Profiling and Optimizing AI Trainings

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Agenda

1. Introduction
    - Systems' Topology
    - GPU communication (NCCL)
2. NVIDIA Nsight Systems
    - Nsys command
    - Nsight client
3. Paraver
    - Nsys2prv
    - Paraver client
4. Exercises

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Why code profiling?

"You can have 1.000.000 GPU hours for FREE!..."

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"You can have 1.000.000 GPU hours for FREE!..."

Only condition:

- Prove that all these hours will be used efficiently

Questions that need answers...

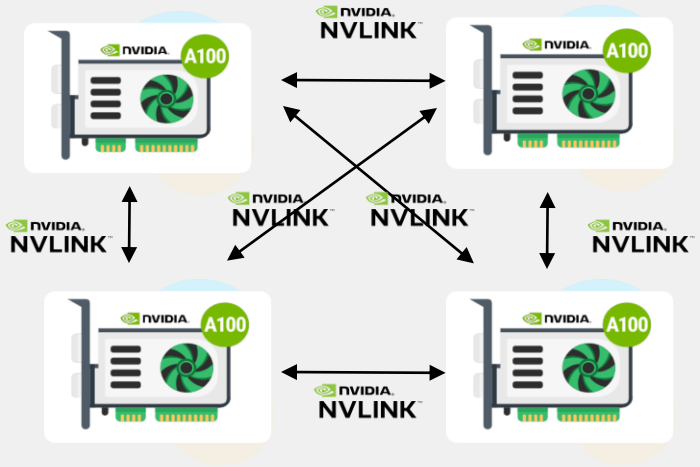
Profiling is the process of measuring and analyzing a program's runtime behavior in order to understand how it uses system resources.

- Is my GPU "starving" for data ?
  - *Maybe the data loader is taking longer than expected..*
- Is the batch size optimized for memory?
  - *Small batch sizes might be underutilizing the available resources...*
- How much time is spent on Communication vs. Computation?
  - *Communication between gpus is blocking unrelated computations..*
- Is my model sharding degree causing too much intra-node or inter-node latency?
  - *Maybe the partition degree I have chosen is too high my hardware topology, and the available bandwidth is limiting...*
- Where is the "Bubble" in my Pipeline?
  - *Pipeline parallelism (PP) introduces GPU dependencies, slowing down out training...*

How do GPUs communicate?

Intra-Node

- NVLink cables
  (Leonardo 64GiB HBM2e NVLink 3.0 (200 GB/s)
- NVSwitch (>4 GPUs node) + NVLink
- PCIe (cpu-gpu, slow)



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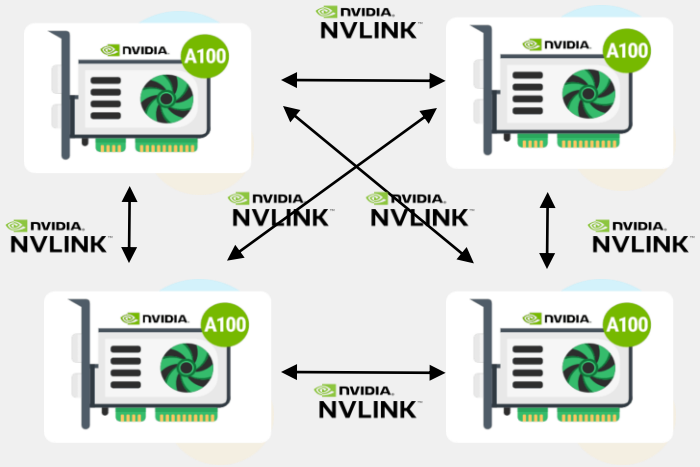
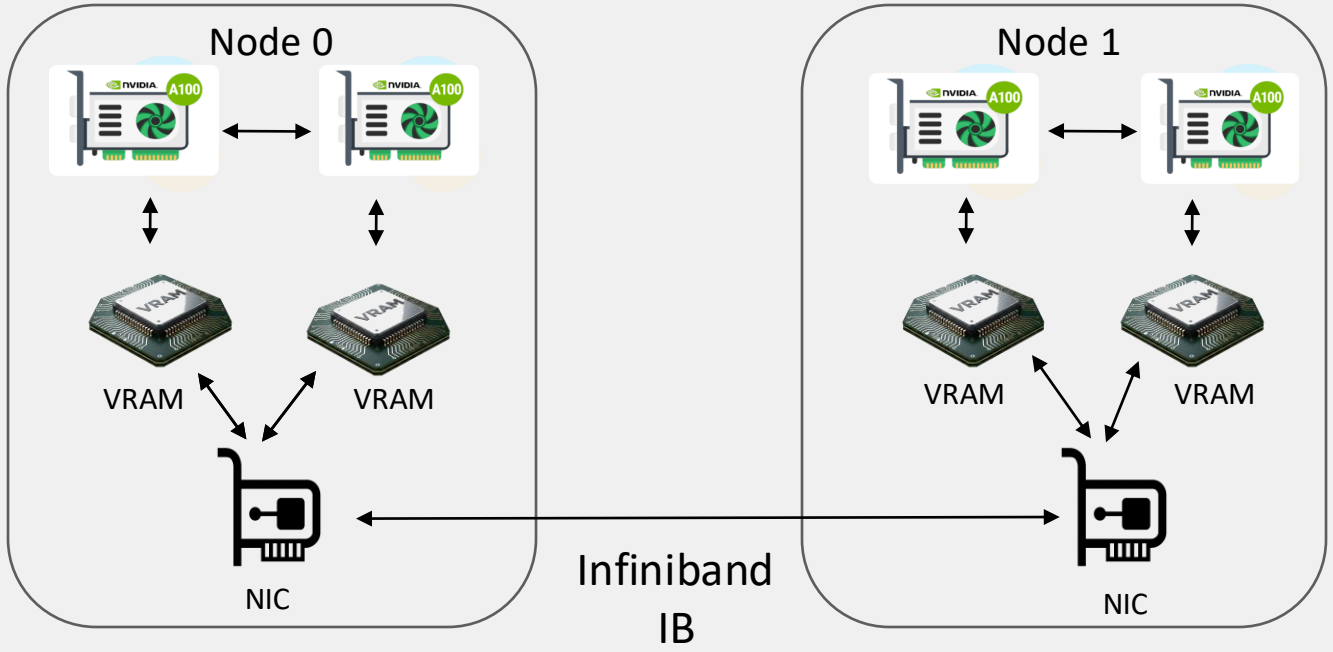


Inter-Node

- InfiniBand GPU inter-node Remote Direct Memory Access
  (Leonardo 200 Gbps~25GB/s NVIDIA Mellanox HDR InfiniBand)
- Ethernet (fallback, slow)



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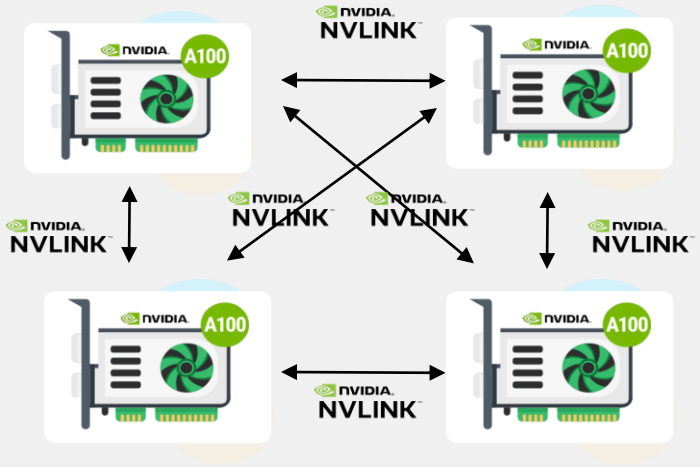

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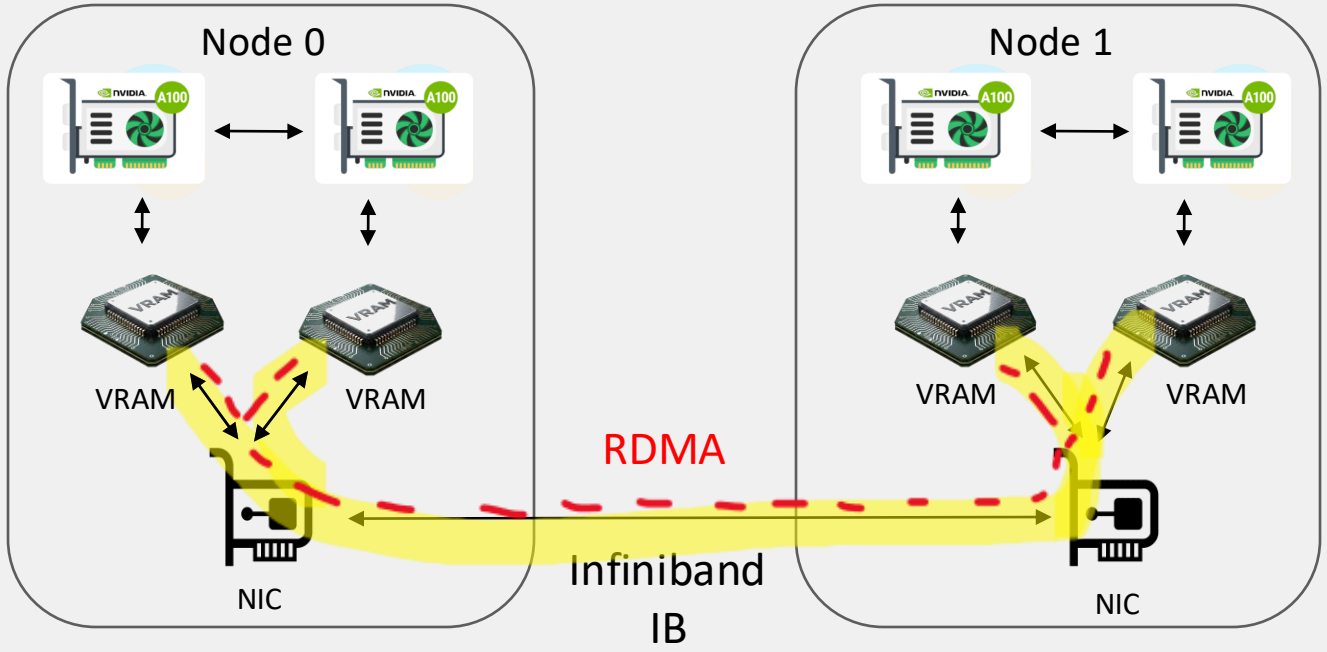


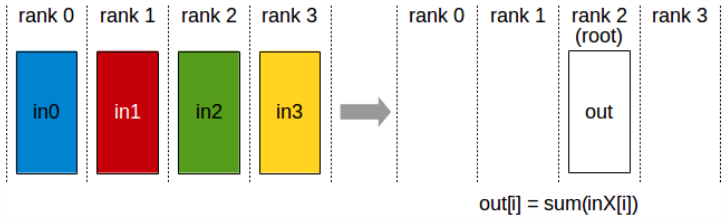
How do GPUs communicate?

NCCL: NVIDIA Collective Communication Library

- Implements multi-GPU and multi-node communication primitives optimized for NVIDIA GPUs and networking.

Reduce

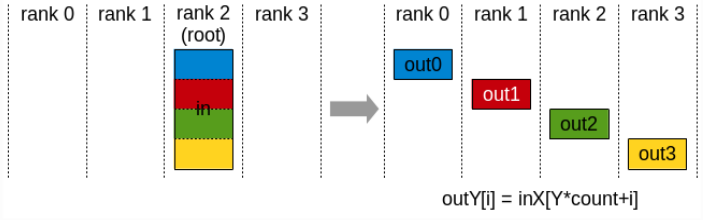
The Reduce operation performs the same operation as AllReduce, but stores the result only in the receive buffer of a specified root rank.



Reduce operation: one rank receives the reduction of input values across ranks.

Scatter

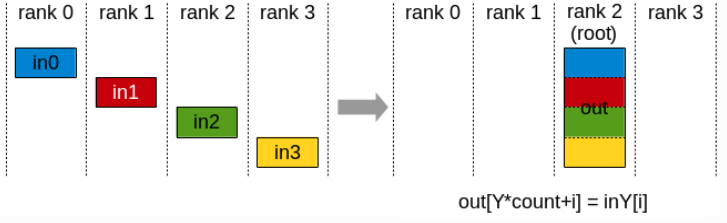
The Scatter operation distributes a total of N*k values from the root rank to k ranks, each rank receiving N values.



Scatter operation: root rank distributes data to all ranks.

Gather

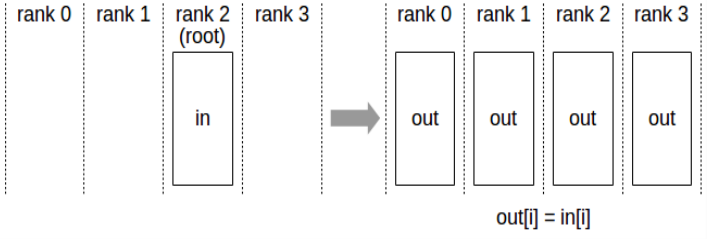
The Gather operation gathers N values from k ranks into an output buffer on the root rank of size k*N.



Gather operation: root rank receives data from all ranks.

Broadcast

The Broadcast operation copies an N-element buffer from the root rank to all the ranks.



Broadcast operation: all ranks receive data from a "root" rank.

How do GPUs communicate?

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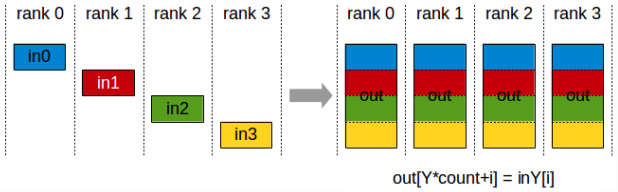
AllGather

The AllGather operation gathers N values from k ranks into an output buffer of size k*N, and distributes that result to all ranks.

The output is ordered by the rank index. The AllGather operation is therefore impacted by a different rank to device mapping.

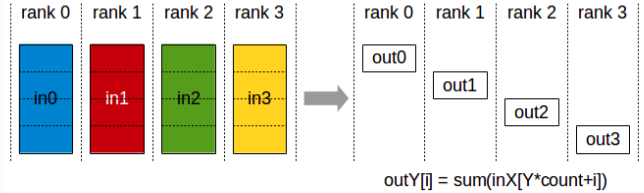


AllGather operation: each rank receives the aggregation of data from all ranks in the order of the ranks.

ReduceScatter

The ReduceScatter operation performs the same operation as Reduce, except that the result is scattered in equal-sized blocks between ranks, each rank getting a chunk of data based on its rank index.

The ReduceScatter operation is impacted by a different rank to device mapping since the ranks determine the data layout.

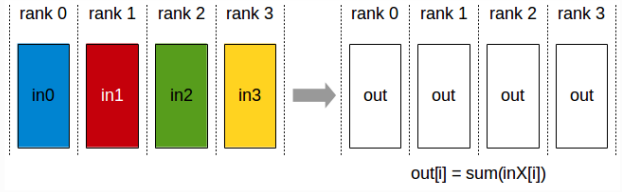


Reduce-Scatter operation: input values are reduced across ranks, with each rank receiving a subpart of the result.

AllReduce

The AllReduce operation performs reductions on data (for example, sum, min, max) across devices and stores the result in the receive buffer of every rank.

In a *sum* allreduce operation between *k* ranks, each rank will provide an array in of N values, and receive identical results in array out of N values, where out[i] = in0[i]+in1[i]+...+in(k-1)[i].

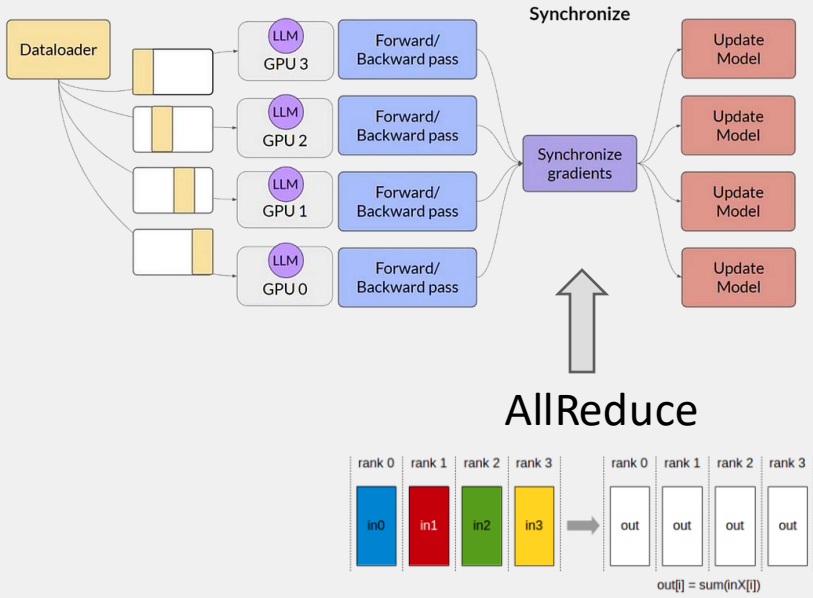


All-Reduce operation: each rank receives the reduction of input values across ranks.

DDP Communication

Collective	Role
AllReduce	Aggregates gradients across all GPUs after backward pass. This is the default and the most performance-critical operation in DDP.
Broadcast	Used at initialization to broadcast model weights from a master rank to all other ranks, ensuring consistent start states before training.

Distributed Data Parallel (DDP)



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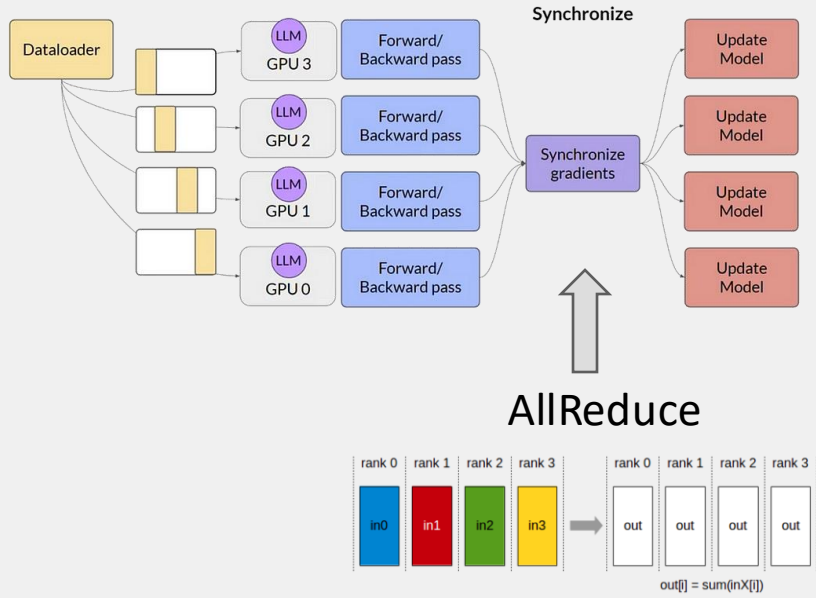


Trace Pattern:

Forward GEMM → Backward GEMM→ AllReduce (bucketed)

*GEMM: CUDA kernel for General Matrix Multiplication

Larger Model VRAM requirements - example

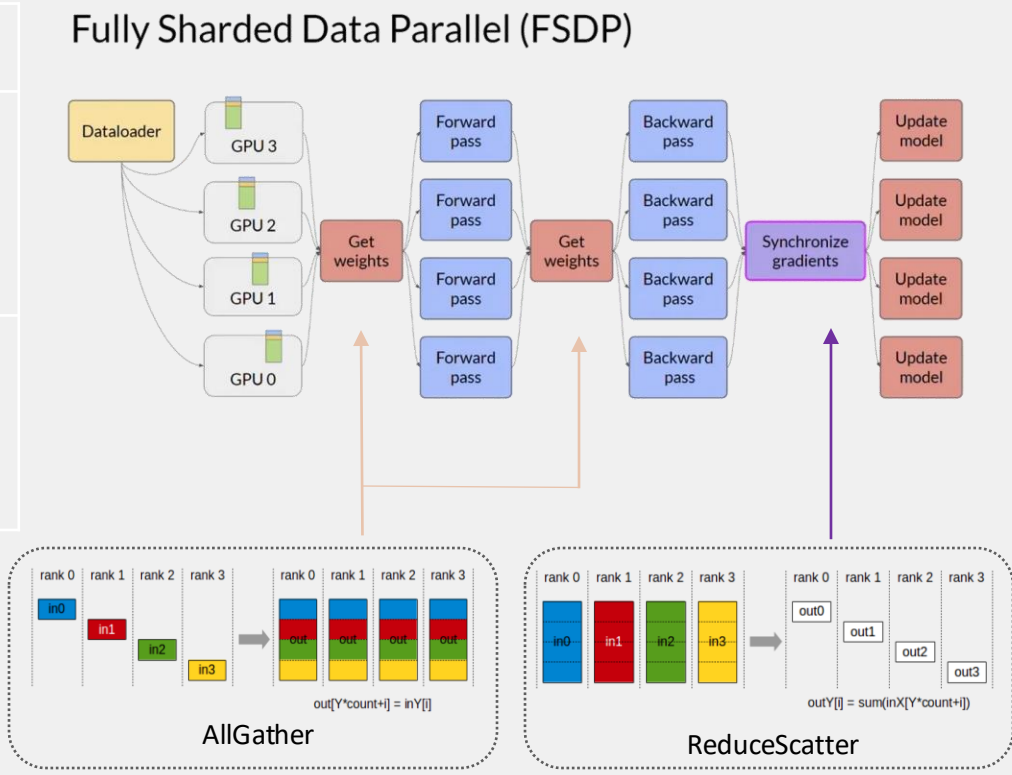
- **Training static states**:
  - Weights
  - Gradients
  - Optimizer states
- **ADAM optimizer**:
  - Master Weights (FP32)
  - Momentum & variance (FP32) for each model parameter
- **Dynamic or live states:**
  - Activations (depends batch size, hidden layers, sequence length, etc.)
  - Activation gradients
  - Communication & precision casting buffers
  - Etc.

Dynamic states can vary in this example 8-20GB or more

Component	Per Billion Params	Mistral 7B Total	Equal partitions (4 GPUS)
Model weights	x2bytes → 2 GB (FP16/BF16)	14 GB	3.5 GB / GPU
Gradients	x2bytes →2 GB (FP16/BF16)	14 GB	3.5 GB / GPU
Optimizer States	3x4bytes → 12 GB (Adam)	84 GB	21 GB / GPU
Total Static	16 GB	112 GB	**28** GB / GPU

FSDP Communication

Collective	Role
AllGather	During forward and backward pass, before computing a layer, the full parameter shard is assembled across GPUs, so that so each GPU can compute activations, attention matrices, etc. (Q-K-V projection weights, embeddings, MLP weigths)
ReduceScatter	After backward pass, gradient shards are reduced and scattered back across GPUs.



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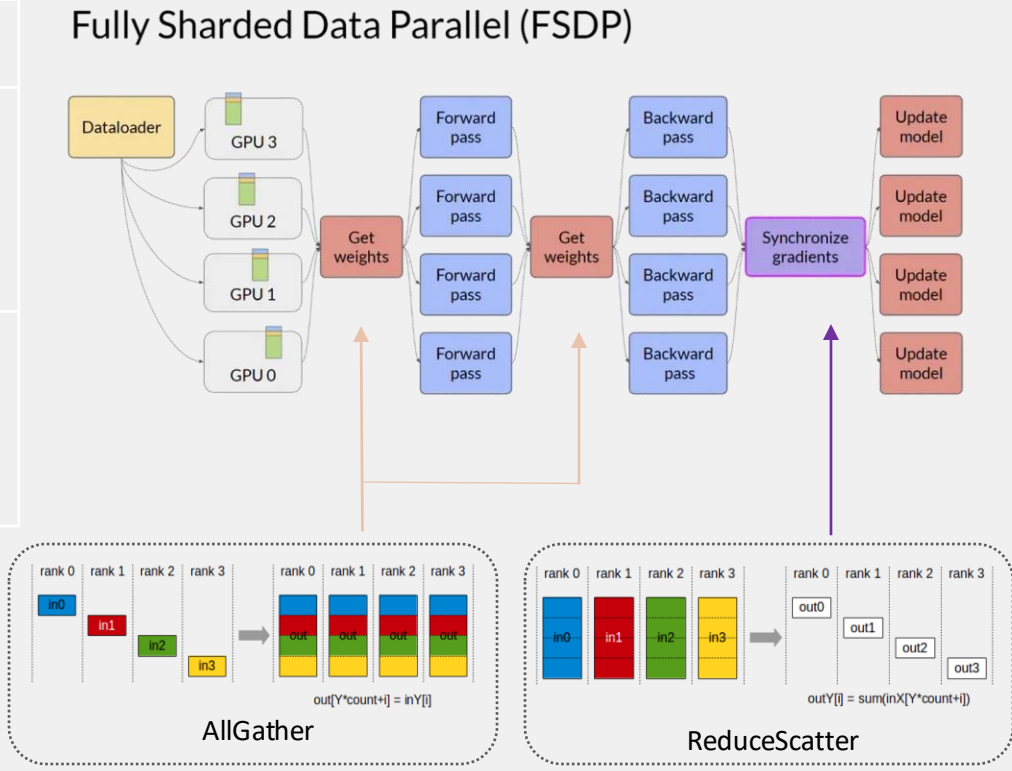
ReduceScatter	After backward pass, gradient shards are reduced and scattered back across GPUs.

Trace Pattern:

AllGather → Forward GEMM → AllGather → Backward GEMM→ ReduceScatter

FSDP compared to DDP:

- More frequent collectives
- Smaller collective sizes
- Higher sensitivity to latency
- More opportunity for commumication-computation overlap



Deepspeed Communication - ZeRO1

Feature	ZeRO Stage 1
Parameter storage	Replicated
Gradient storage	Replicated
Optimizer state	Sharded
Forward communication	None
Backward communication	AllReduce
Optimizer communication	Minimal
Memory efficiency	Medium
Communication frequency	Low

Trace Pattern:

ZeRO1: Backward GEMM → AllReduce (large buckets) [Similar to DDP]

Deepspeed Communication - ZeRO2

Feature	ZeRO Stage 1	ZeRO Stage 2
Parameter storage	Replicated	Replicated
Gradient storage	Replicated	Sharded
Optimizer state	Sharded	Sharded
Forward communication	None	None
Backward communication	AllReduce	ReduceScatter
Optimizer communication	Minimal	Minimal
Memory efficiency	Medium	High
Communication frequency	Low	Medium

Trace Pattern:

ZeRO1: Backward GEMM → AllReduce (large buckets) [Similar to DDP]

ZeRO2: Backward GEMM→ ReduceScatter

Deepspeed Communication - ZeRO3

Feature	ZeRO Stage 1	ZeRO Stage 2	ZeRO Stage 3
Parameter storage	Replicated	Replicated	Sharded
Gradient storage	Replicated	Sharded	Sharded
Optimizer state	Sharded	Sharded	Sharded
Forward communication	None	None	AllGather (per layer)
Backward communication	AllReduce	ReduceScatter	AllGather, ReduceScatter
Optimizer communication	Minimal	Minimal	Minimal
Memory efficiency	Medium	High	Very High
Communication frequency	Low	Medium	High

Trace Pattern:

ZeRO1: Backward GEMM → AllReduce (large buckets) [Similar to DDP]

ZeRO2: Backward GEMM→ ReduceScatter

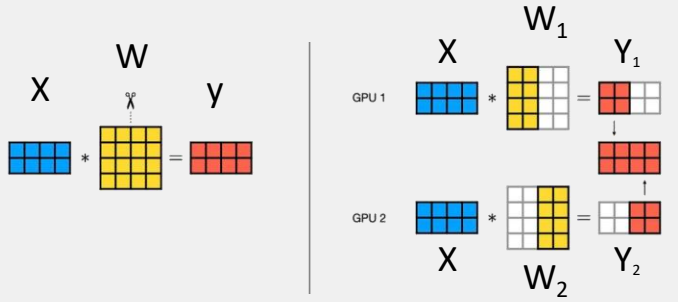
ZeRO3: AllGather → Forward GEMM → AllGather → Backward GEMM→ ReduceScatter [Similar to FSDP]

MegatronLM Communication

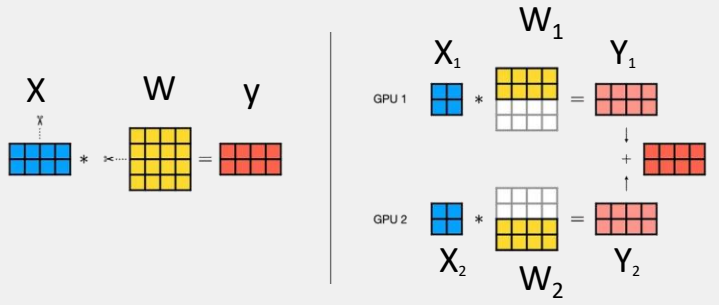
Parallelism Type	Collective Used	Forward	Backward
Data Parallel	AllReduce	-	After backward on weight updates
Pipeline Parallel	Send / Recv (P2P)	Transfer activations (outputs) between pipeline stages	Transfer gradients between pipeline stages
Tensor Parallel	-	ColumnParallelLinear -> RowParallelLinear	-
	AllGather	ColumnParallelLinear -> ColumnParallelLinear (rare)	-
	AllReduce	RowParallelLinear -> ColumnParallelLinear	ColumnParallelLinear layer input gradients only * (all other gradients are computed locally on each rank)

Linear Layer: Y = W*X + b

Column Parallel Linear



Row Parallel Linear



* $dX=dYW^T$, $W=[\ W_1;W_2;\ldots;W_{TP\text{-}ranks}\ ]$, $Y=[\ Y_1,Y_2,\ldots,Y_{TP\text{-}ranks}\ ]$

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Nvidia Nsight Systems - Terminology

Kernel: function executed on the GPU.

- ampere_bf16_gemm → matrix multiplication
- attn_fwd_kernel → attention
- ncclDevKernl_AllReduce → communication

CUDA API: CPU-GPU interface, set of functions that allow out program to launch kernels, allocate GPU memory, copy data, synchronize execution, etc.

- cudaMalloc, cudaMemcpy, cudaStreamSynchronize, etc.

NVTX: lightweight annotation API to create custom markers and labels in the code. Used in torch.cuda.nvtx.

- "Batch X", "forward", "backward", "data loading X"

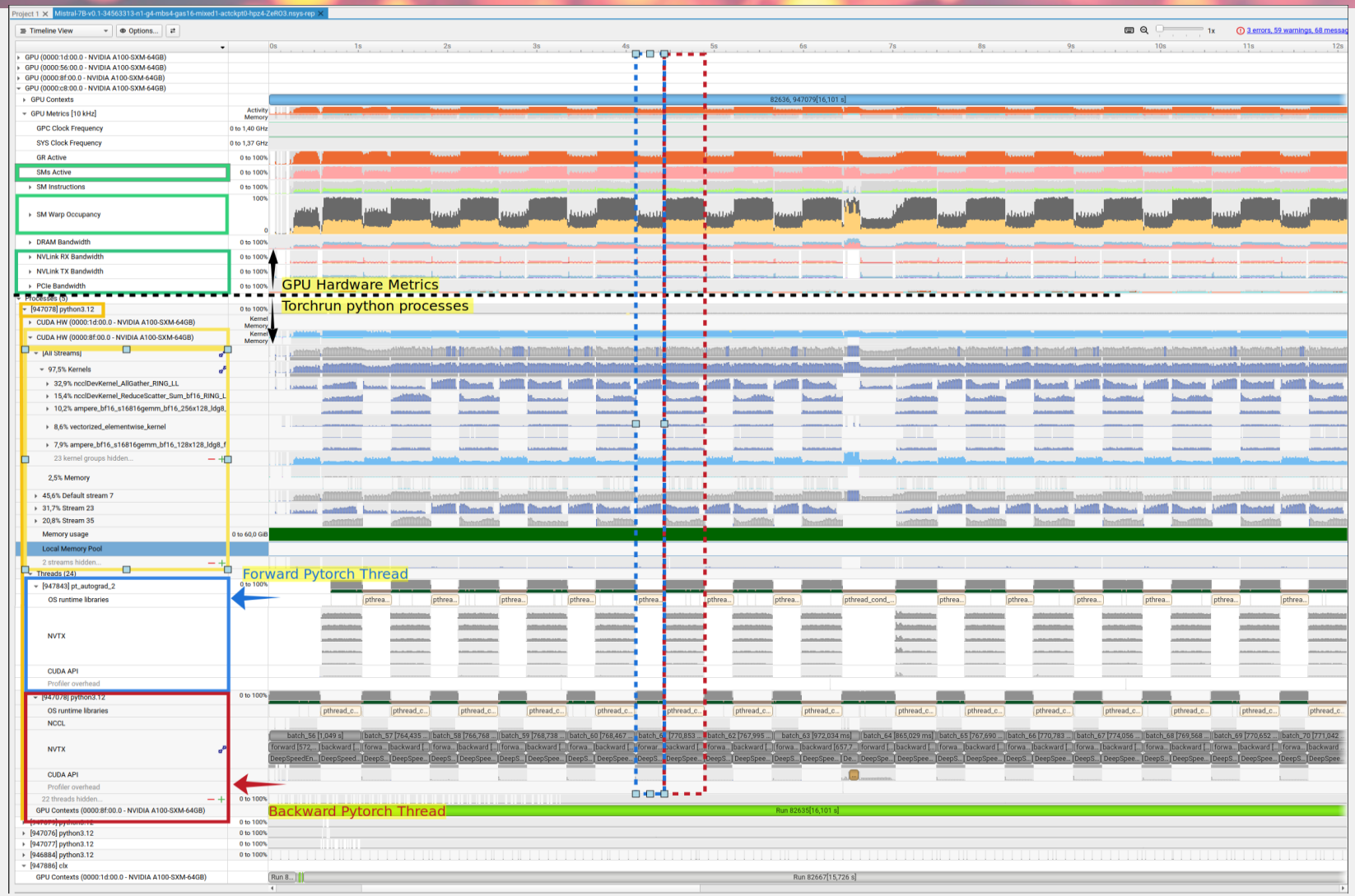
Stream Processors (SM): A compute unit inside the GPU. The A100 has 108 SMs.

GPU Thread: Smallest execution unit

Warp: Group of GPU threads that execute together (commonly 32)

- **SM Active %:** Percentage of time SMs are doing work.
- **SM Instructions Tensor Active**: Tensor core activity for accelerate tensor multiplication
- **Warp Occupancy**: How many warps are ready to run per SM
- **(CUDA) Stream**: Execution queue

Nvidia Nsight Systems - Events View



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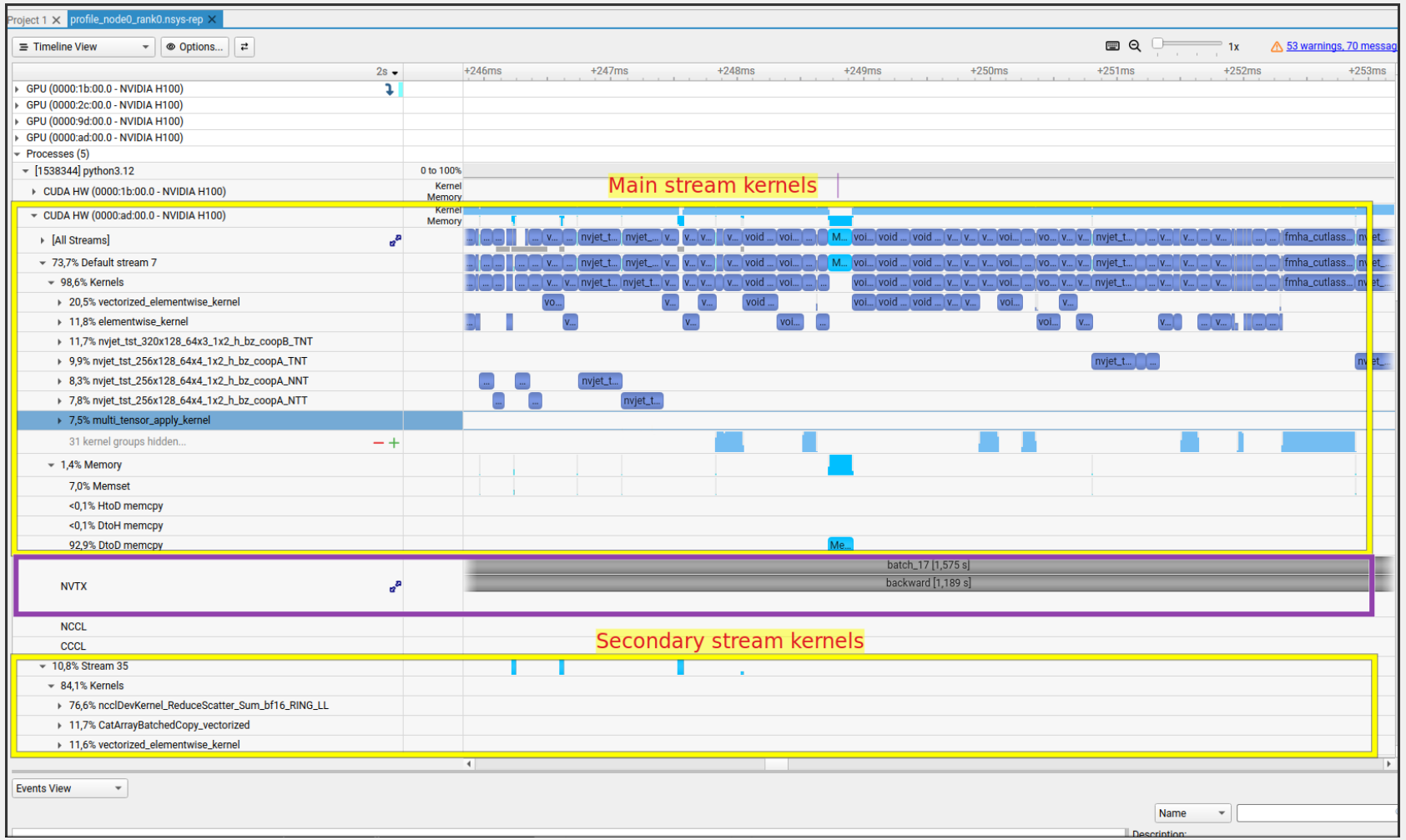
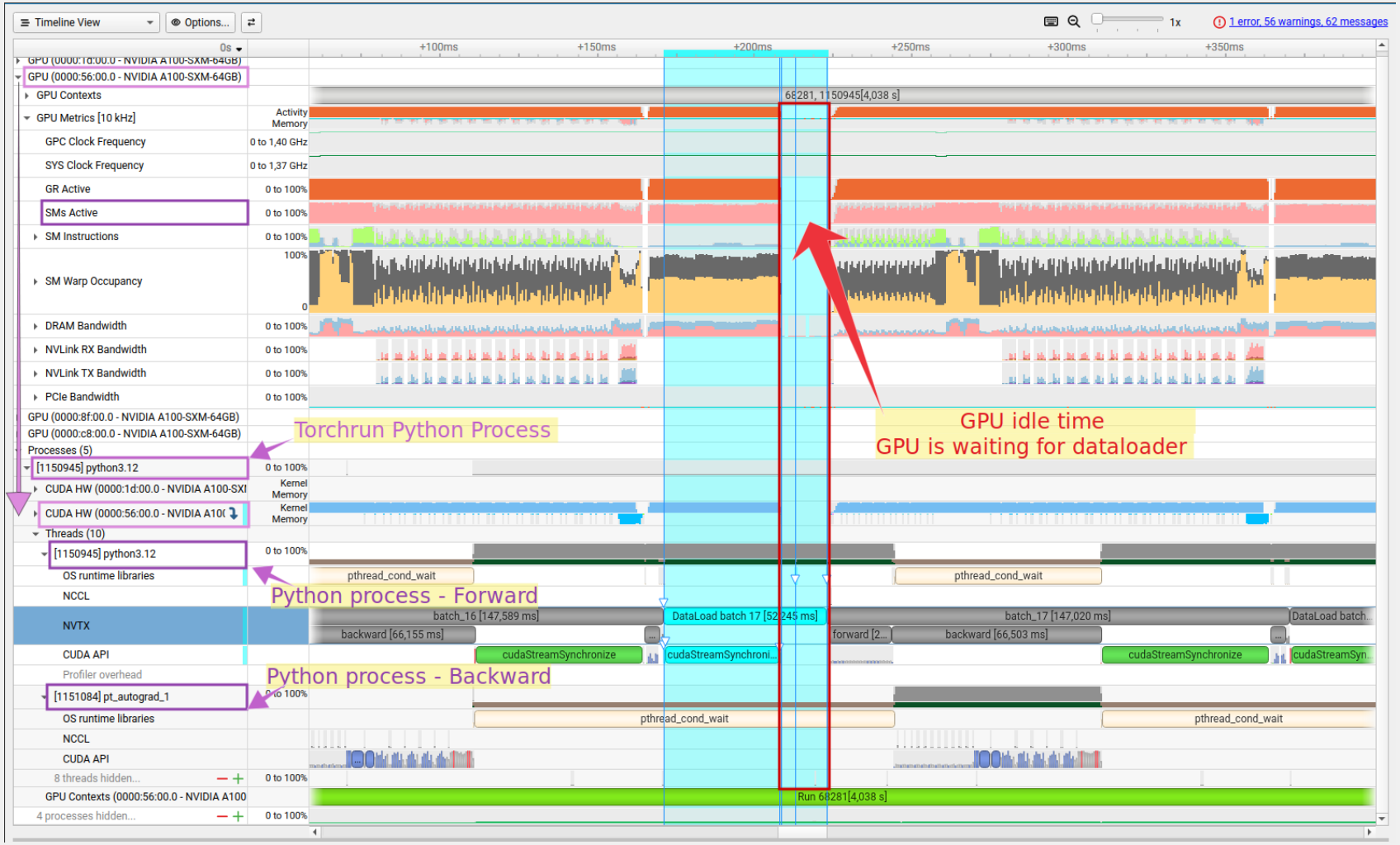
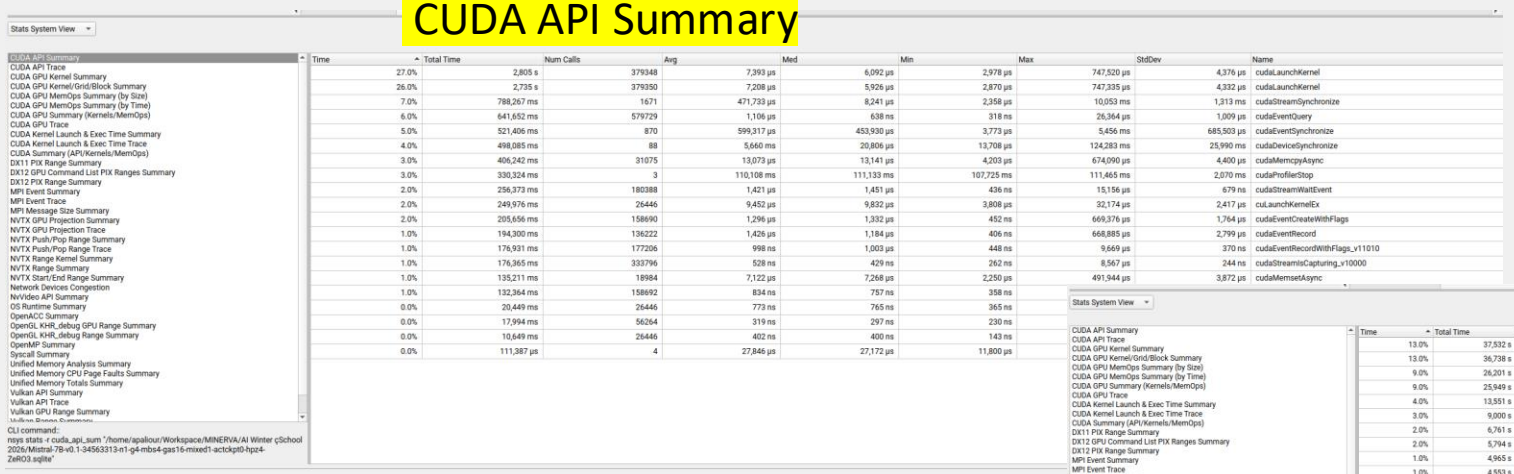


Nvidia Nsight Systems – Idle time

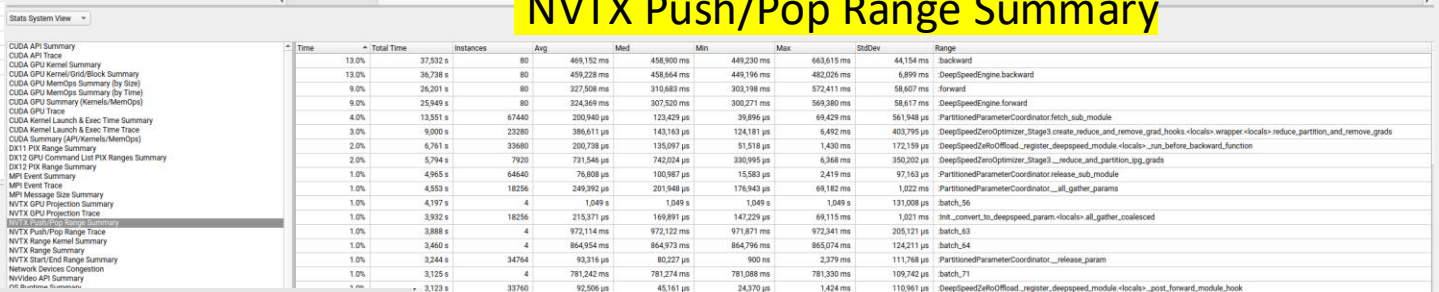


Nvidia Nsight Systems – Stats View

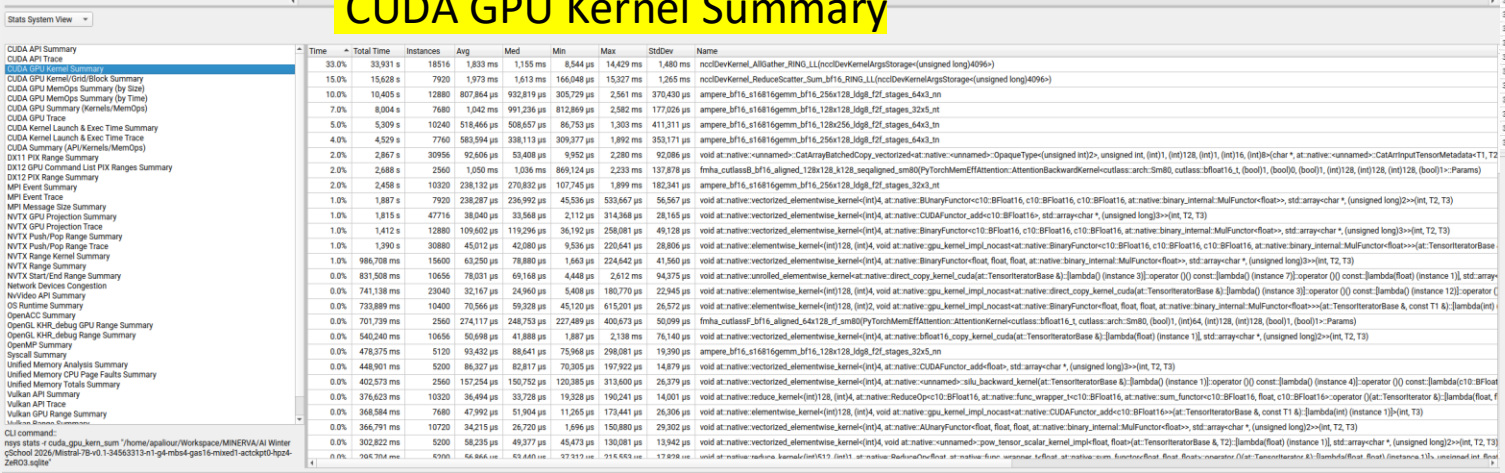
CUDA API Summary



NVTX Push/Pop Range Summary



CUDA GPU Kernel Summary



Nvidia Nsight Systems – nsys command

'nsys' command

```
[apaliour@login05 ~]$ module purge
[apaliour@login05 ~]$ module load cuda/12.6
[apaliour@login05 ~]$ which nsys
/leonardo/prod/opt/compilers/cuda/12.6/none/bin/nsys
[apaliour@login05 ~]$ nsys
 usage: nsys [--version] [--help] <command> [<args>] [application] [<application args>]

 The most commonly used nsys commands are:
        profile       Run an application and capture its profile into a nsys-rep file.
        launch        Launch an application ready to be profiled.
        start         Start a profiling session.
        stop          Stop a profiling session and capture its profile into a nsys-rep file.
        cancel        Cancel a profiling session and discard any collected data.
        service       Launch the Nsight Systems data service.
        stats         Generate statistics from an existing nsys-rep or SQLite file.
        status        Provide current status of CLI or the collection environment.
        shutdown      Disconnect launched processes from the profiler and shutdown the profiler.
        sessions list List active sessions.
        export        Export nsys-rep file into another format.
        analyze       Identify optimization opportunities in a nsys-rep or SQLITE file.
        recipe        Run a recipe for multi-node analysis.
        nvprof        Translate nvprof switches to nsys switches and execute collection.

 Use 'nsys --help <command>' for more information about a specific command.

 To run a basic profiling session:   nsys profile ./my-application
 For more details see "Profiling from the CLI" at https://docs.nvidia.com/nsight-systems
```

'nsys profile' sub-command

```
[apaliour@login05 ~]$ nsys profile --help

usage: nsys profile [<args>] [application] [<application args>]

# ======================================================================
# NSYS Configuration
# ======================================================================
# Recommended NSYS options for ML training profiling:
#   --trace=cuda,nvtx,osrt,cudnn,ucx,nccl,cublas : Trace GPU kernels, NVTX markers, OS runtime, cuDNN, UCX, NCCL, cuBLAS
#   --force-overwrite true              : Overwrite existing profile files
#   --cuda-memory-usage=true            : Track CUDA memory allocations and usage
#   --gpuctxsw=true                     : Track GPU context switches (optional, rarely a bottleneck)
#   --gpu-metrics-devices=all           : Collect GPU metrics (SM utilization, memory throughput, etc.)
#   --gpu-metrics-frequency=10000       : Sample GPU metrics at 10kHz for fine granularity
#   --capture-range=cudaProfilerApi     : Use cudaProfiler start/stop for precise capture (requires NVTX markers in code)
#   --capture-range-end=stop            : End capture when cudaProfilerStop is called
#   --sample=cpu                        : CPU sampling for host-side bottlenecks
#   --backtrace=dwarf                   : Detailed backtraces for CPU samples
#   --cudabacktrace=kernel              : Collect backtraces for CUDA kernel launches
#   --stats=true                        : Generate summary statistics
#   --export=sqlite                     : Export results in SQLite format for advanced analysis
#   --output=<path>                     : Set output file path (already used)
#
# ======================================================================
```

'nsys profile' example

```
nsys profile
  --trace=cuda,nvtx,osrt,cudnn,cublas
  --cuda-memory-usage=true
  --gpuctxsw=true
  --gpu-metrics-devices=all
  --gpu-metrics-frequency=10000
  --capture-range=cudaProfilerApi
  --capture-range-end=stop
  --cudabacktrace=kernel
  --stats=true
  --force-overwrite=true
  --output=./exercise_2_DeepSpeed/profiler/Mistral-7B-v0.1-34563983-n1-g4-mbs4-gas16-mixed1-actckpt0-hpz4-ZeRO3-badcomm1/nsys/profile_node%q{SLURM_NODEID}
  singularity exec
     --nv
     --bind /leonardo
     --bind /leonardo_work
     /leonardo_work/tra26_minwinsc/containers/ai-profiling-workshop.sif
         accelerate launch
             --config_file ./exercise_2_DeepSpeed/accelerate_config.yaml-H8OGt1r6yDfrb
             --rdzv_backend=c10d
             --machine_rank 0
             -m exercise_2_DeepSpeed.train
             --data-path /leonardo_work/tra26_minwinsc/DATA/alpaca-cleaned/alpaca_data_cleaned.json
             --model-path /leonardo_work/tra26_minwinsc/models/Mistral-7B-v0.1
              --epochs 1
              --no-validation
              --profile
              --data-sample 5000
              --dataloader-num-workers 8
              --batch-size 4
              --gradient-accumulation-steps 16
              --deepspeed-config ./exercise_2_DeepSpeed/ds_configs/stage-3/ds_config_mixed-precision_no-activation-checkpointing_comm-overhead.json
```

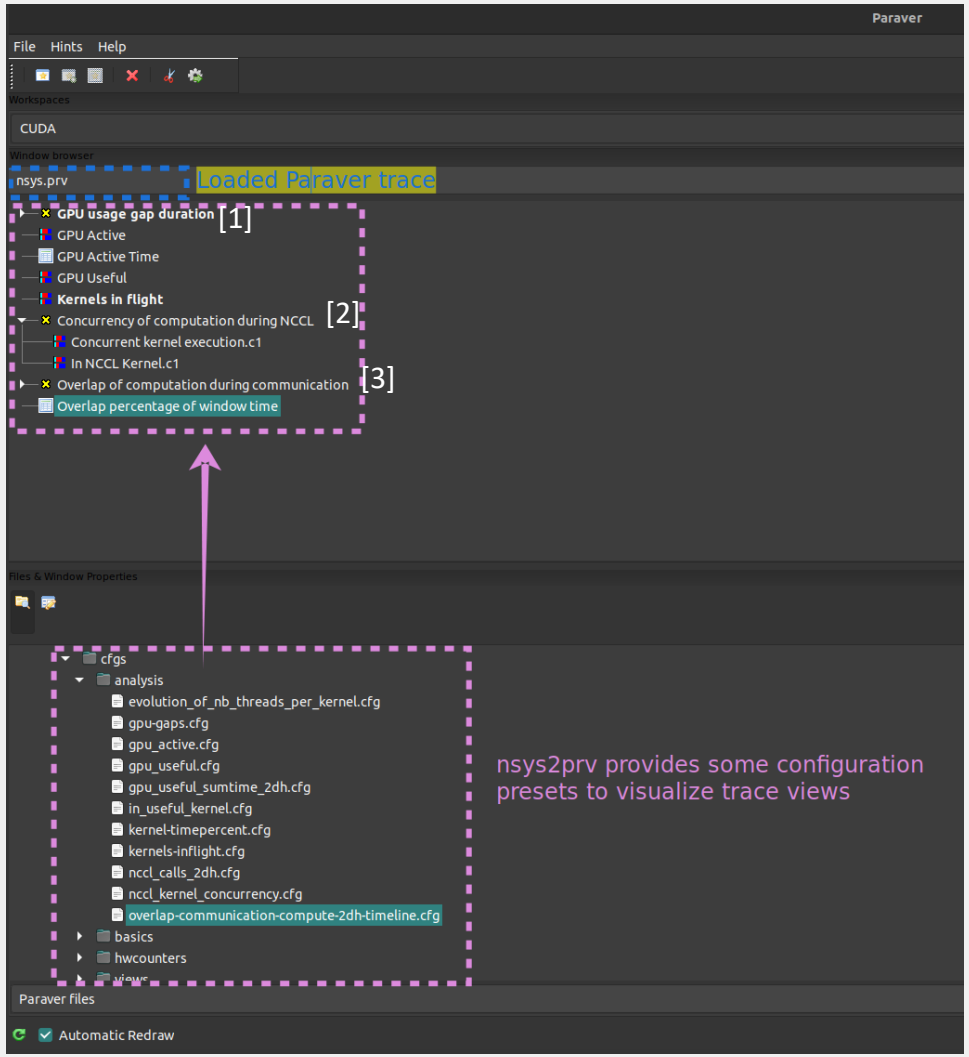
"nsys profile" options

Application to profile

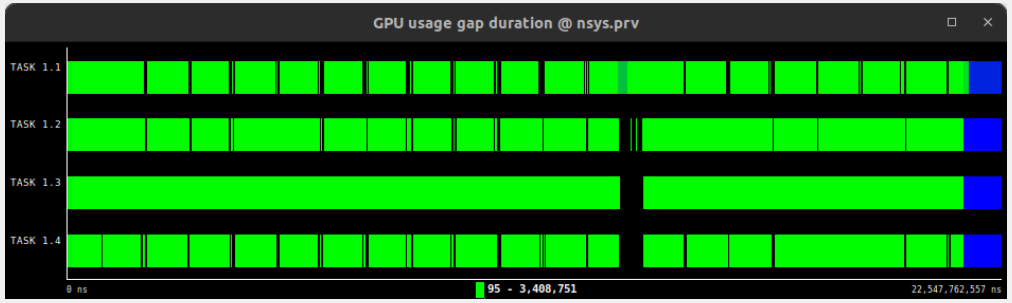
Agenda

1. Introduction
   - NCCL
   - Systems' Topology
2. NVIDIA Nsight Systems
   - Nsys command
   - Nsight client
3. **Paraver**
   - **Nsys2prv**
   - **Paraver client**
4. Demo
5. Hands-on Exercises

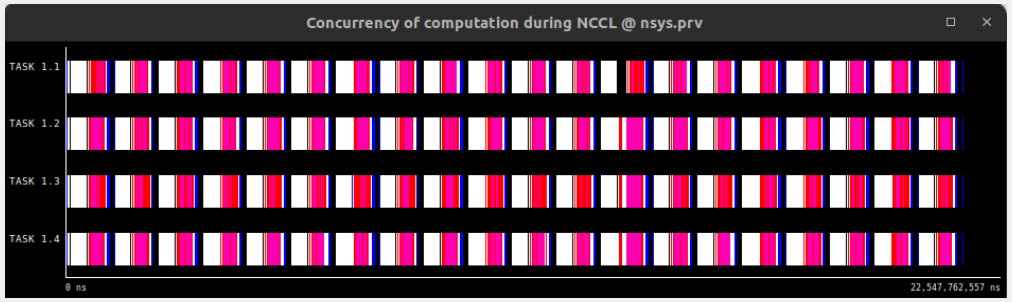
Paraver



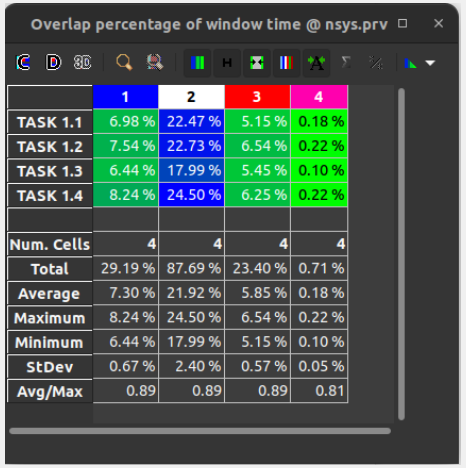
[1]



[2]

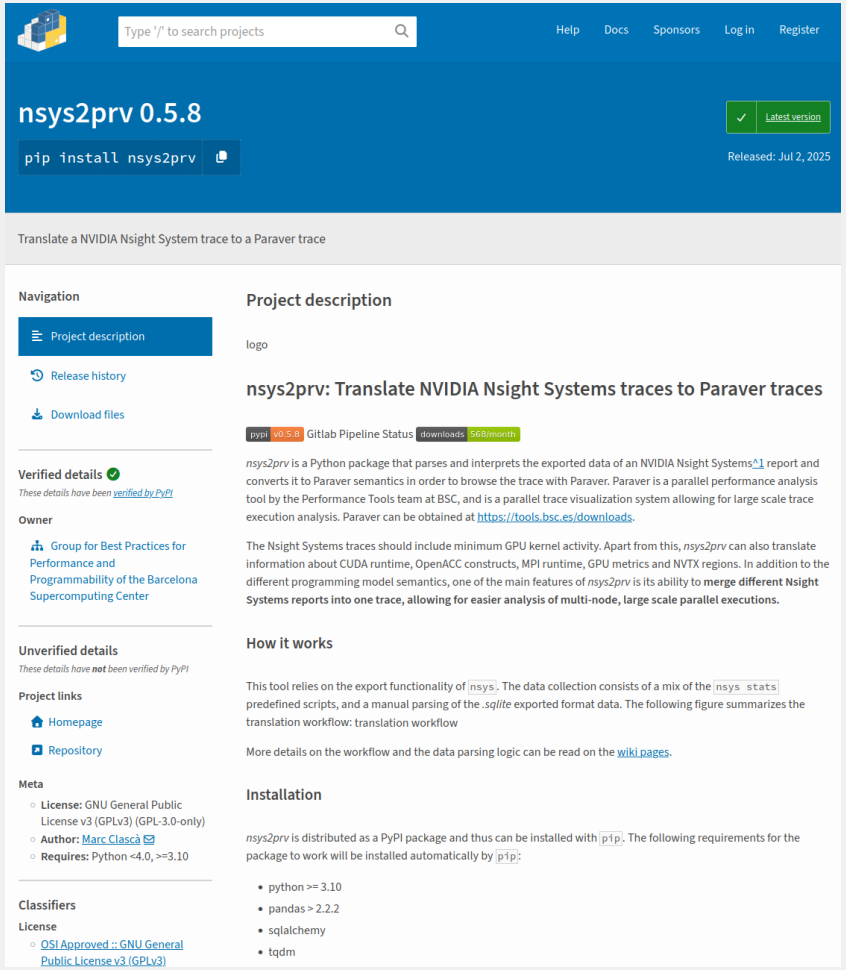


[3]

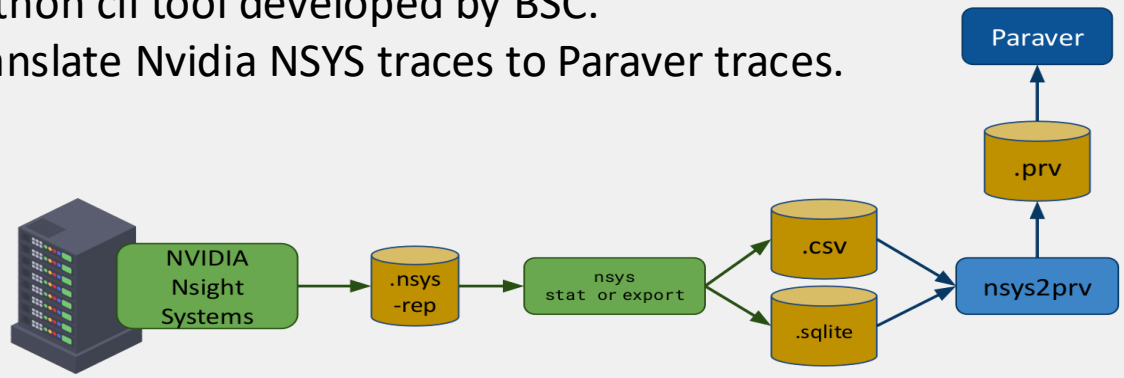


	1	2	3	4
TASK 1.1	6.98 %	22.47 %	5.15 %	0.18 %
TASK 1.2	7.54 %	22.73 %	6.54 %	0.22 %
TASK 1.3	6.44 %	17.99 %	5.45 %	0.10 %
TASK 1.4	8.24 %	24.50 %	6.25 %	0.22 %
Num. Cells	4	4	4	4
Total	29.19 %	87.69 %	23.40 %	0.71 %
Average	7.30 %	21.92 %	5.85 %	0.18 %
Maximum	8.24 %	24.50 %	6.54 %	0.22 %
Minimum	6.44 %	17.99 %	5.15 %	0.10 %
StDev	0.67 %	2.40 %	0.57 %	0.05 %
Avg/Max	0.89	0.89	0.89	0.81

nsys2prv – Trace translation



- Python cli tool developed by BSC.
- Translate Nvidia NSYS traces to Paraver traces.

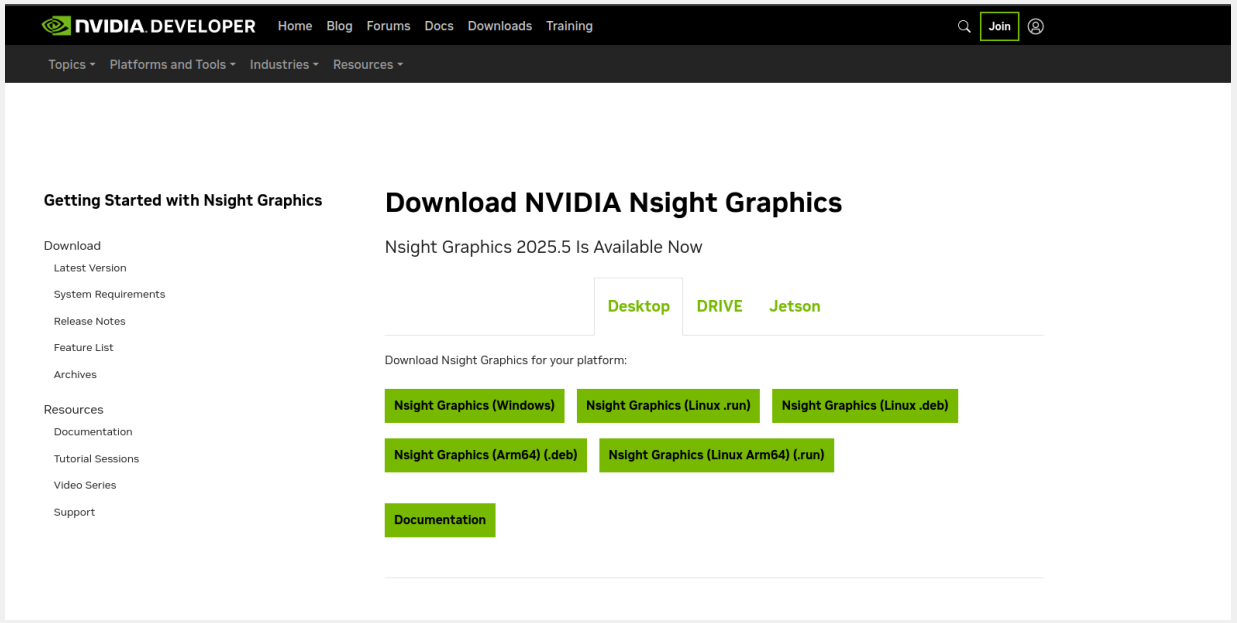



```
❯ nsys2prv --help
nsys2prv v0.5.8
usage: nsys2prv [-h] [-v] [-f FILTER_NVTX] [-t TRACE] [-m] [--force-sqlite] [-s] [-z] source_rep [source_rep ...] output

Translate a NVIDIA Nsight System trace to a Paraver trace

positional arguments:
  source_rep            Nsight source report file
  output                Paraver output trace name

options:
  -h, --help            show this help message and exit
  -v, --version         Show version and exit. (default: None)
  -f FILTER_NVTX, --filter-nvtx FILTER_NVTX
                        Filter by this NVTX range (default: None)
  -t TRACE, --trace TRACE
                        Comma separated names of events to translate: [mpi_event_trace, nvtx_pushpop_trace, nvtx_startend_trace, cuda_api_trace, gpu_metrics, openacc, nccl,
                        graphs] (default: None)
  -m, --multi-report    Translate multiple reports of the same execution into one trace. (default: False)
  --force-sqlite        Force Nsight System to export SQLite database (default: False)
  -s, --sort            Sort trace at the end (default: False)
  -z, --compress        Compress trace at the end with gzip (default: False)

The nsys executable needs to be in the PATH, or the environment variable NSYS_HOME needs to be set. If using postprocessing, the PARAVER_HOME variable needs to be set.
```

Agenda

1. Introduction
   - Systems' Topology
   - GPU communication (NCCL)
2. NVIDIA Nsight Systems
   - Nsys command
   - Nsight client
3. Paraver
   - Nsys2prv
   - Paraver client
4. **Exercises**

Download and setup Nsight



- Download Nvidia Nsight Systems @ https://developer.nvidia.com/nsight-graphics/get-started
- Install on your computer

3. Validate client is running

If in Linux, prefer to download ".deb" and install with:

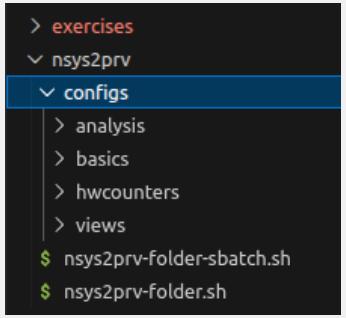
```
> sudo dpkg install
NVIDIA_Nsight_Graphics_2025.5.0.25335.deb
```

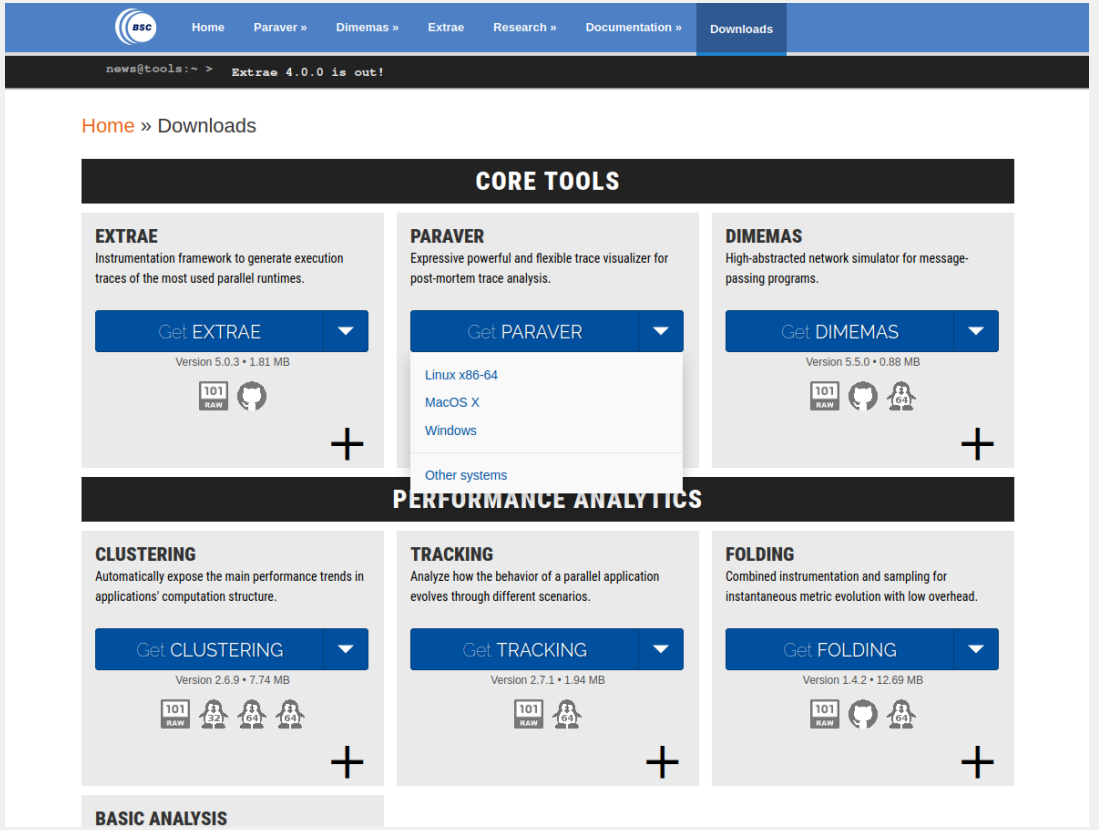
You can check your CPU architecture by running:

```
> arch
```

Download and setup Paraver

1. Download Paraver
   @ https://tools.bsc.es/downloads
2. Install on your computer
3. On Linux/MacOS
   - [Optional] Move folder to ~/Applications
   - Run "bin/wxparaver.bin" on terminal
4. On Windows
   - Run bin/wxparaver.bin.exe
5. Download nsys2prv configuration files stored inside the workshop directory:
   - sys2prv/configs





Exercises

- Repository under path "/leonardo_work/tra26_minwinsc/training-profiling-workshop"
- Copy to your home folder: `cp -R /leonardo_work/tra26_minwinsc/training-profiling-workshop ~/`
- Check contents of the copied folder `cd ~/training-profiling-workshop/exercises && ls -la`

```
[apaliour@login07 ~]$ ls -la training-profiling-workshop/exercises/
total 52
drwxrwsrwx.  9 apaliour interactive  4096 feb 24 14:40 .
drwxrwsrwx.  8 apaliour interactive  4096 feb 22 19:49 ..
drwxrwsrwx. 23 apaliour interactive  4096 feb 25 01:36 .cache
drwxrwsrwx.  4 apaliour interactive  4096 feb 10 15:09 datasets
drwxrwsrwx.  2 apaliour interactive  4096 feb 24 09:59 exercise_0_Communication_Tests
drwxrwsrwx.  6 apaliour interactive  4096 feb 24 14:02 exercise_1_DDP
drwxrwsrwx.  7 apaliour interactive  4096 feb 25 01:41 exercise_2_DeepSpeed
drwxrwsrwx.  7 apaliour interactive  4096 feb 24 16:20 exercise_3_MegatronLM
-rw-rw-rw-.  1 apaliour interactive     0 feb 10 15:19 __init__.py
-rw-rw-rw-.  1 apaliour interactive 13560 feb 25 00:40 slurm.sh
drwxrwsrwx.  4 apaliour interactive  4096 feb 16 16:05 utils
```

- `bash slurm.sh --help`

```
Usage: slurm.sh [OPTIONS] [-- EXTRA_ARGS]

Options:
  -n, --nodes           Number of nodes (default: 1)
  -g, --gpus-per-node   GPUs per node (default: 4)
  -q, --queue           Queue/QOS for SLURM job (default: acc_bench)
  -a, --account         Account name (default: bsc99)
  -p, --partition       Partition on HPC (default: acc)
  -e, --exercise        Exercise number (0, 1, 2, or 3) (required)
  -h, --help            Show this help message

Extra arguments after '--' will be passed to the training script.

  --slow-dataloading                Enable slow dataloading example for exercise 1 (DDP) (default: disabled)
  --mixed-precision                 Enable mixed precision training using 'bf16' (default: disabled)
  --micro-batch-size N              Set micro batch size to N (default: 4)
  --gradient-accumulation-steps N   Set gradient accumulation steps to N (default: 1)
  --activation-checkpointing        Enable activation/gradient checkpointing (default: disabled)
  --ds-hpz-partition N              Set DeepSpeed HPZ partition size to N, for exercise 2 (DeepSpeed) only. Refers to number of GPUs per model replica (default
: 2)
  --ds-stage2                       Use DeepSpeed stage 2 partitioning instead of stage 3, for exercise 2 (DeepSpeed) only (default: stage 3)
  --tp N                            Set tensor parallelism to N, for exercise 3 (MegatronLM) only (default: 1, i.e. no tensor parallelism)
  --pp N                            Set pipeline parallelism to N, for exercise 3 (MegatronLM) only (default: 1, i.e. no pipeline parallelism)
  --no-profile                      Disable profiling with NSYS (default: profiling enabled)
  --nsys2prv                        After profiling, automatically translate NSYS output to Paraver traces using nsys2prv (default: disabled)

Example:
  slurm.sh -n 1 -g 4 -e 1 -a tra26_minwinsc -p boost_usr_prod -- --mixed-precision --gradient-accumulation-steps 4
```

Exercises

- *Exercise 0* - Intra-node topology discovery and communication validation
  - "exercise_0_Communication_Tests/"
  - Run `bash slurm.sh -e 0`

- *Exercise 1* – Finetune **Llama-3.1-1B** with Accelerate & DDP
  - "exercise_1_DDP/"
  - Run `bash slurm.sh -e 1`
    - slow-dataloading, mixed-precision, gradient-accumulation-steps, micro-batch-size
- *Exercise 2* – Finetune **Mistral-7B-v0.1** with Accelerate & DeepSpeed
  - "exercise_2_DeepSpeed/"
  - Run `bash slurm.sh -e 2`
    - mixed-precision, gradient-accumulation-steps, micro-batch-size, activation-checkpointing, ds-hpz-partition, ds-stage2, ds-heavy-comm, ds-no-overlap
- *Exercise 3* – Pretrain **Mistral-7B-v0.1** with MegatronLM
  - "exercise_3_MegatronLM/"
  - Run `bash slurm.sh -e 3`
    - tp, pp, micro-batch-size, global-batch-size

Exercises

- Repo can be found on MINERVA Github: https://github.com/minerva4ai-eu/training-profiling-workshop
  - Only one branch: *leonardo*

- After running each exercise (1,2,3) for the 1st time, inside its folder will be created the following folder:

  - *logs/* - containing slurm logs per JOB ID
  - *profiler/* - containing gpu monitoring plots and nsys profiles, also paraver traces is "--nsys2prv" enabled

    - *gpus-monitor/* - logs and plots of gpus' memory, utilization %, watt per node
    - *nsys/* - code profiling traces of type ".nsys-rep" and ".prv"

Exercise 0 – Intranode comm tests

```
bash slurm.sh -e 0
```

```
============== Test 1: PCIe P2P Read ==============
Description: Test direct GPU-to-GPU PCIe read connectivity (P2P) using 'nvidia-smi topo -p2p r'.
 Checking intra-node P2P read PCIe communication with 'nvidia-smi topo -p2p r'...
       GPU0    GPU1    GPU2    GPU3
 GPU0  X       OK      OK      OK
 GPU1  OK      X       OK      OK
 GPU2  OK      OK      X       OK
 GPU3  OK      OK      OK      X

Legend:

  X    = Self
  OK   = Status Ok
  CNS  = Chipset not supported
  GNS  = GPU not supported
  TNS  = Topology not supported
  NS   = Not supported
  U    = Unknown
------------------------------------------------
```

```
============== Test 2: PCIe P2P Write ==============
Description: Test direct GPU-to-GPU PCIe write connectivity (P2P) using 'nvidia-smi topo -p2p w'.
 Checking intra-node P2P write PCIe communication with 'nvidia-smi topo -p2p w'...
       GPU0    GPU1    GPU2    GPU3
 GPU0  X       OK      OK      OK
 GPU1  OK      X       OK      OK
 GPU2  OK      OK      X       OK
 GPU3  OK      OK      OK      X

Legend:

  X    = Self
  OK   = Status Ok
  CNS  = Chipset not supported
  GNS  = GPU not supported
  TNS  = Topology not supported
  NS   = Not supported
  U    = Unknown
------------------------------------------------
```

```
============== Test 3: NVLink P2P ==============
Description: Test direct GPU-to-GPU NVLink connectivity using 'nvidia-smi topo -p2p n'.
 Checking intra-node P2P NVLink communication with 'nvidia-smi topo -p2p n'...
       GPU0    GPU1    GPU2    GPU3
 GPU0  X       OK      OK      OK
 GPU1  OK      X       OK      OK
 GPU2  OK      OK      X       OK
 GPU3  OK      OK      OK      X

Legend:

  X    = Self
  OK   = Status Ok
  CNS  = Chipset not supported
  GNS  = GPU not supported
  TNS  = Topology not supported
  NS   = Not supported
  U    = Unknown
------------------------------------------------
```

```
============== Test 4: GPU Topology ==============
Description: Show the full GPU, NIC, and CPU topology using 'nvidia-smi topo -m'. Useful for understanding all de
vice interconnections.
 Checking intra-node GPUs topology with 'nvidia-smi topo -m'...
       GPU0    GPU1    GPU2    GPU3    NIC0    NIC1    NIC2    NIC3    CPU Affinity    NUMA Affinity   GPU NUMA
ID
 GPU0   X      NV4     NV4     NV4     PXB     NODE    NODE    NODE    0-15    0               N/A
 GPU1   NV4     X      NV4     NV4     NODE    PXB     NODE    NODE    0-15    0               N/A
 GPU2   NV4     NV4     X      NV4     NODE    NODE    PXB     NODE    0-15    0               N/A
 GPU3   NV4     NV4     NV4     X      NODE    NODE    NODE    PXB     0-15    0               N/A
 NIC0   PXB     NODE    NODE    NODE     X      NODE    NODE    NODE
 NIC1   NODE    PXB     NODE    NODE    NODE     X      NODE    NODE
 NIC2   NODE    NODE    PXB     NODE    NODE    NODE     X      NODE
 NIC3   NODE    NODE    NODE    PXB     NODE    NODE    NODE     X

Legend:

  X    = Self
  SYS  = Connection traversing PCIe as well as the SMP interconnect between NUMA nodes (e.g., QPI/UPI)
  NODE = Connection traversing PCIe as well as the interconnect between PCIe Host Bridges within a NUMA node
  PHB  = Connection traversing PCIe as well as a PCIe Host Bridge (typically the CPU)
  PXB  = Connection traversing multiple PCIe bridges (without traversing the PCIe Host Bridge)
  PIX  = Connection traversing at most a single PCIe bridge
  NV#  = Connection traversing a bonded set of # NVLinks

NIC Legend:

  NIC0: mlx5_0
  NIC1: mlx5_1
  NIC2: mlx5_2
  NIC3: mlx5_3

------------------------------------------------
```

```
============== Test 5: InfiniBand State ==============
Description: Show the InfiniBand state using 'ibstat'. Useful for understanding the network interconnections.
 Checking InfiniBand state with 'ibstat'...
CA 'mlx5_0'
        CA type: MT4123
        Number of ports: 1
        Firmware version: 20.39.2048
        Hardware version: 0
        Node GUID: 0x0800380001c2f7b8
        System image GUID: 0x0800380001c2f7b8
        Port 1:
                State: Active
                Physical state: LinkUp
                Rate: 100
                Base lid: 10209
                LMC: 0
                SM lid: 5
                Capability mask: 0xa651e848
                Port GUID: 0x0800380001c2f7b8
                Link layer: InfiniBand
CA 'mlx5_1'
        CA type: MT4123
        Number of ports: 1
        Firmware version: 20.39.2048
        Hardware version: 0
        Node GUID: 0x0800380001c3356a
        System image GUID: 0x0800380001c3356a
        Port 1:
                State: Active
                Physical state: LinkUp
                Rate: 100
                Base lid: 6302
                LMC: 0
                SM lid: 5
                Capability mask: 0xa651e848
                Port GUID: 0x0800380001c3356a
                Link layer: InfiniBand
CA 'mlx5_2'
        CA type: MT4123
        Number of ports: 1
        Firmware version: 20.39.2048
        Hardware version: 0
        Node GUID: 0x0800380001c33568
        System image GUID: 0x0800380001c33568
        Port 1:
                State: Active
                Physical state: LinkUp
                Rate: 100
                Base lid: 6107
                LMC: 0
                SM lid: 5
                Capability mask: 0xa651e848
                Port GUID: 0x0800380001c33568
                Link layer: InfiniBand
CA 'mlx5_3'
        CA type: MT4123
        Number of ports: 1
        Firmware version: 20.39.2048
        Hardware version: 0
        Node GUID: 0x0800380001c2f7ba
        System image GUID: 0x0800380001c2f7ba
        Port 1:
                State: Active
                Physical state: LinkUp
                Rate: 100
                Base lid: 10400
                LMC: 0
                SM lid: 5
                Capability mask: 0xa651e848
                Port GUID: 0x0800380001c2f7ba
                Link layer: InfiniBand
================================================

Communication tests completed!
```

Exercise 1a – DDP

1a. `bash slurm.sh -e 1 -- --slow-dataloading` vs `bash slurm.sh -e 1`

Description:
The "--slow-dataloading" example simulates a bad case of on-the-fly batch embedding process, without spawning data loading workers* nor using the "pinned memory"** for faster CPU-GPU copy.

Goal:
Recognize GPU idle times during data loading and compare with version that pre-computes batch embeddings, spawns parallel data loading workers and user "pinned memory" when copying CPU-GPU.

* "data loading workers": CPU threaded process to handle asynchronous batch preprocessing and GPU loading.
** "pin memory": Host RAM area which the OS prohibits from being swapped (reindexed or moved to disk), also "paged memory".

Exercise 1a – DDP [Optional]

Task:
Designate the part of code to profile and create our own profiling tagged sections.

Description:
When profiling a python code with nsys using the CUDA API, we need to insert some simple code lines designating the part of the code we want to profile, as well as, tag with custom names sub-section of interest.

Using the torch.cuda.nvtx library we can make that happen:

- `torch.cuda.cudart().cudaProfilerStart()` : Insert line where profiling starts collecting information
- `torch.cuda.cudart().cudaProfilerStop()` : Insert line where profiling stops
- `nvtx.range_push("Section name")` : the beginning of a custom tagged code section named "Section name"
- `nvtx.range_pop()` : the end of a custom tagged code section, must come after a `nvtx.range_push()` .

Tip – Can be avoided if `nvtx.range_push("Section name")` is used in a python "with" statement, e.g.

```
with nvtx.range_push("Section name"):
    <tagged section code> …
```

ToDo:
Insert the beginning and end of the code to be profiled and add your own custom NVTX tags inside the epoch training loop of file "exercises/exercise_1_DDP/train_todo.py", inside function `train_epoch()` .

!! Make sure to rename train.py->train_original.py and train_todo.py -> train.py to run your own code. !!

Exercise 1b – DDP

1b. `bash slurm.sh -e 1` vs `bash slurm.sh -e 1 -- --mixed-precision`

Description:
Running all matrix multiplications during training under FP32 precision provides us with great accuracy and stability. However, as models scale up in parameters, FP32 computations become almost impossible to carry out in efficient time, as well as store in GPU VRAM. Mixed precision*, solves this issue by downscaling the precision of crucial computations down to FP16/BF16, bringing computation time and memory requirements down to almost half.

Goal:
Locate the use of FP32 and BF16 precision matrix multiplication kernels (GEMMs).

* **Mixed Precision**: The training technique of keeping models weight and gradients in FP16/BF16 for speed and memory optimization and the optimizer states in FP32 for training stability.

Exercise 1c – DDP

1c. `bash slurm.sh -e 1 -- --mixed-precision --gradient-accumulation-steps 16`

Description:
Gradient accumulation is part of set of training techniques that allows us to aggregate the gradients of multiple forward-backward iterations, before upgrading the model's weights. Along those lines, it also contributes by decreasing training time, since we do not need to communicate gradients or compute new weights as frequently. Thus, each aggregated batch becomes a micro-batch to the bigger effective global batch size.

Goal:
Recognize the essential difference in communications and weights' update done.

Exercise 2a – DeepSpeed

2a. `bash slurm.sh -e 2 -- --mixed-precision --gradient-accumulation-steps 16`

vs

`bash slurm.sh -e 2 -- --mixed-precision --gradient-accumulation-steps 16 --ds-stage2`

Description:
The major difference between DeepSpeed ZeRO2 and ZeRO3 is the partitioning of model weights. In ZeRO2 each device retains its own whole copy of the model weight, in this case in BF16 precision, while in ZeRO3 these weights are also sharded between ranks. This sharding, introduces a communication overhead during forward/backward passes, compared to ZeRO2.

Goal:
Compare traces of these two case and estimate the overhead introduced when training in ZeRO3. Is the overhead worth the gains ?

Exercise 2b – DeepSpeed

2b. `bash slurm.sh -e 2 -n 2 -- --mixed-precision --gradient-accumulation-steps 16 --micro-batch-size 8 --ds-no-overlap`

vs `bash slurm.sh -e 2 -n 2 -- --mixed-precision --gradient-accumulation-steps 16 --micro-batch-size 8`

Description:
DeepSpeed ZeRO3 partitions all trainable parameters, model weights, gradients and optimizer states. However, that dictates the frequent communication between GPUs during forward and backward passes, especially when running in multi-node setups. In this example we will double the resources and the workload (2 nodes, 8 GPUs & 8*16*8=256 global batch size). However, the in one trace communication is not being overlapped with computation. In both case ds-hpz-partition is 4. So, we employ also DDP, because in 8 GPUs we can fit 2 model copies.

Goal:
Compare traces of between ZeRO3 fine-tuning that does not overlap any communication with computations to the case where non-blocking communications are overlapped with computation wherever possible.

Tips: Looking for differences in communication and computation times. Nsight Stats view and Paraver communications overlap configuration can be of help.

* **hpz-partition-size**: Hierarchical Partition Size is a DeepSpeed parameter that denotes the number of GPUs among which one model copy is sharded

Exercise 3 – MegatronLM

3a. `bash slurm.sh -e 3 -- --pp 1 --tp 4 --nsys2prv`
vs `bash slurm.sh -e 3 –n 2 -- --pp 2 --tp 4 --nsys2prv`

Description:
MegatronLM, as mentioned earlier, follows a per layer sharding strategy which optimizes the communication requirements between GPUs using Pipeline and Tensor Parallelism. When PP=1, we shard all model layers' tensors between the GPUs inside only 1 node. When using PP=2, the first half of the layers' are assigned to one node and the rest are assigned to a second node. Setting TP=4, means that tensors per PP stage are sharded between 4 GPUs inside one node.

However, PP>1 introduces an inherent dependency between the different pipeline stages, according to which later stages of the model need the output of previous stages to perform a forward pass and equivalently need the gradients of the next stages to perform the backward pass. This dependency causes GPUs idle times, which are referred to as the "Pipeline Bubble".

Goal:
Compare Paraver trace of PP=1 and PP=2 and recognize the phenomenon of "Pipeline Bubble".

Tip: Run a communication-computation overlap configuration and locate activity delays between different groups of GPUs

Thank you

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