2022 APAC HPC-AI Communications Performance with UCX: Dataframe Merging

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In this task, we are to run a dataframe merging benchmark on Gadi nodes, which communicates with each other via UCX (Unified Communication X).

1 Introduction

The benchmark is run on 16 GPUs, on each of which is a worker there with left and right dataframe distributed throughout all GPUs. It is our task that each worker merges its left and right dataframe, which means that a worker need communicate with others at scale.

There are two major metrics — bandwidth as well as throughput — to measure the performance of the benchmark we run. We tried to discover the instinct meaning of the two by means of investigating and interpreting the codes provided.

1.1 Bandwidth

For a particular worker, its bandwidth is defined to the average of the amount of data it communicated with all other workers of left and the right dataframe, divided by wall time. Without lost of generality, let's consider the worker with rank 0, then its bandwidth could be expressed as:

Bandwidth =
$$\frac{bw_{left} + bw_{right}}{2}$$

, where the bandwidth of left or right data
frame is bw =
$$\frac{\displaystyle\sum_{i=1}^{15} size\ of\ \text{Dataframe transferred}_i}{\displaystyle\sum_{i=1}^{15} \text{Wall time}_i}.$$

1.2 Throughput

The throughput of an iteration is defined as:

$$\label{eq:Throughput} \text{Throughput} = \frac{\text{\# chunks} \times \text{Data processed}}{\text{Wall time}}$$

, where "Data processed" indicates the total amount of data being transferred and processed by all workers during each iteration.

We believe that there should be some relation between the two metrics yet that throughput is more comprehensive, so we put more emphasis on it.

2 Optimized Configurations

We tried various sorts of UCX options. Most of them were exported as environment variables in the cluster.cfg.

2.1 Enable Hardware Tag Matching

In Tag Matching, the software holds a list of matching entries called matching list. Each matching entry contains a tag and a pointer to an application buffer. The matching list is used to steer arriving messages to a specific buffer according to the message tag. The action of traversing the matching list and finding the matching entry is called Tag Matching.

Sending messages with numeric tags accelerates the processing of incoming messages, leading to better CPU utilization and lower latency for expected messages. Currently, *Hardware Tag Matching* is supported for the accelerated RC (*Reliable Connected*) and DC (*Dynamic Connected*) transports, and we found that it can be enabled by setting the following environment parameters:

- UCX_RC_MLX5_TM_ENABLE=y
- UCX_DC_MLX5_TM_ENABLE=y

By setting these two environment parameters, the bandwidth improved to 521.87 MiB/s (102.9% speedup), and the throughput improved from 4.27 GiB/s to 4.36 GiB/s (102.1% speedup).

2.2 Use mutex for Multithreading Support

The environment variable UCX_USE_MT_MUTEX is set to n by default, which means not using mutex for multithreading support and using spinlock instead.

Both **spinlock** and **mutex** are common synchronization mechanism. The difference between them is: the mechanism that **mutex** uses is sleep-waiting, while the mechanism that **spinlock** uses is busy-waiting. That is, when a thread tries to lock a **mutex** and it does not succeed, it will go to sleep, immediately allowing another thread to run. As for **spinlock**, as long as the **spinlock** polling is blocking the only available CPU core, no other thread can run and the lock won't be unlocked either.

There are some pros and cons for both of them, listed below:

Since we have no idea which one is more efficient for the task, we've tried both of them and gained the following results:

Throughput with spinlock $4.27~\mathrm{GiB/s}$

Throughput with mutex 4.71 GiB/s

We've found out that we should choose **mutex** instead of **spinlock**, i.e., having UCX_USE_MT_MUTEX set to y, to get better performance, the bandwidth increased

Pros & Cons for mutex & spinlock

	Pros	Cons
mutex	Having better adaptability.	Costs more resources since require switches.
spinlock	Costs less resources, compared to mutex .	Spend more user time since threads waiting at its core.

to 509.99 MiB/s (100.5% speedup), and the throughput increased from 4.27 GiB/s to 4.71 GiB/s (110.3% speedup).

2.3 Enable *Non-blocking* Mode

The option UCXPY_NON_BLOCKING_MODE determines whether to use non-blocking progress mode to receive and send data. We discovered that the performance improves if we enable non-blocking mode, i.e, setting UCXPY_NON_BLOCKING_MODE to 1: the bandwidth increased to 590.62 MiB/s (116.4% speedup), and the throughput increased from 4.27 GiB/s to 4.96 GiB/s (116.1% speedup).

2.4 Switch Rendezvous protocol to Active Messages scheme

There is a environment parameters that manipulate communication scheme in *Rendezvous* protocol. Although there are only 3 options: get_zcopy, put_zcopy, auto, documented in detail, we found that there are several other schemes such as get_ppln, put_ppln (these two might refer to pipe-lined get / put), am, rkey_ptr; among all these schemes am, which stands for *Active Messages*, worked better than any other scheme above.

After setting UCX_RNDV_SCHEME=am, the bandwidth increased to 546.51 MiB/s (107.7% speedup), and the throughput increased from 4.27 GiB/s to 5.54 GiB/s (129.7% speedup), which is a significant improvement.

2.5 Other parameters & options

2.5.1 Adjust the initial pool size for memories

In the dask training, the lecturer mentioned that we can adjust the <code>--rmm_pool_size</code> parameter to determine the size of memory to allocate at the beginning while initializing a cluster. RMM is memory manager from RAPIDS. Since memory allocation is an expensive operation, allocating a big chunk of memory improves performance.

Similarly, we found the parameter --rmm-init-pool-size in file run-cluster.sh, and we thought about that setting the initial memory size which exactly same as usage may reduce waste of memory and maybe improve the performance.

Without any optimal configuration, the performance do increase if we make the initial pool size smaller. The default --rmm-init-pool-size is set to 3×10^{10} . If we set to 2.5×10^{10} , the throughput increased from 4.27 GiB/s to 4.74 GiB/s; if setting to 2×10^{10} , the throughput increased from 4.27 GiB/s to 4.35 GiB/s (101.9% speedup).

However, with the optimal configurations, setting --rmm-init-pool-size smaller doesn't guaranteed that the performance would be better. The best throughput we could achieve with --rmm-init-pool-size set to 3×10^{10} is 8.98 GiB/s. If we set it to 2.5×10^{10} and 2×10^{10} , then the throughput would come to 8.25 GiB/s and 8.27 GiB/s, respectively, which is a bit worse than the best performance.

2.5.2 Enable various optimizations for homogeneous environment

Setting UCX_UNIFIED_MODE to y enables various optimizations intended for homogeneous environment. According to the document, enabling this mode implies that the local transport resources/devices of all entities which connect to each other are the same. The throughput comes from 4.27 GiB/s to 4.39 GiB/s (102.8% speedup) if we enable this mode. Although it brought improvement to the performance, this option would conflict to UCX_RNDV_SCHEME=am. Since the latter option could bring better performance to the task, we decided not to enable this mode.

2.5.3 Modify the memory pool buffer grow rate

There are two options that determine how much buffers are added every time the memory pool grows. UCX_TCP_RX_BUFS_GROW, UCX_TCP_TX_BUFS_GROW determines for the receive/send memory pool respectively. We wonder that whether modifying the buffer grow rate could bring better performance for us. Therefore, we've tried to increase the buffer grow rate. The default value of UCX_TCP_RX_BUFS_GROW and UCX_TCP_TX_BUFS_GROW are both 8. If we set both of them to 16, the throughput increases from 4.27 GiB/s to 4.68 GiB/s (109.6% speedup). Nevertheless, if we combine these two options with other optimal configurations, it seems that changing these two options does not guaranteed the result be optimized.

2.5.4 Use GPU Direct RDMA for HCA to access GPU pages

This option, UCX_IB_GPU_DIRECT_RDMA is default to try. It made no noticeable difference in comparison to the baseline. So we guessed that it might be enabled in baseline.

2.5.5 Reduce the threshold to switch to *Rendezvous* protocol

It is auto of the option UCX_RNDV_THRESH in UCX default and 8192 in UXC-Py default. We used to reduce its value for the purpose of utilizing the *Rendezvous* protocol more. Nonetheless, the result was not apparent.

2.5.6 Enlarge copy-out buffer for TCP sending and receiving

The pair of options, UCX_TCP_TX_SEG_SIZE along with UCX_TCP_RX_SEG_SIZE, which determines the size of send/receive copy-out buffer respectively, are said to have some impact when the amount of communication is quite large at scale. We tried to enlarge their values, yet the outcome was still not sufficient enough to distinguish from baseline.

3 Conclusion

3.1 All optimal config

Combining the above options altogether, we have:

Table 1: Optimized combination of UCX configurations

- UCX_RC_TM_ENABLE=y
- UCX_DC_TM_ENABLE=y
- UCX_USE_MT_MUTEX=y
- UCXPY_NON_BLOCKING_MODE=1
- UCX_RNDV_SCHEME=am
- UCX_IB_GPU_DIRECT_RDMA=y
- UCX_RNDV_THRESH=1024
- UCX_TCP_TX_SEG_SIZE=64k
- UCX_TCP_RX_SEG_SIZE=512k

These configurations have been appended to the original cluster.cfg. In addition, we also submit a file optimized.cfg exporting all of them only so that one could easily source it.

3.2 Result

As the problem description mentioned, our objective is to achieve best bandwidth and throughput performance. We need to run 100 iterations, running on 16 GPUs of 4 nodes, and each 10^6 and 2.5×10^7 rows per chunk, for small data set and large data set, respectively. By modifying the parameters above, we achieve the following results:

Table 2: Average bandwidth of 100 times (With Ordinary Volta GPUs)

${\bf Chunk\ size}$	Default	Optimized Configurations
10^{6}	$507.21~\mathrm{GiB/s}$	$1.06~\mathrm{GiB/s}$
2.5×10^7	405.89 MiB/s	$1.15~\mathrm{GiB/s}$

Table 3: Average throughput of 100 times (With Ordinary Volta GPUs)

Chunk size	Default	Optimized Configurations
10^{6}	$3.95~\mathrm{GiB/s}$	$9.28~\mathrm{GiB/s}$
2.5×10^7	$4.40~\mathrm{GiB/s}$	$12.37~\mathrm{GiB/s}$

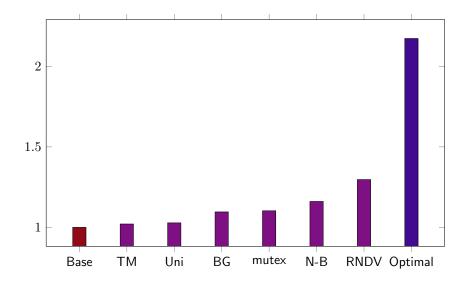


Figure 1: Bar graph of throughput speedup

Figure 1 illustrate the bar graph of throughput speedup of different options. Base, TM, Uni, Uni, BG, mutex, N-B, RNDV and Optimal represent baseline, *Hardware Tag Matching*, unified mode, buffer grow rates, non-blocking mode, *Rendezvous* scheme and the optimal combination respectively.

The output files created by benchmark are also submitted.

4 Result running on DGX-A100 nodes

We are told that there're two DGX-A100 servers in NCI Gadi, where we may run dataframe merging better, and we may earn some bonus points with the result of running on DGX-A100 nodes. We are curious about the performance with DGX-A100 nodes, thus we also experimented with the DGX servers, the results are listed below:

It's worth noting that although we mentioned that setting UCX_RNDV_SCHEME to am could optimize the performance, this option somehow doesn't work well with DGX A100 servers. Switching this parameter to *Active Messages* makes the performance worse in this case, making the throughput drop drastically from 88.29 GiB/s to 34.89 GiB/s. On the contrary, switch back to default scheme

Table 4: Average bandwidth of 100 times (With DGX-A100s)

Chunk size	Default	Optimized Configurations
10^{6}	$2.41~\mathrm{GiB/s}$	$2.37~\mathrm{GiB/s}$
2.5×10^7	$10.04~\mathrm{GiB/s}$	$3.36 \; \mathrm{GiB/s^1}$ $10.19 \; \mathrm{GiB/s^2}$

Table 5: Average throughput of 100 times (With DGX-A100s)

${\bf Chunk\ size}$	Default	Optimized Configurations
10^{6}	$16.66~\mathrm{GiB/s}$	$16.69~\mathrm{GiB/s}$
2.5×10^7	88.29 GiB/s	$34.89 \; \mathrm{GiB/s^3}$ $89.00 \; \mathrm{GiB/s^4}$

makes the performance a bit better, which makes the throughput increases to $89.00~\mathrm{GiB/s}.$