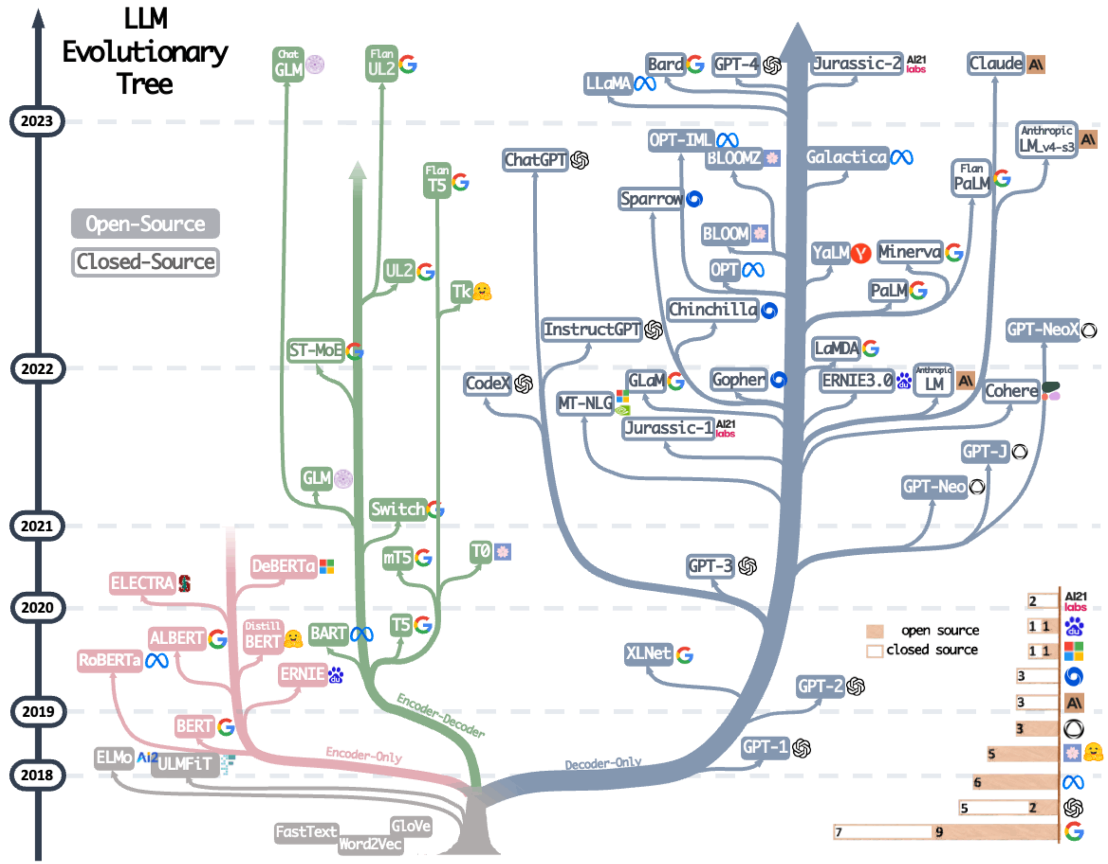
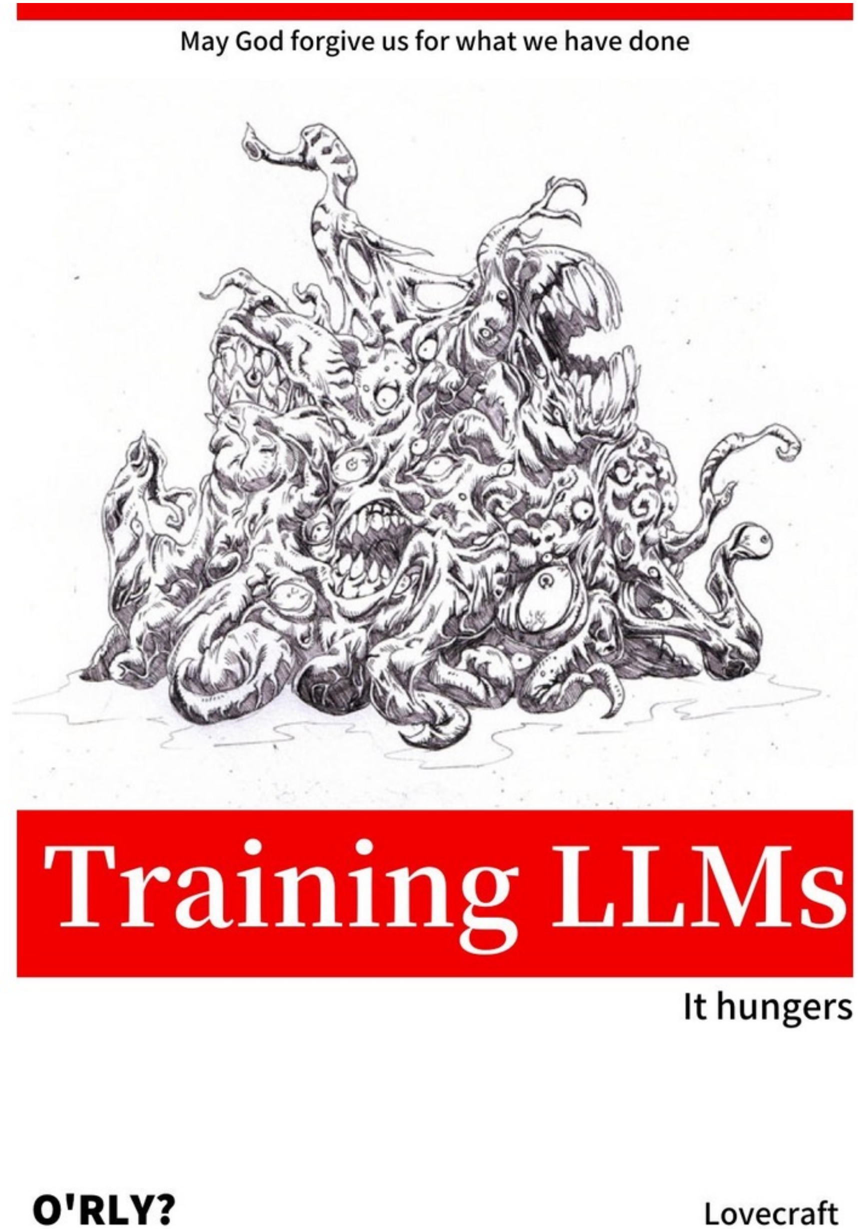


Figure 2: Visualization from Yang et al. (2023)



Recent Work (2017 – Now)

- **Recent Work**

Life-Cycle of the LLM

1. Data collection + preprocessing
2. **Pre-training**
   - Architecture decisions: `{model_size, hyperparameters, parallelism, lr_schedule, ...}`
3. Supervised Fine-Tuning
   - Instruction Tuning
   - Alignment
4. Deploy (+ monitor, re-evaluate, etc.)

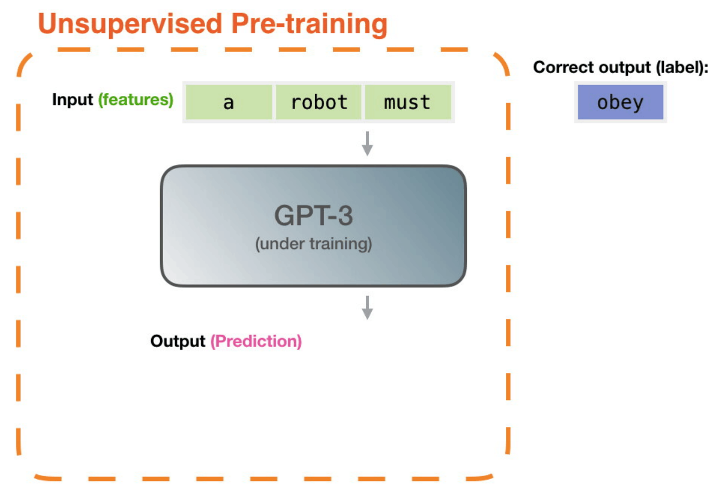


Figure 3: **Pre-training**: Virtually all of the compute used during pretraining phase[1].

1. Figure from [The Illustrated Transformer]

Life-Cycle of the LLM: Pre-training

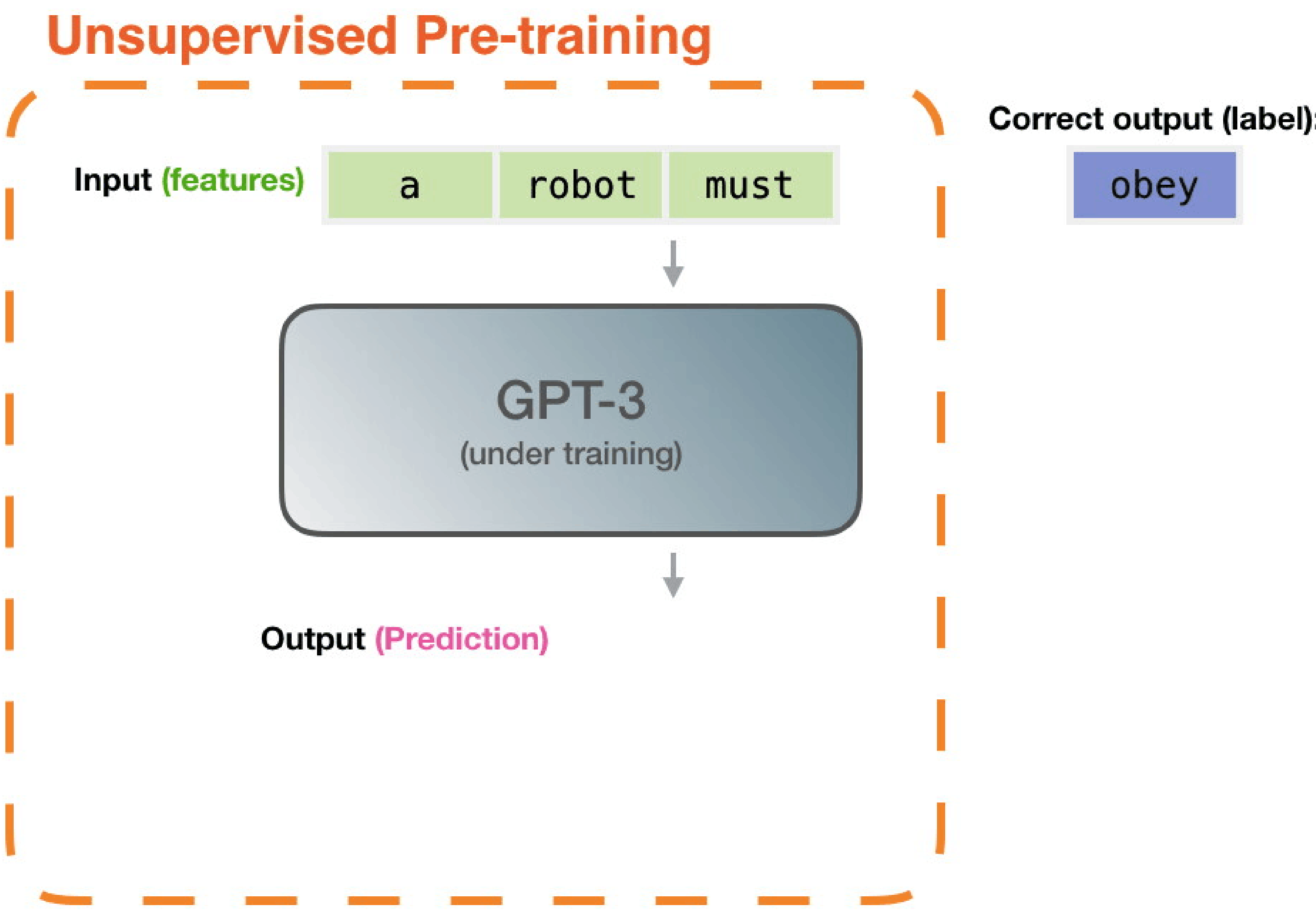


Figure 4: **Pre-training**: Virtually all of the compute used during pretraining phase

Life-Cycle of the LLM: Fine-Tuning

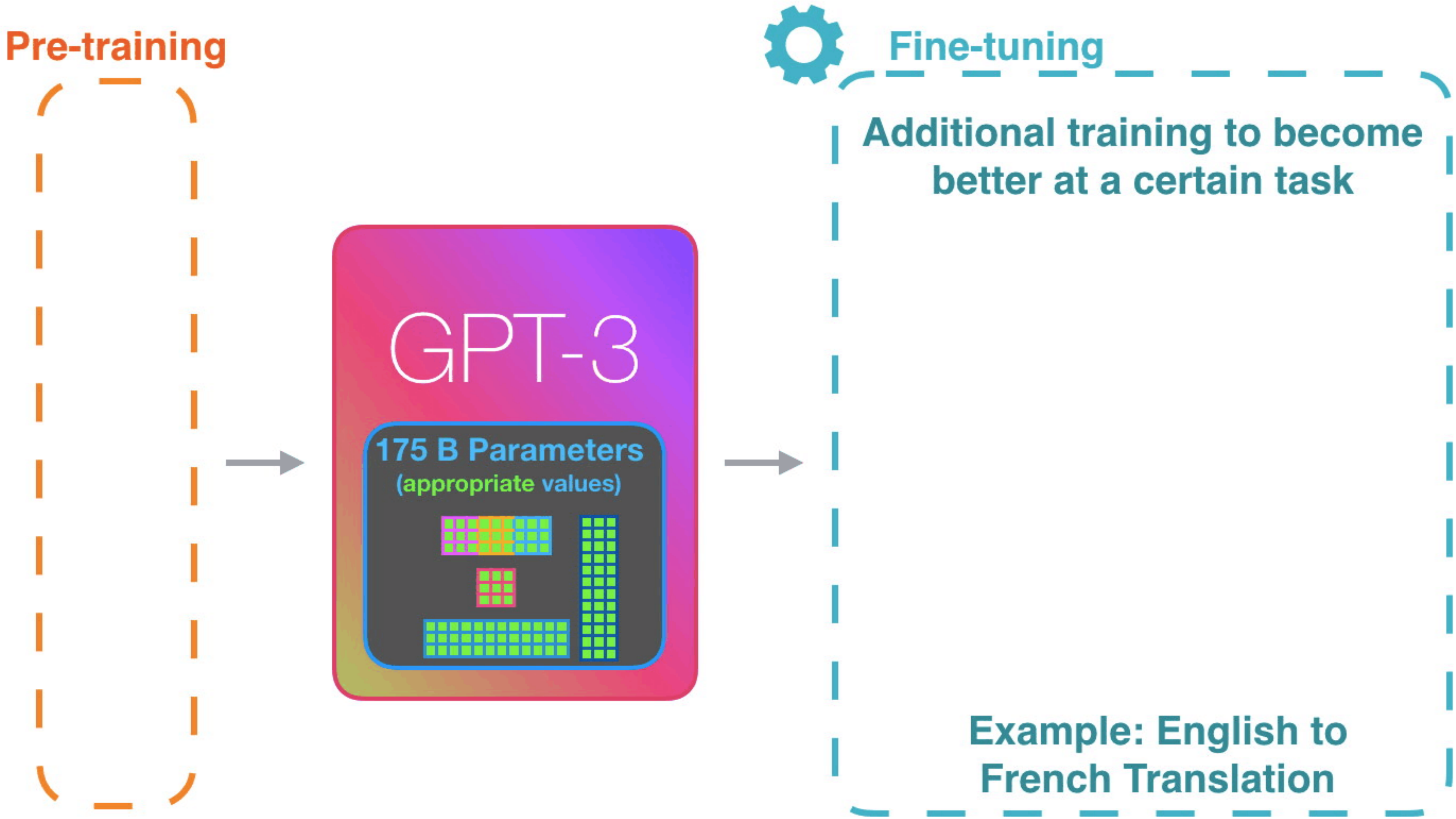
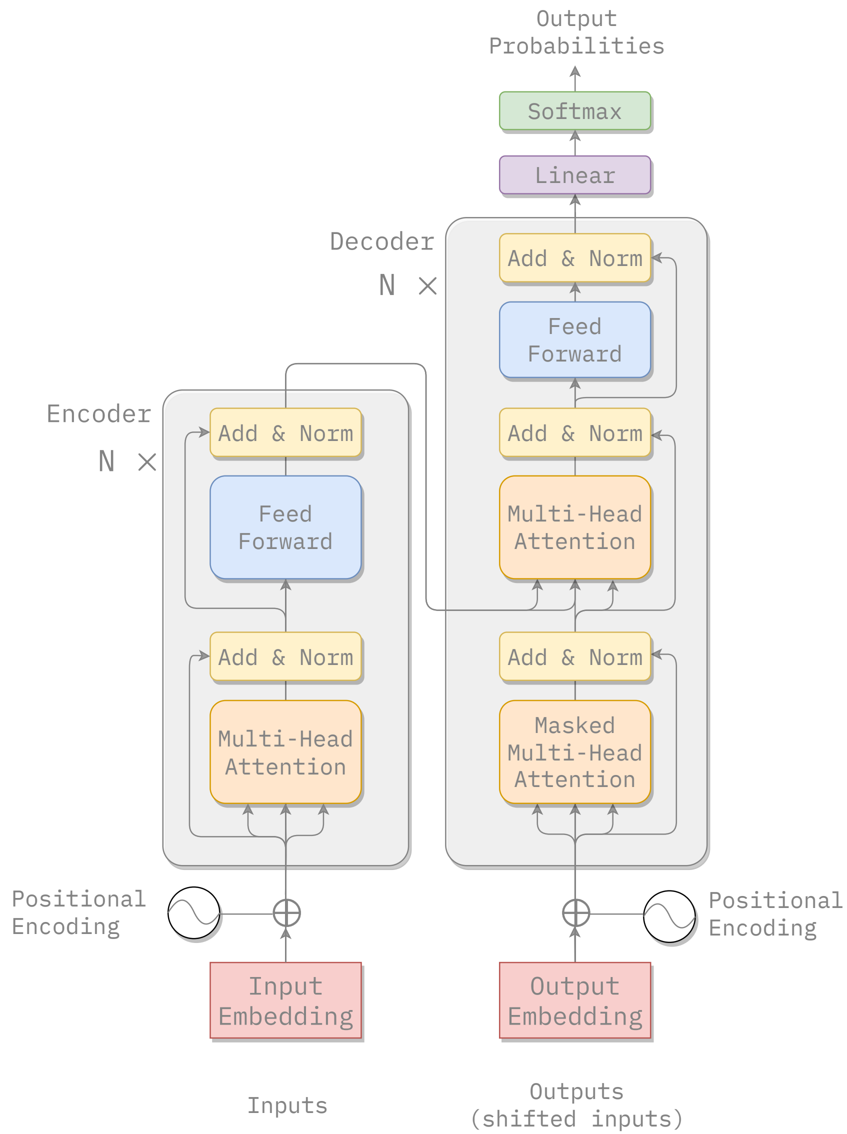


Figure 5: **Fine-tuning**[1]: Fine-tuning actually updates the model's weights to make the model better at a certain task.

1. Figure from [The Illustrated Transformer]

Transformer Architecture



Vaswani et al. (2017)

Forward Pass

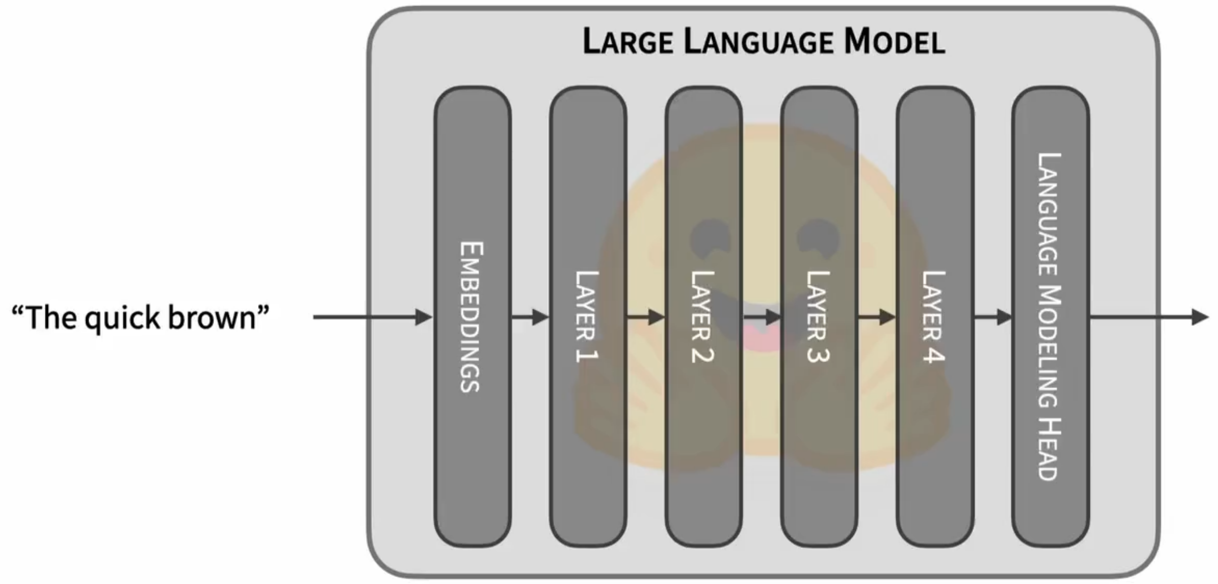


Figure 6: Language Model trained for causal language modeling. Video from: 🤗 Generation with LLMs

Generating Text

Figure 7: Language Model trained for causal language modeling. Video from: 🤗 [Generation with LLMs]

Parallelism Overview

> ***Modern parallelism techniques*** *enable the training of large language models*

Parallelism Concepts[1]

- **DataParallel (DP)**:
  - The same setup is replicated multiple times, and each being fed a slice of the data.
  - The processing is done in parallel and all setups are synchronized at the end of each training step.
- **TensorParallel (TP)**:
  - Each tensor is split up into multiple chunks.
  - So, instead of having the whole tensor reside on a single gpu, each shard of the tensor resides on its designated gpu.
    - During processing each shard gets processed separately and in parallel on different GPUs and the results are synced at the end of the step.
    - This is what one may call horizontal parallelism, as he splitting happens on horizontal level.

1. 🤗 Model Parallelism

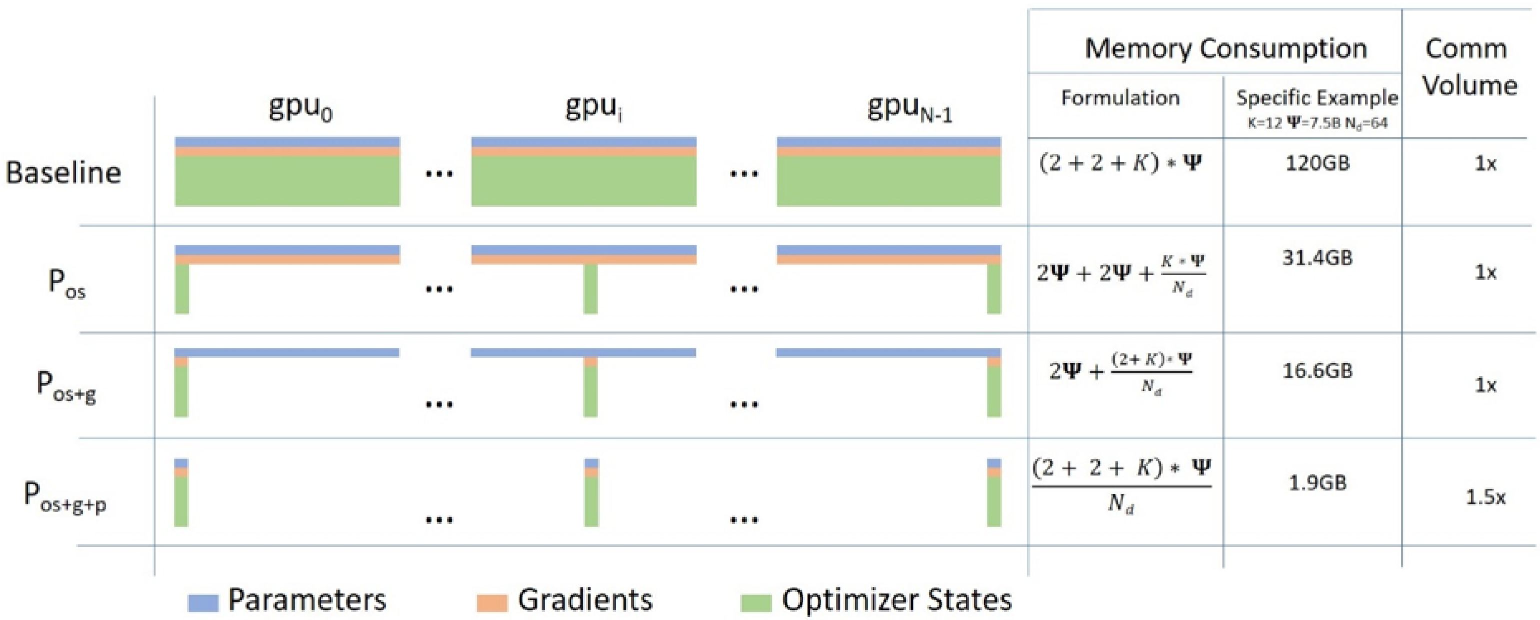
Parallelism Concepts[1]

- **PipelineParallel (PP)**:
  - Model is split up vertically (layer-level) across multiple GPUs, so that only one or several layers of the model are places on a single gpu.
    - Each gpu processes in parallel different stages of the pipeline and working on a small chunk of the batch.
- **Zero Redundancy Optimizer (ZeRO)**:
  - Also performs sharding of the tensors somewhat similar to TP, except the whole tensor gets reconstructed in time for a forward or backward computation, therefore the model doesn't need to be modified.
  - It also supports various offloading techniques to compensate for limited GPU memory.
- **Sharded DDP**:
  - Another name for the foundational ZeRO concept as used by various other implementations of ZeRO.

1. 🤗 Model Parallelism

Data Parallelism

- **Data Parallelism**:
  - The simplest and most common parallelism technique. Workers maintain *identical copies* of the *complete* model and work on a *subset of the data*.
  - `DDP` supported in PyTorch native.
- ZeRO Data Parallel
  - ZeRO powered data parallelism is shown below[1]



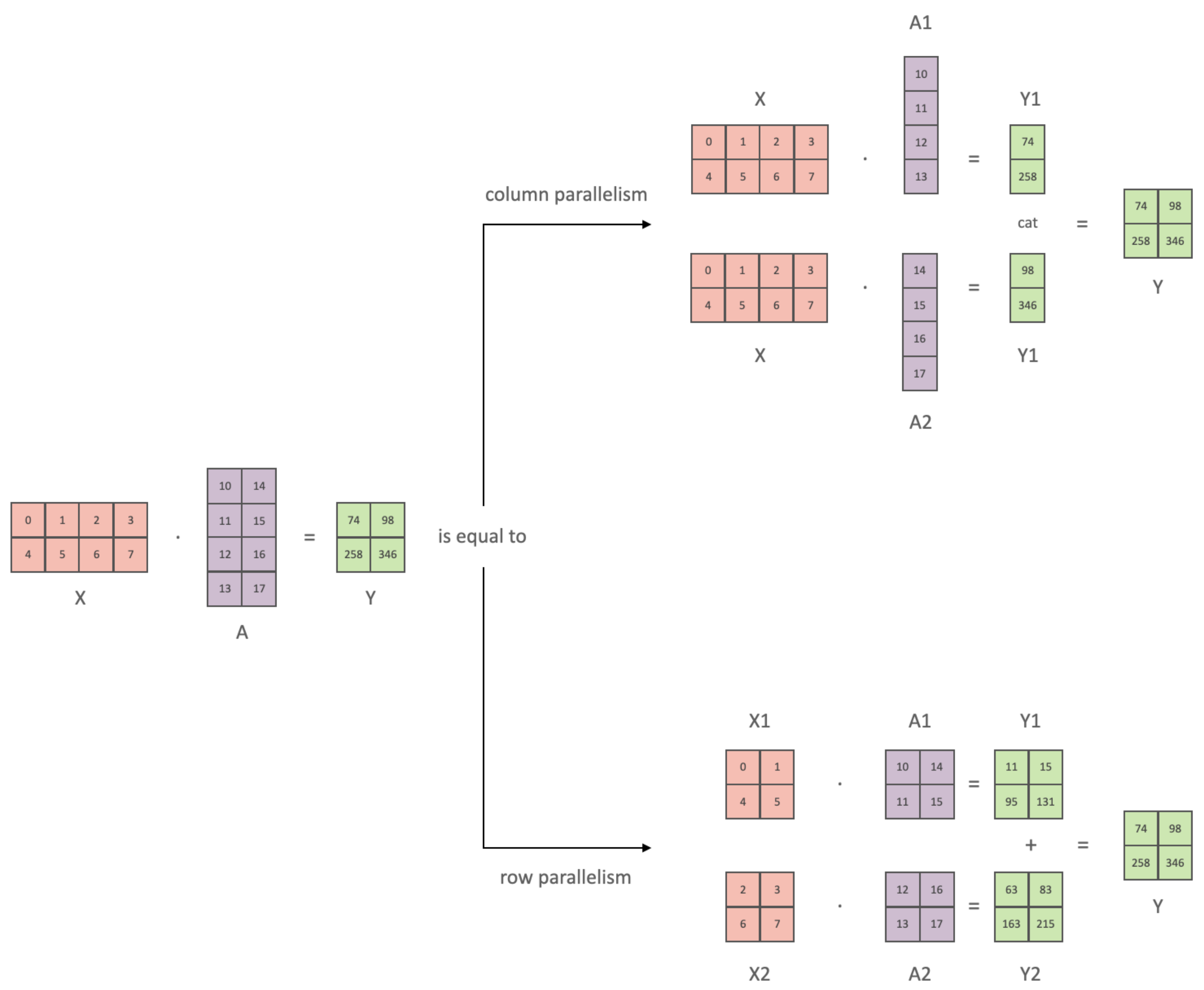
1. [Blog Post]

Tensor Parallelism[1]

- In **Tensor Paralleism** each GPU processes only a slice of a tensor and only aggregates the full tensor for operations that require the whole thing.
  - The main building block of any transformer is a fully connected nn.Linear followed by a nonlinear activation GeLU.
    - `Y = GeLU(XA)`, where X and Y are the input and output vectors, and A is the weight matrix.
  - If we look at the computation in matrix form, it’s easy to see how the matrix multiplication can be split between multiple GPUs:

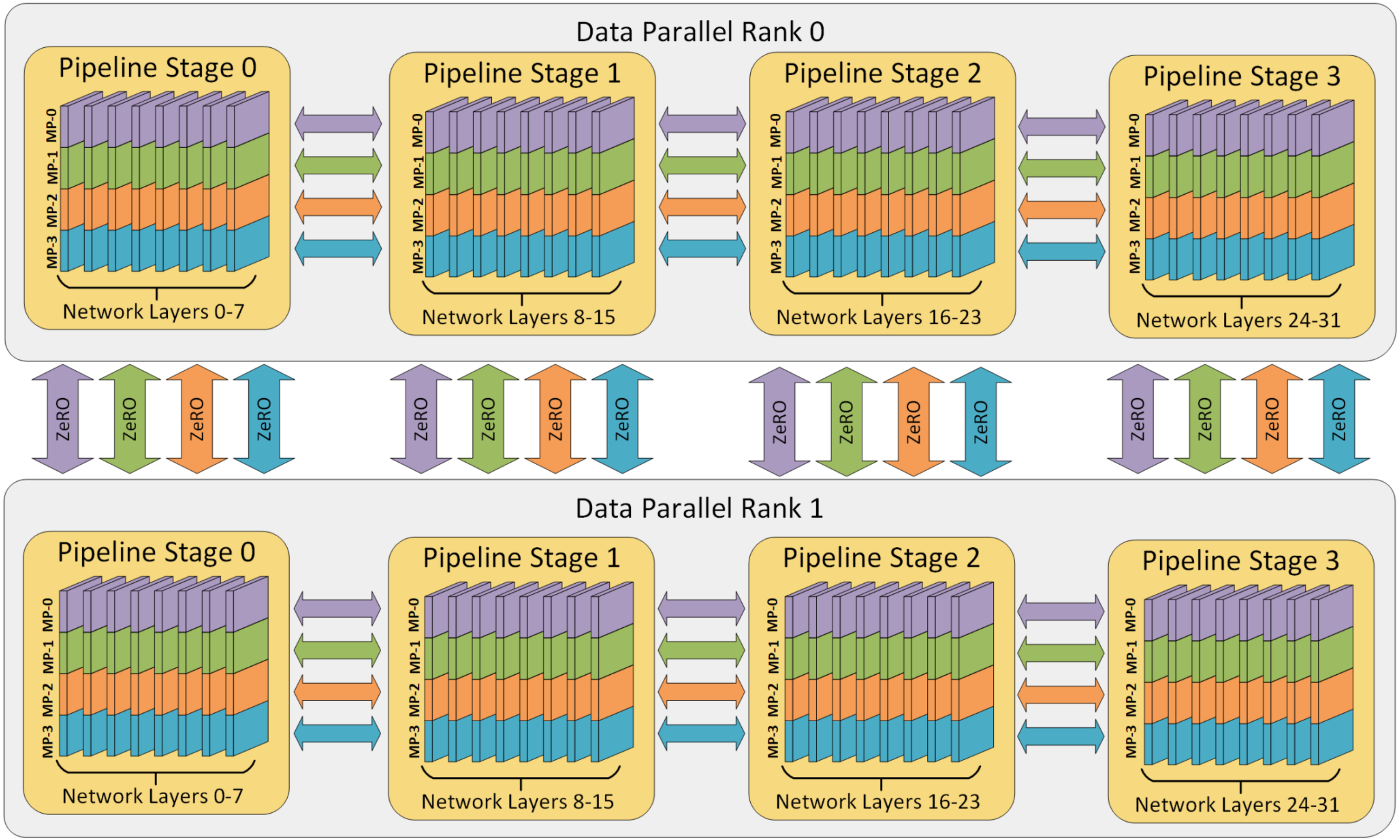
1. [Efficient Large-Scale Language Model Training on GPU Clusters]

Tensor Parallelism



3D Parallelism

- `DP` + `TP` + `PP` (3D) Parallelism



3D Parallelism illustration. Figure from: https://www.deepspeed.ai/

3D Parallelism

- DP + TP + PP (3D) Parallelism

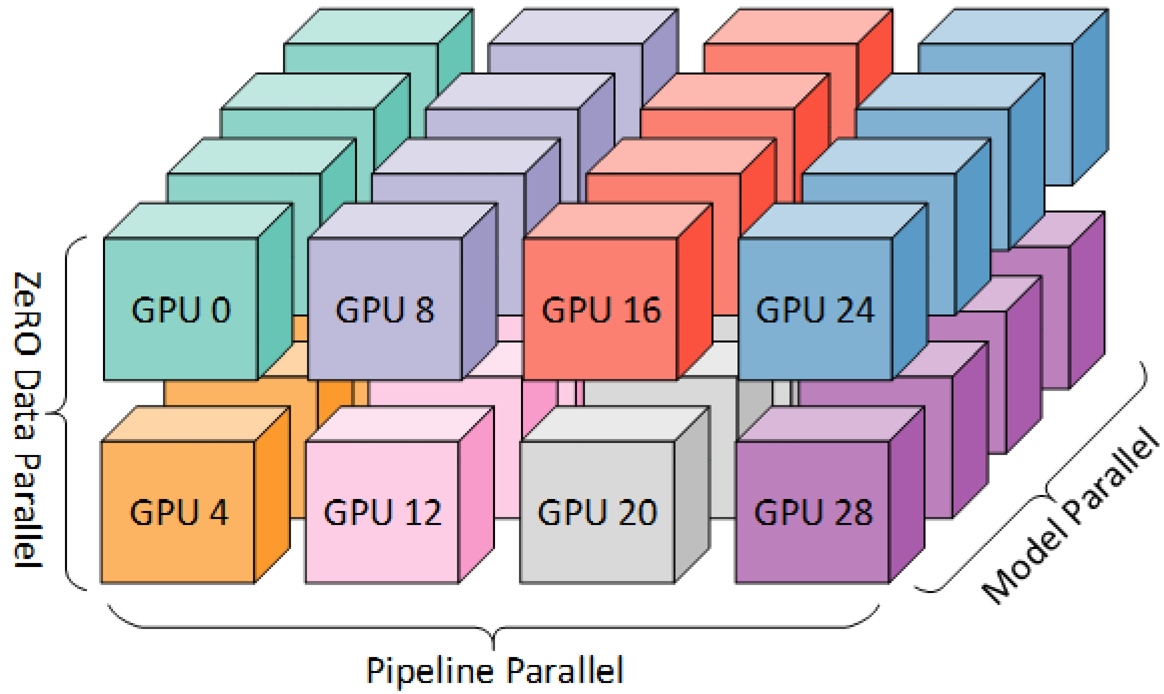


Figure taken from [3D parallelism: Scaling to trillion-parameter models]

Running on ALCF

- We've provided a virtual environment complete with all dependencies for running argonne-lcf/Megatron-DeepSpeed

```bash
# navigate to directory -------------------------------------
WORKSHOP_DIR="/lus/grand/projects/fallwkshp23/"
PROJECTS_DIR="${WORKSHOP_DIR}/foremans/projects"
PROJECT_DIR="${PROJECTS_DIR}/argonne-lcf/Megatron-DeepSpeed"
cd "${PROJECT_DIR}"
# load conda module and activate venv -------------------------
module load conda/2023-10-04; conda activate base
source venvs/polaris/2023-10-04/bin/activate
# set runtime environment variables ---------------------------
export IBV_FORK_SAFE=1
export CUDA_DEVICE_MAX_CONNECTIONS=1
# set environment variables for running -----------------------
SEQ_LEN=1024
MICRO_BATCH=1
SP_TYPE="megatron"
MODEL_SIZE_KEY="GPT1_5B"
# launch training --------------------------------------------
./ALCF/train-gpt3.sh
```

Running on ALCF

- Executable:

```
MODEL_SIZE_KEY="GPT1_5B" SEQ_LEN=1024 MICRO_BATCH=1 SP_TYPE="megatron" ./ALCF/train-gpt3.sh
```

▼ **Output**

```
+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+
ALCF_DIR: /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lcf/Me
+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+
source-ing /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lcf/M
Setting up MPI on Polaris from x3210c0s1b0n0
++ SetupMPI() +++++++++++++++++++++++++++++++++
Using HOSTFILE: /var/spool/pbs/aux/1126584.polaris-pbs-01.hsn.cm.polaris.alcf.anl.gov
NHOSTS: 2
NGPU_PER_HOST: 4
NGPUS: 8
+++++++++++++++++++++++++++++++++++++++++++++++
Skipping setupThetaGPU() on x3210c0s1b0n0
Setting up MPI on Polaris from x3210c0s1b0n0
USING PYTHON: /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lc
[...]
```

Running on ALCF

Once the text has *finally* stopped printing, you should see output similar to the following:

```
Job started at: 2023-10-11-092906 on x3210c0s1b0n0
[...]
Writing logs to: /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lcf/Megatron-DeepS
to view output: tail -f $(tail -1 logfiles)
i.e. tail -f /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lcf/Megatron-DeepSpeed
```

- To watch / view the output:

```
tail -fn 1000 $(tail -1 logfiles) | less
```

- will look like[1]:

```
Job started at: 2023-10-11-092906 on x3210c0s1b0n0
Training GPT-3 with GPT13B parameters
Writing logs to: /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lcf/Megatron-DeepS
to view output: tail -f $(tail -1 logfiles)
i.e. tail -f /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lcf/Megatron-DeepSpeed
using: /lus/grand/projects/fallwkshp23/foremans/locations/polaris/projects/argonne-lcf/Megatron-DeepSpeed/venvs
[...]
```

1. 🚀 W&B Run: `soft-wave-264`

Getting Started at ALCF

- We provide below the **details** for installing / getting started on ALCF (Polaris)
- Installation:
  1. Clone GitHub repo:

```
git clone https://github.com/argonne-lcf/Megatron-DeepSpeed
```

  2. Load Conda module:
     - Polaris:

```
if [[ "$(hostname)==x3*" ]]; then
    export MACHINE="Polaris"
    export CONDA_DATE="2023-10-04"
    module load conda/${CONDA_DATE}
    conda activate base
fi
```

     - ThetaGPU:

```
if [[ "$(hostname)==theta*" ]]; then
    export MACHINE="ThetaGPU"
    export CONDA_DATE="2023-01-10"
    module load conda/${CONDA_DATE}
    conda activate base
fi
```

Getting Started

3. Setup virtual environment[1]:

```bash
cd Megatron-DeepSpeed
# create a new virtual environment
mkdir -p "venvs/${MACHINE}/${CONDA_DATE}"
python3 -m  venv "venvs/${MACHINE}/${CONDA_DATE}" --system-site-packages
source "venvs/${MACHINE}/${CONDA_DATE}/bin/activate"
```

4. Create a new folder where we'll install dependencies:

```bash
mkdir -p "deps/${MACHINE}"
cd "deps/${MACHINE}"
```

1. **On-top of** the base `conda` environment (`--system-site-packages`)

Install Dependencies

Dao-AILab/flash-attention | saforem2/ezpz | NVIDIA/apex

- The new release supports three different implementations of FlashAttention: (`v1.0.4`, `v2.x`, `triton`)
- FlashAttention `v2.x` may have numerical instability issues. For the best performance, we recommend using FlashAttention + Triton
- `Dao-AILab/flash-attention`:
  - `v1.0.4`:

    ```
    python3 -m pip install flash-attn==1.0.4
    ```

  - `v2.x`:

    ```
    git clone https://github.com/Dao-AILab/flash-attention
    cd flash-attention
    python3 setup.py install
    ```

  - `openai/triton`:

    ```
    git clone -b legacy-backend https://github.com/openai/triton
    cd triton/python
    python3 -m pip install cmake pybind11
    python3 -m pip install .
    ```

Running

- The ALCF/ directory contains shell scripts for setting up the environment and specifying options to be used for training.

- ALCF/
  ```
  ├── args.sh
  ├── launch.sh
  ├── model.sh
  ├── setup.sh
  ├── submit-pbs.sh
  ├── submit.sh
  └── train-gpt3.sh
  ```

- Various options can be specified dynamically at runtime by setting them in your environment, e.g.:

```bash
# Set env. vars to use:
MODEL_SIZE_KEY="GPT25B"
SEQ_LEN=1024
USE_FLASH_ATTN=1
MICRO_BATCH=1
GAS=1
SP_TYPE="megatron"
ZERO_STAGE=1
# Launch training:
./ALCF/train-gpt3.sh
```

Details

Explicitly:

- ALCF/train-gpt3.sh: **Main entry point for training**. This script will:
  - Source the rest of the required ALCF/*.sh scripts below
- ALCF/models.sh: Contains some example model architectures for GPT3-style models
- ALCF/args.sh: Logic for parsing / setting up runtime options for Megatron and DeepSpeed
- ALCF/setup.sh: Locate and activate virtual environment to be used, ensure MPI variables are set properly
- ALCF/launch.sh: Identify available resources and build the command to be executed
  - i.e. figure out how many: `{nodes, GPUs per node, GPUs total}`, to pass to `mpi{run,exec}`
  - then, use this to launch `mpiexec <mpiexec-args> python3` `pretrain_gpt.py` `<gpt-args>`

DeepSpeed4Science

- Long Sequence Support for GenSLM Model

Argonne NATIONAL LABORATORY ⟷ DeepSpeed4Science ⟷ DeepSpeed

Latent space of biologically meaningful properties for SARS-CoV-2 genomes

Looooooooooong Sequence Lengths

Argonne NATIONAL LABORATORY ⟷ DeepSpeed4Science ⟷ DeepSpeed

Table 2: Long sequence length support from microsoft/Megatron-DeepSpeed

Sequence Length	Old Megatron-DeepSpeed (TFLOPS)	New Megatron-DeepSpeed (TFLOPS)
2k	25	68
4k	28	80
8k	OOM	86
16k	OOM	92
32k	OOM	100
64k	OOM	106
128k	OOM	119
256k	OOM	94

Looooooooong Sequence Lengths

- Working with [Microsoft DeepSpeed] team to enable longer sequence lengths (context windows) for LLMs[1]
  - Release: **DeepSpeed4Science Overview and Tutorial**

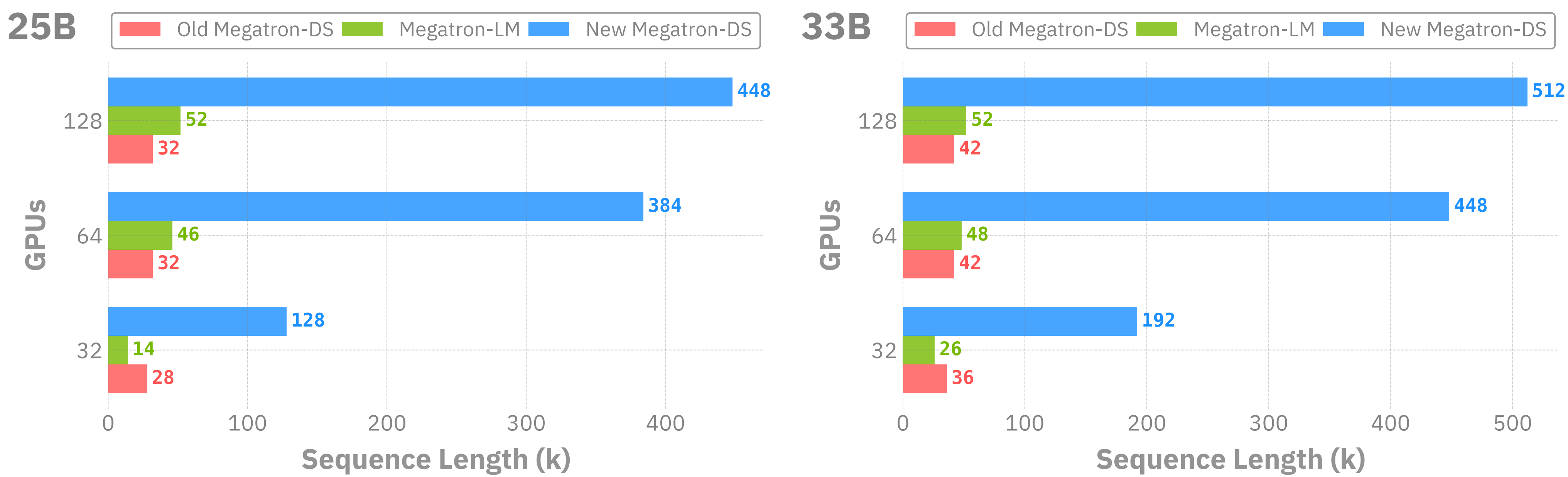


Figure 8: Maximum (achievable) `SEQ_LEN` for both `25B` and `33B` models [WIP]

1. The described experiments were performed on 4 NVIDIA DGX A100-40GB nodes, all using TPSIZE=32[^tpsize], connected through 8 HDR InfiniBand (200Gb/s per HDR).↩

Looooooooong Sequence Lengths

- We can evaluate the performance of our model by looking at two different metrics for throughput: `samples_per_sec` and `TFLOPS`.
  - Explicitly, we see that we are able to scale up to significantly longer sequences: (`420k / 128k ~ 3.3x`) with only a minimal impact on throughput performance: (`81 / 105 ~ 77%`)[1].

Table 3: Impact on TFLOPS as a function of increasing sequence length. Table from: `throughput/TFLOPS`

Name	Sequence Length (k)	(`seq_len / min_seq_len`)	TFLOPS	TFLOPS (% of peak)
GPT25B	420	**3.28125**	81.77225	**77.867**
GPT25B	400	3.125	90.62	86.297
GPT25B	360	2.8125	81.6325	77.7348
GPT25B	360	2.8125	82.6824	78.7346
GPT25B	192	1.5	115.8228	110.2927
GPT25B	128	1	106.672	101.5788
GPT25B	128	1	105.014	100.00

1. `throughput/TFLOPS`

Links

1. Hannibal046/Awesome-LLM awesome
2. Mooler0410/LLMsPracticalGuide
3. Large Language Models (in 2023)
4. The Illustrated Transformer
5. Generative AI Exists because of the Transformer
6. GPT in 60 Lines of Numpy
7. Better Language Models and their Implications
8. 🧪 Progress / Artefacts / Outcomes from 🌸 Bloom BigScience

Acknowledgements

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References

Vaswani, Ashish, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. 2017. "Attention Is All You Need." https://arxiv.org/abs/1706.03762.

Yang, Jingfeng, Hongye Jin, Ruixiang Tang, Xiaotian Han, Qizhang Feng, Haoming Jiang, Bing Yin, and Xia Hu. 2023. "Harnessing the Power of LLMs in Practice: A Survey on ChatGPT and Beyond." https://arxiv.org/abs/2304.13712.

Yao, Shunyu, Dian Yu, Jeffrey Zhao, Izhak Shafran, Thomas L. Griffiths, Yuan Cao, and Karthik Narasimhan. 2023. "Tree of Thoughts: Deliberate Problem Solving with Large Language Models." https://arxiv.org/abs/2305.10601.