Tools in action An example with Pytorch

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slides on LUMI in /project/project_465002175/Slides/AMD/

hands-on exercises: https://hackmd.io/@sfantao/lumi-training-tal-2025#Pytorch-example

hands-on source code: /project/project_465002175/Exercises/AMD/Pytorch

Agenda

- 1. Intro to Pytorch and its dependencies
- 2. Controlling affinity
- 3. Profiling rocprof and omnitools.

All suggestions presented here are transversal to any Al or HPC application!

Python applications can leverage the same tooling as non-python applications!

Scripting examples are suggestions and can always be adapted!



Pytorch highlight

- Official page: https://pytorch.org/
- Code: https://github.com/pytorch/pytorch
- Python[™]-based framework for machine learning
 - Auto-differentiation on tensor types
- GPU-enabled
 - ROCm support for MI250x (and others)
 - Hipification as part of the build system
 - C/C++ libraries with proper bindings for Python
 - Python code does <u>NOT</u> need changing using the same CUDA conventions
- Other related packages:
 - Torch vision/audio, triton, many others
- Many more build on it
 - vLLM, Deepspeed, Megatron-LM



Pytorch install – our base environment

module purge

module load CrayEnv

module load PrgEnv-cray/8.5.0

module load craype-accel-amd-gfx90a

module load cray-python



Setup the GPU environment and the Cray Python environment

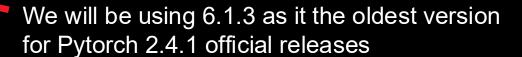


Recent Pytorch builds need recent user-level ROCm versions.

This path provides more recent ROCm modules.

module use /appl/local/containers/test-modules

module load rocm/6.1.3.lua



Pytorch install – running the examples

- For simplicity and improve the demonstration we leverage interactive runs on existing node allocation
- We run beforehand:

```
N=1; salloc -p standard-g \
--threads-per-core 1 \
--exclusive \
-N $N \
--gpus $((N*8)) \
-t 4:00:00 --mem 0
```



We are reserving **N nodes**, in this case only one node, using **one of the two available hardware threads**per core. We we'll be using the **8 GCDs** available in each node.

- This is a good way to experiment and converge to the correct job description.
- Don't forget to release your allocations once you are done!
- Once you consolidate your job description you can leverage batch jobs.
 - Salloc options translate directly to sbatch options.



Pytorch install – system python

Native install from Pytorch python wheels

Where do we want to install things - don't use your home folder!

Package install version can mix the Pytorch version as well as the ROCm it was build against.

This is where Pytorch project posts the wheel files - browse it to see what versions and ROCm combinations are available.

pip3 install -t \$PWD/pip-installs --pre torch==2.4.1+rocm6.1

--index-url https://download.pytorch.org/whl/

Collecting torch==2.4.1+rocm6.1

PYTHONPATH=\$PWD/pip-installs \

Make the frershly install Pytorch available to your Python runs

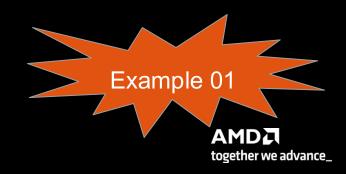
srun --jobid=\$jobid -n1 --gpus 8 \

python -c 'import torch; print("I have this many devices:", torch.cuda.device count())'

> I have this many devices: 8



Should yield the number of GCDs in the node.

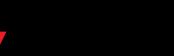


Pytorch install – virtual environments



Virtual environments are convenient to manage python package installation in ones user-space

Leverage the venv module to create the virtual environment



We are happy to leverage system's already installed packages

The folder where the virtual environment will be installed

python -m venv --system-site-packages cray-python-virtualenv

source cray-python-virtualenv/bin/activate



Activate the environment. It will be leveraged by the install and run.



Install and run as before. No need to specify install location – the environment is doing it for you.

pip3 install --pre torch==2.4.1+rocm6.1 --index-url https://download.pytorch.org/whl/ srun --jobid=\$jobid -n1 --gpus 8 \

python -c 'import torch; print("I have this many devices:", torch.cuda.device_count())'



Pytorch install – conda environment



- Conda environment adds the package-manager functionality to a virtual environment
- One can tune the Python version to use as we won't be leveraging the system one anymore.
 - No module load cray-python needed!

curl -LO https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
bash ./Miniconda3-* -b -p miniconda3 -s

Download and install a minimal conda (miniconda).

source \$PWD/miniconda3/bin/activate base conda create -y -n pytorch python=3.11

source \$PWD/miniconda3/bin/activate pytorch

Create and activate a conda environment to install Pytorch based on Python 3.11

Install and run as before - Conda package manager doesn't have ROCm enabled Pytorch installs

```
pip3 install --pre torch==2.4.1+rocm6.1 --index-url https://download.pytorch.org/whl/srun --jobid=$jobid -n1 --gpus 8 \
python -c 'import torch; print("I have this many devices:", torch.cuda.device_count())'
```



Pytorch install – conda environment install from source

- Installing Pytorch from source is not recommended on LUMI
 - Too old default ROCm to build against.
- It might be useful in some cases: builds with symbols for debugging.

We need a recent enough compiler – we'll use gcc

module load PrgEnv-gnu/8.5.0 gcc/10.3.0

Clone a given version of Pytorch and all its third_party components

git clone -b v2.4.1 --recursive \

https://github.com/pytorch/pytorch pytorch-source

Createand activate conda environment to manage the install conda create -y -n pytorch-from-source python=3.11

source \$wd/miniconda3/bin/activate pytorch-from-source

Install requirements for Pytorch and some build tools. pip install -r \$wd/pytorch-source/requirements.txt

conda install -y cmake ninja

Sometimes we need to solve some library clashes between conda and the system. We force the removal of the conda libstdc++ so that we use the system one.

rm -rf \$wd/miniconda3/envs/pytorch-from-source/lib/libstdc++.so



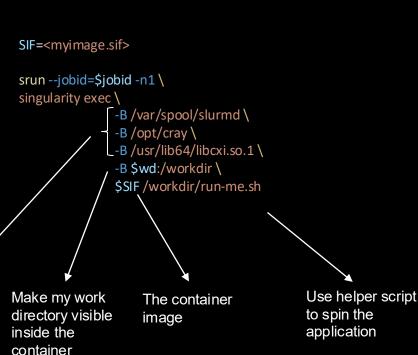


Pytorch install – Singularity containers

- Control better the Pytorch environment
- Less strain on the filesystem
 - All application installation is loaded as a single file
- Enable more recent ROCm versions
- Transferable and arguably more portable
- Some containers available under:
 - /appl/local/containers/sif-images/

Any cons?

- Updating the environment and installing more packages may require rebuild the container
- Containers can't currently be build on LUMI:
 - Needs containers to be built elsewhere and copied to the system
- Submitting jobs has to be done more carefully.





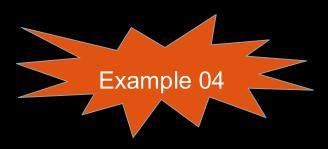
Make relevant pieces of

inside the container

native environment visible

Pytorch install – Singularity containers

SIF=/appl/local/containers/sif-images/lumi-pytorch-rocm-6.1.3-python-3.12-pytorch-v2.4.1.sif rm -rf \$wd/run-me.sh cat > \$wd/run-me.sh << EOF #!/bin/bash -e # Start conda environment inside the container \\$WITH_CONDA # Run application python -c 'import torch; print("I have this many devices:", torch.cuda.device count())' **EOF** chmod +x \$wd/run-me.sh srun --jobid=\$jobid -n1 --gpus 8 \ singularity exec \ -B /var/spool/slurmd \ -B /opt/cray \



The container image to use:

Pytorch 2.4.1 on top of ROCm 6.1.3

One could leverage a script to describe what is going to be executed inside the container.

This script has to load the container Conda environment. A special variable is set in the container to facilitate that.

Run as before.

Invoke singularity to start the container and execute the script created above.

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-B /usr/lib64/libcxi.so.1 \

\$SIF /workdir/run-me.sh

-B \$wd:/workdir \

Controlling device visibility

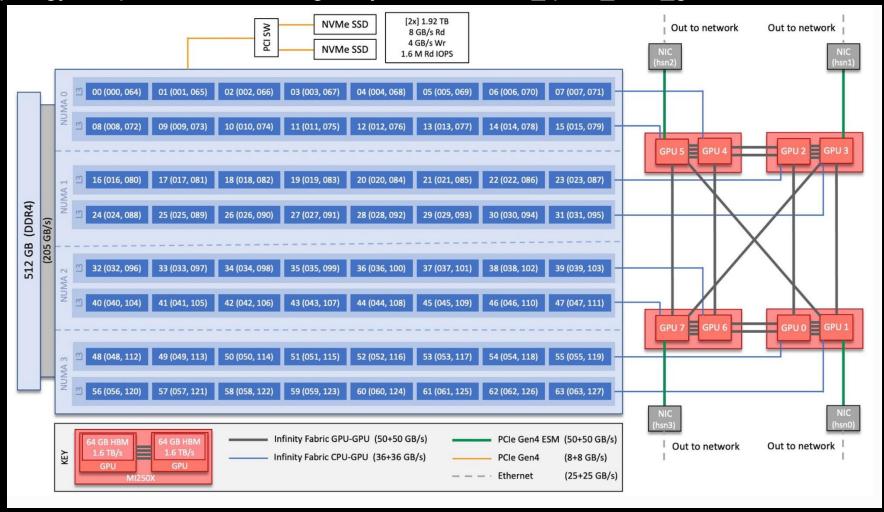
- Controlling visibility
 - HIP_VISIBLE_DEVICES=0,1,2,3 python -c 'import torch; print(torch.cuda.device_count())'
 - ROCR_VISIBLE_DEVICES=0,1,2,3 python -c 'import torch; print(torch.cuda.device_count())'
 - SLURM sets ROCR_VISIBLE_DEVICES
 - Implications of both ways of setting visibility blit kernels and/or DMA
 - Considerations:
 - Does my app expects GPU visibility to be set in the environment?
 - Does my app expects arguments to define target GPUs
 - Does my app make any assumption on the device based on other information:
 - MPI rank
 - CPU-range
 - Auto-determined
 - How many processes using the same GPU:
 - Contention vs occupancy
 - Runtime scheduling limits
 - Increased scheduling complexity
 - Imbalance

Most Pytorch applications and driver scripts assume the GPU to be used corresponds to the local rank!!!



What CPUs I have available and their NUMA domain? GPU[0] Iscpu : (Topology) Numa Node: 3 : (Topology) Numa Affinity: 3 GPU[0] : (Topology) Numa Node: 3 GPU[1] What GPUs I have **GPU[1]** : (Topology) Numa Affinity: 3 rocm-smi –showtopo **GPU[2]** : (Topology) Numa Node: 1 **GPU[2]** : (Topology) Numa Affinity: 1 GPU[3] : (Topology) Numa Node: 1 GPU[3] : (Topology) Numa Affinity: 1 NUMA node0 CPU(s): 0-15,64-79 GPU[4] : (Topology) Numa Node: 0 **NUMA node1 CPU(s):** 16-31,80-95 GPU[4] : (Topology) Numa Affinity: 0 **NUMA** node2 CPU(s): 32-47,96-111 : (Topology) Numa Node: 0 **GPU[5] NUMA** node3 CPU(s): 48-63,112-127 GPU[5] : (Topology) Numa Affinity: 0 **GPU[6]** : (Topology) Numa Node: 2 : (Topology) Numa Affinity: 2 **GPU[6]** : (Topology) Numa Node: 2 **GPU[7]** : (Topology) Numa Affinity: 2 **GPU[7]**

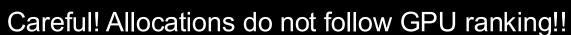
ORNL topology - https://docs.olcf.ornl.gov/systems/crusher_quick_start_guide.html



Check what SLURM is giving us:

```
srun -c 7 -N 2 -n 16 --gpus 16 \
bash -c 'echo "$SLURM_PROCID -- GPUS $ROCR_VISIBLE_DEVICES -- $(taskset -p $$)"' \
| sort -n -k1
```

```
0 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54249's current affinity mask: fe
1 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54250's current affinity mask: fe00
2 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54251's current affinity mask: fe0000
3 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54252's current affinity mask: fe000000
4 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54253's current affinity mask: fe00000000
5 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54254's current affinity mask: fe0000000000
6 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54255's current affinity mask: fe00000000000
7 -- GPUS 0,1,2,3,4,5,6,7 -- pid 54256's current affinity mask: fe00000000000000
8 -- GPUS 0,1,2,3,4,5,6,7 -- pid 110083's current affinity mask: fe
9 -- GPUS 0,1,2,3,4,5,6,7 -- pid 110084's current affinity mask: fe00
10 -- GPUS 0,1,2,3,4,5,6,7 -- pid 110085's current affinity mask: fe0000
11 -- GPUS 0,1,2,3,4,5,6,7 -- pid 110086's current affinity mask: fe000000
12 -- GPUS 0,1,2,3,4,5,6,7 -- pid 110087's current affinity mask: fe00000000
14 -- GPUS 0,1,2,3,4,5,6,7 -- pid 110089's current affinity mask: fe00000000000
15 -- GPUS 0,1,2,3,4,5,6,7 -- pid 110090's current affinity mask: fe00000000000000
```







Check what SLURM is giving us:

sort -n -k1

```
0 -- GPUS 0,1,2,3,4,5,6,7 -- pid 13819's current affinity mask: fe00000000000
2 -- GPUS 0,1,2,3,4,5,6,7 -- pid 13821's current affinity mask: fe0000
3 -- GPUS 0,1,2,3,4,5,6,7 -- pid 13822's current affinity mask: fe000000
4 -- GPUS 0,1,2,3,4,5,6,7 -- pid 13823's current affinity mask: fe
5 -- GPUS 0,1,2,3,4,5,6,7 -- pid 13824's current affinity mask: fe00
6 -- GPUS 0,1,2,3,4,5,6,7 -- pid 13825's current affinity mask: fe00000000
7 -- GPUS 0,1,2,3,4,5,6,7 -- pid 13826's current affinity mask: fe0000000000
8 -- GPUS 0,1,2,3,4,5,6,7 -- pid 94670's current affinity mask: fe00000000000
9 -- GPUS 0,1,2,3,4,5,6,7 -- pid 94671's current affinity mask: fe0000000000000
10 -- GPUS 0,1,2,3,4,5,6,7 -- pid 94672's current affinity mask: fe0000
11 -- GPUS 0,1,2,3,4,5,6,7 -- pid 94673's current affinity mask: fe000000
12 -- GPUS 0,1,2,3,4,5,6,7 -- pid 94674's current affinity mask: fe
13 -- GPUS 0, 1, 2, 3, 4, 5, 6, 7 -- pid 94675's current affinity mask: fe00
14 -- GPUS 0,1,2,3,4,5,6,7 -- pid 94676's current affinity mask: fe00000000
15 -- GPUS 0,1,2,3,4,5,6,7 -- pid 94677's current affinity mask: fe0000000000
```

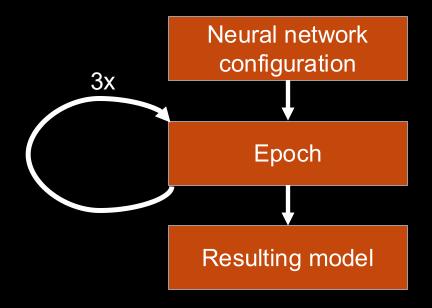


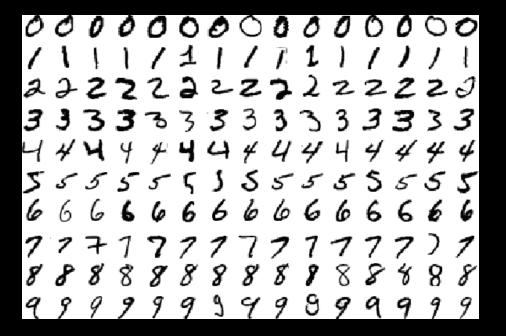
Great! CPUs are properly bound to the GPUs!



Pytorch example app – MNIST distributed learning

- Popular computer vision training dataset
- Al training iterate over epochs and a given sample batch is considered in each epoch
- Provided example runs over 3 epochs (properly trained models need much more than than!)
- MNIST training considers number images with different formats.





Pytorch example app – MNIST distributed learning

- What provides distributed capability:
 - Pytorch Distribute Data Parallel (DDP) Batches of different data run concurrently
 - Other more sophisticated methods available
 - Frameworks like Deepspeed and Horovod can also enable distributed training.

import torch.distributed as dist

dist.init process group(backend='nccl', init method='env://', world size=int(os.environ['WORLD SIZE']), rank=int(os.environ['RANK']))

Let's use RCCL collectives library.

LUMI Advanced Training

Well be learning about the distributed setting from the environment

> Capture some env vars to adjust my distributed training

- ... Epoch 0 Loss 0.148397 Global batch size 2048 on 16 ranks
- ... Epoch 1 Loss 0.147906 Global batch size 2048 on 16 ranks
- Epoch 2 Loss 0.147717 Global batch size 2048 on 16 ranks

Pytorch example app – MNIST distributed learning – RCCL

- RCCL should be set to use only high-speed-interfaces Slingshot
- The problem one might see on startup:

```
NCCL error in: /workdir/pytorch-
example/pytorch/torch/csrc/distributed/c10d/ProcessGroupNCCL.cpp:1269, unhandled
system error, NCCL version 2.12.12
```

Check error origin by setting RCCL specific debug environment variables:

```
Node has interfaces other than Slingshot export NCCL_DEBUG=INFO

These are the correct ones.

NCCL INFO NET/Socket: Using [0]nmn0:10.120.116.65<0> [1]hsn0:10.253.6.67<0> [2]hsn1:10.253.6.68<0> [3]hsn2:10.253.2.12<0> [4]hsn3:10.253.2.11<0>

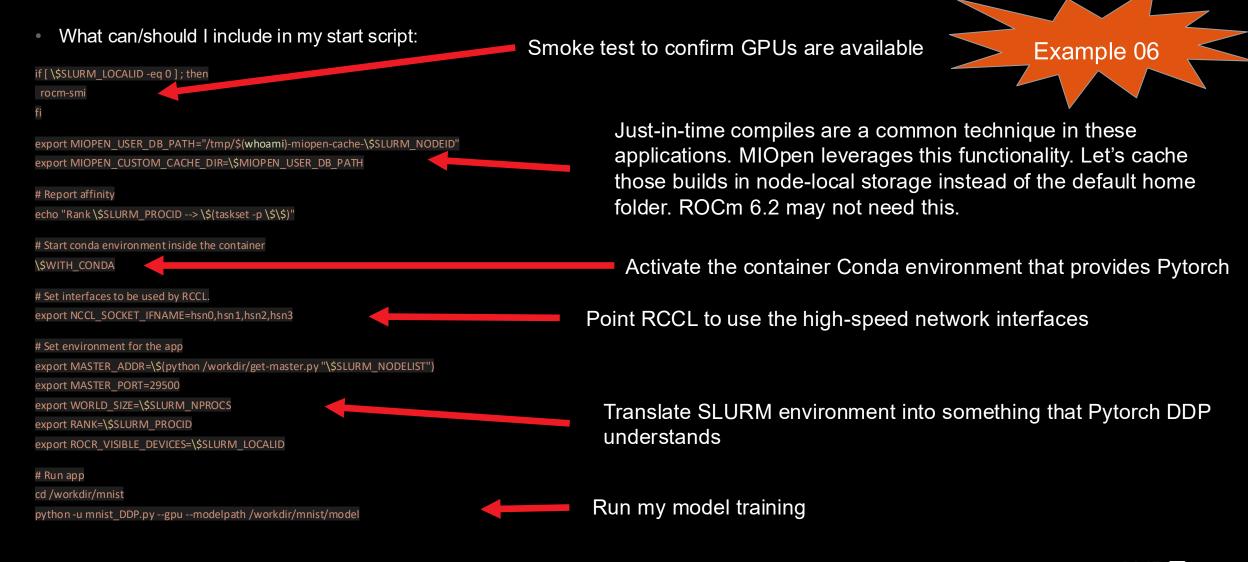
NCCL INFO /long_pathname_so_that_rpms_can_package_the_debug_info/data/driver/rccl/src/init.cc:1292
```

• The fix: export NCCL_SOCKET_IFNAME=hsn0,hsn1,hsn2,hsn3

Point RCCL to use all 4 high-speed interfaces. It will know how to bind them based on the node topology.



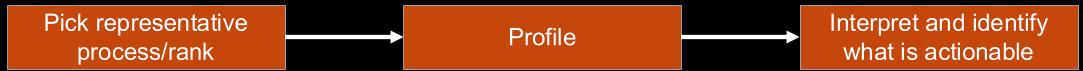
Pytorch example app – MNIST distributed learning - script





Pytorch example app — MNIST distributed learning - rocprof

- Rocprof profiler client is the easiest way to get started with GPU profiling.
- It is available as part of the ROCm stack and, therefore, available in the containers
- It is seldomly useful to profile every single process/rank of your app:
 - Profilling more than needed = more potential profiling overhead
 - Misleading conclusions



pcmd="
if [\$RANK -eq 2]; then
 pcmd='rocprof --hip-trace'
fi

Command to prepend to my application instantiation

We want to profile only for one rank – in this case rank #2

Run command as before except to the prepended profiling command

\$pcmd python -u mnist_DDP.py --gpu --modelpath /workdir/mnist/model

More than one rank to be profiled? Use, -o myresults.\$RANK.csv, to make sure sure there are no races generating the profile files

Pytorch example app – MNIST distributed learning - rocprof

Bound by RCCL communication! 274458.5 s + 30.16 s 30.20 s 30.22 s 30.24 s 30.26 s 30.28 s 30.32 s 30.34 s 30.36 s 30.40 s 30.30 s 30.38 s Thread 50305 ▲ GPU6 12 Thread 1 ncclKerne... ernel_SendRecv_RING_SIMP... Thread 2 ncclKernel_SendRecv_RING_SIMPLE_Su Thread 66 ◆ COPY 1 Flow Events **Current Selection** Slice Details ncclKernel_SendRecv_RING_SIMPLE_Sum_int8_t(ncclDevComm*, unsigned long, Preceding flows Name ncclWork*) Slice hipExtLaunchKernel Category Delay Start time 30s 277ms 317us Thread NULL (CPU HIP API 2) Duration 52ms 383us Arguments Thread duration 0s (0.00%) Thread BeginNs -274488790966731 **Process** GPU6 12 Data 🕶 NULL Slice ID 53978 DurationNs -52383950 EndNs ncclKernel_SendRecv_RING_SIMPLE_Sum_int8_t(ncclDevComm*, unsigned long

Example 07

Collectives kernels dominate profile

Comms are important! - RCCL AWS-CXI plugin

- LUMI, Frontier (and others) directly attaches AMD Instinct™ MI250x Accelerator to the Slingshot Network
 - Enable collectives computation on devices
 - Minimize the role of the CPU in the control path expose more asynchronous computation opportunities
 - Lowest latency for network message passing is from GPU HBM memory

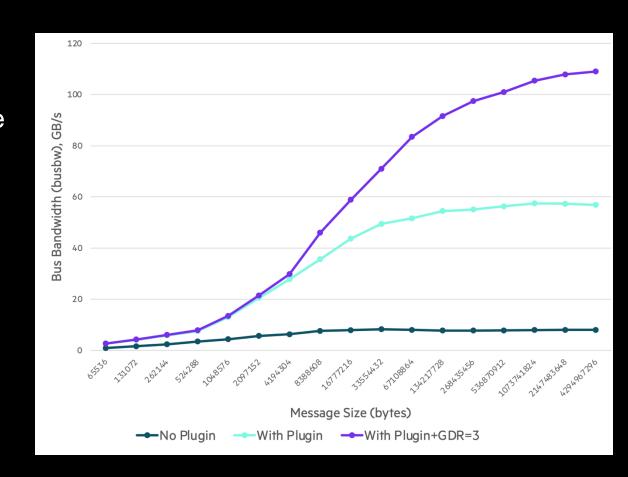


- CXI plugin is a runtime dependency. Requires: HPE Cray libfabric implementation
 - https://github.com/rocm/aws-ofi-rccl
 - 3-4x faster collectives
- Included in the LUMI provided containers! If not using the LUMI containers make sure you have that in your environment:

```
export NCCL_DEBUG=INFO
export NCCL_DEBUG_SUBSYS=INIT
# and search the logs for:
[0] NCCL INFO NET/OFI Using aws-ofi-rccl 1.4.0
```

Configuring RCCL environment (cont.)

- RCCL should be set configured to use GPU RDMA:
 - export NCCL_NET_GDR_LEVEL=PHB
- On upcoming ROCm versions (6.2) this won't be needed – it is default.
- Why should I spend time with all this?
 - 3-4x better bandwidth utilization with plugin
 - 2x better bandwidth utilization with RDMA
 - Can scale further!
- Careful using external containers! You may need to be setting plugin yourself!



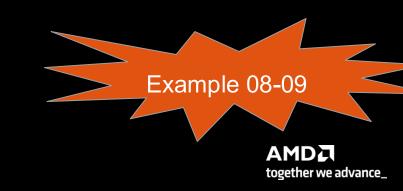


- Obtain more thorough trace information and visualization
 - https://github.com/AMDResearch/omnitrace
- Omnitrace install outside the container can be used
 - The host/container ROCm levels should match.

module use module use /appl/local/containers/test-modules module load rocm/6.1.3.lua omnitrace/1.12.0-rocm6.1.x

SIF=/appl/local/containers/sif-images/lumi-pytorch-rocm-6.1.3-python-3.12-pytorch-v2.4.1.sif

- Configuration file:
 - omnitrace-avail -G omnitrace.cfg –all
 - export OMNITRACE_CONFIG_FILE=/workdir/omnitrace-config.cfg
 - Override environment with command line arguments if needed



- Sample learn about the native stack trace along side GPU activity
- GPU activity is <u>never</u> sampled even in sampling mode
- Adjust configuration file according to the needs:

OMNITRACE_USE_SAMPLING = true

OMNITRACE_USE_ROCM_SMI = false

OMNITRACE_SAMPLING_CPUS = none

OMNITRACE_SAMPLING_GPUS = 2

Let's do sampling!

Not interested in sampling GPU hardware metrics (frequency, temperature...)

Not interested in sampling CPU hardware metrics

Targeting GPU #2 only used by Rank #2

Execution similar to rocprof:

Oct. 24th 2025

```
pcmd="

if [ $RANK -eq 2 ] ; then

pcmd='omnitrace-sample -- '

fi
$pcmd python -u mnist_DDP.py --gpu --modelpath /workdir/mnist/model
```

Prepend omnitrace sampling driver for rank #2

We need to add a few more bindings to singularity:

srun --jobid=\$jobid -N \$((Nodes)) -n \$((Nodes*8)) --gpus \$((Nodes*8)) --cpu-bind=mask_cpu:\$MYMASKS \

```
singularity exec \
...\
-B $wd:/workdir \
-B $OMNITRACE_dir/omnitools \
-B /usr/lib64/libpciaccess.so.0 \
$SIF /workdir/run-me.sh
```

Make omnitrace available in the container

Omnitrace does PCIe info loading – so we need to enable that

...and make sure the environment inside the container is set accordingly:

export PATH=\$OMNITRACE_dir/bin:\$PATH
export LD_LIBRARY_PATH=\$OMNITRACE_dir/lib:\$LD_LIBRARY_PATH
export PYTHONPATH=\$OMNITRACE_dir/lib/python/site-packages:\$LD_LIBRARY_PATH

Makes sure all Omnitrace bits are available in my environment.



Example 08

Native stack flame graph:



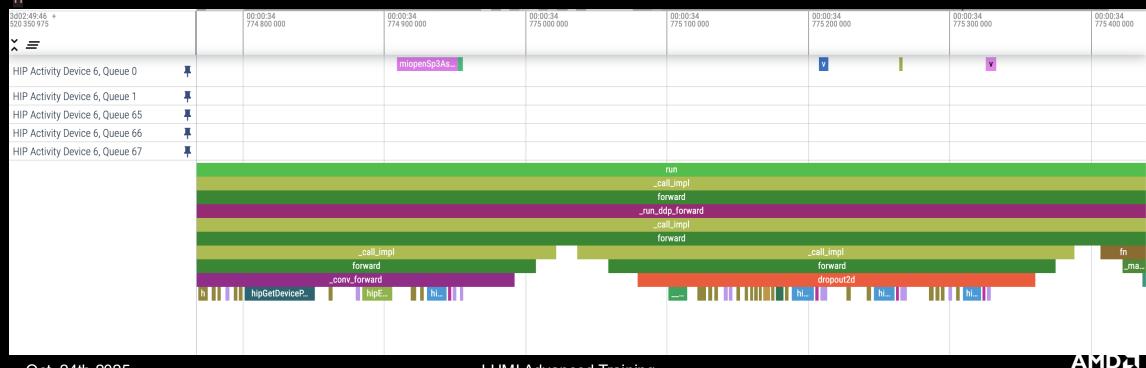


Sampling the Python and C/C++ parts of the code – omnitrace-python if [\\$RANK -eq 2]; then

omnitrace-python-3.10 -- mnist_DDP.py --gpu --modelpath /workdir/mnist/model

Omnitrace expects the Python script as opposed to the Python executable Match relevant python version

python -u mnist_DDP.py --gpu --modelpath /workdir/mnist/model



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Example 9

- Obtain detailed kernel performance counters
 - https://github.com/AMDResearch/omniperf

module use module use /appl/local/containers/test-modules module load rocm/6.1.3.lua omniperf/2.1.0

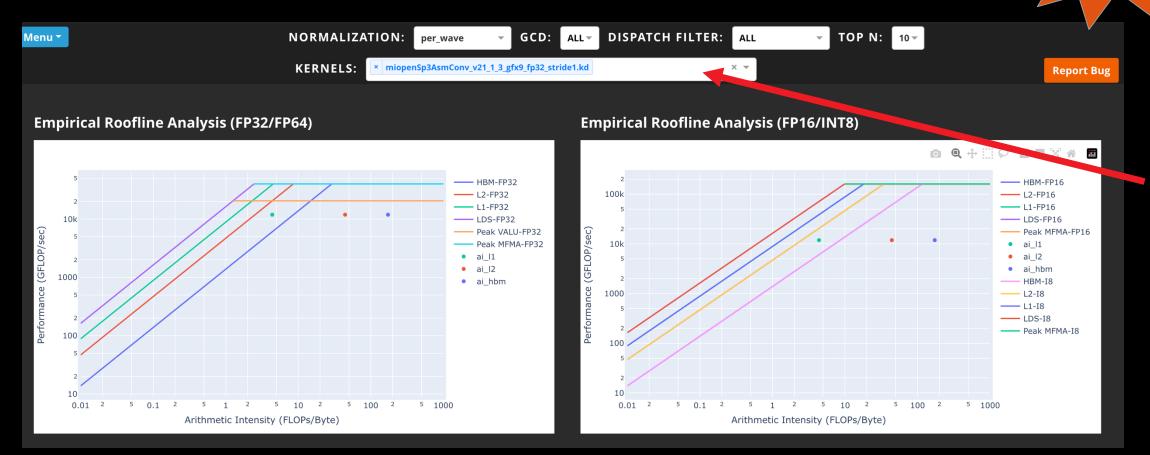


- Virtual environment is used to extend the existing Python environment inside the container.
- Omniperf needs replaying the application many times
 - Could be challenging to profile individual ranks as all need replaying.

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- Analyze in or outside the container):
 - omniperf analyze -p workloads/pytorch/MI200/ --gui

Example 10



Select kernel of interest

HBM-FP32

L2-FP32

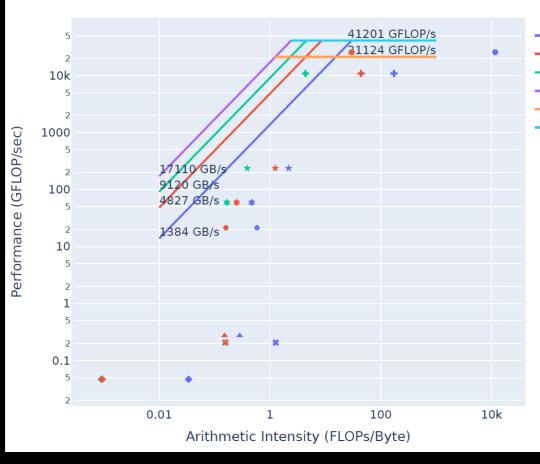
L1-FP32

ai l1 ai l2

ai hbm

LDS-FP32 Peak VALU-FP32 Peak MFMA-FP32

- Analyze in or outside the container):
 - **Roofline PDFs**



Example 10

Kernel Names and Markers



Kernel

names

Leveraging framework profiler infrastructure

Example 11

- Al frameworks typically provide hooks for developers to gather profiling information
- An example with Pytorch:

Invoke the profiler from torch.profiler import profile, record function, ProfilerActivity for epoch in range(args.epochs): Enable profiling for epoch number 3 prof = None if epoch == 3: print("Starting profile...") prof = profile(activities=[ProfilerActivity.CPU, ProfilerActivity.CUDA]) prof.start() for imgs, labels in dataloader: Training for an epoch with torch.amp.autocast('cuda',enabled=args.amp): imgs, labels = imgs.cuda(), labels.cuda() outputs = model(imgs) loss = criterion(outputs, labels) loss = scaler.scale(loss) Finish profiling and generate trace loss.backward() scaler.step(optimizer) scaler.update() Trace file can be viewed in Perfetto UI tool if prof: prof.stop() prof.export_chrome_trace("trace.json")
Oct. 24th 2025 **LUMI Advanced Training**

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