High Performance Computing Proseminar 2024
Assignment 1

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Exercise 1

This exercise consists in familiarizing yourself with SLURM job submission. You received user credentials for the LCC3 cluster. If you did not change the default password, do so immediately. You are responsible for this account during this semester. You can find information about LCC3 at `https://www.uibk.ac.at/zid/systeme/hpc-systeme/leo3/` and information about SLURM job submission at `https://www.uibk.ac.at/zid/systeme/hpc-systeme/common/tutorials/slurm-tutorial.html`. Please run any benchmarks or heavy CPU loads only on the compute nodes, not on the login node. If you want to do some interactive experimentation, use an interactive job as outlined in the tutorial. Make sure to stop any interactive jobs once you are done.

Tasks

- Study how to submit jobs in SLURM, how to check their state and how to cancel them.
- Prepare a submission script that starts an arbitrary executable, e.g. /bin/hostname
- In your opinion, what are the 5 most important parameters available when submitting a job and why? What are possible settings of these parameters, and what effect do they have?
- How do you run your program in parallel? What environment setup is required?

1. Submiting jobs in SLURM consits of first writing a job file where the configuration is written in SLURM specific format. Afterwards we can submit the job using `sbatch filename.sh`. To check their state we can either use `squ` or `squeue` where the latter shows all jobs from all users. `scancel job-id` terminates the job with the according job-id.

2. The following script measures the time required to execute `/bin/hostname`.

```
#!/bin/bash

# Execute job in the partition "lva" unless you have special requirements.
#SBATCH --partition=lva
# Name your job to be able to identify it later
#SBATCH --job-name ps1
# Redirect output stream to this file (if the output is assumed to be larger put it in
    scratch)
#SBATCH --output=output.log
# Maximum number of tasks (=processes) to start in total
#SBATCH --ntasks=1
# Maximum number of tasks (=processes) to start per node
#SBATCH --ntasks-per-node=1
# Enforce exclusive node allocation, do not share with other jobs
#SBATCH --exclusive
/usr/bin/time -v /bin/hostname
```

3. The 5 most important parameters are (IMO)

I `#SBATCH --time=...` which sets the time limit to the given argument (in this format: [[D-]HH:]MM[:SS]). For our purposes it is less important, but generally speaking it makes much sense to limit the duration. An example would be `#SBATCH --time=1:30:00` which configures the job to run for 1.5 hours. If a job takes longer it'll be terminated.

II `#SBATCH --exclusive` is mandatory if we want to make any meaningful (performance) measurement as it reserves the entire machine for this job. If other jobs would run here they could interfere with the cache or main memory access latencies.

III `#SBATCH --output=outputfile.txt` (as well as error) pipes the output stream (or error stream) into an according file. This is useful for debugging textual outputs of our program we submitted.

IV `#SBATCH --mail-user=Karl.Mustermann@xxx.com` in combination with `#SBATCH --mail-type=END,FAIL` is not mandatory but quite nice if we have a long running job and want to be notified whenever the job either terminates or fails. `mail-type` supports the following types: BEGIN, END, FAIL, REQUEUE, STAGE_OUT, TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80, TIME_LIMIT_50, ARRAY_TASKS. (Stage out https://slurm.schedmd.com/burst_buffer.html)

V `#SBATCH --job-name=name` may seem silly to put into this list but it is quite helpful to distinguish from other jobs especially if many are being executed simultaneously.

To run programs on several nodes in parallel utilizing the openMPI functionality we have to setup our configuration in the job file. The following parameters can be adjusted according to the system and the requirements:

```bash
#!/bin/bash

#SBATCH --partition=lva
#SBATCH --job-name myjob
#SBATCH --output=output.log

#SBATCH --ntasks=10
#SBATCH --nodes=10

#SBATCH --exclusive

# load required modules
module load openmpi/3.1.6-gcc-12.2.0-d2gmn55
mpiexec -n $SLURM_NTASKS ./somexec
```

`ntasks` specifies the overall number of task that should be distributed. `nodes` corresponds to the number of individual nodes (not NUMA's but rather machines) while `ntasks-per-socket` specifies how many should run per NUMA node. `ntasks-per-node` sets the tasks per node to a fixed number. And lastly `cpus-per-task` can set the number of CPU's per each task (can occur that CPU's on separate nodes work on one task → unideal for latency and throughput). Afterwards I found out that it really only makes sense to set the ntasks and the nodes and orchestrate the location of each task using mpiexec's parameters bind-to and map-by.

Exercise 2

This exercise consists in running an MPI microbenchmark in order to examine the impact of HPC topologies on performance.

The OSU Micro-Benchmarks suite holds multiple benchmarks that measure low-level performance properties such as latency and bandwidth between MPI ranks (=processes). Specifically, for this exercise, we are interested in the point-to-point ones, which exchange messages between 2 MPI ranks.

Tasks

- Download and build the OSU Micro-Benchmarks available at http://mvapich.cse.ohio-state.edu/download/mvapich/osu-micro-benchmarks-5.8.tgz. Do not forget to set the compiler parameters for configure, e.g. ./configure CC=mpicc CXX=mpic++ ...

- After building, submit SLURM jobs that run the osu_latency and osu_bw executables.
- Create a table and figures that illustrate the measured data and study them. What effects can you observe?
- Find out more about the hardware that you're running on, e.g. by using lstopo –of txt (available via module load hwloc). Modify your experiment such that the 2 MPI ranks are placed on different cores of the same socket, different sockets of the same node, and different nodes.
- Amend your table and figures to include these additional measurements. What effects can you observe? How can you verify rank placement without looking at performance?
- How stable are the measurements when running the experiments multiple times?
- Insert the measured time for latency (size 0) and bandwidth (size 1048576) into the comparison spreadsheet: https://docs.google.com/spreadsheets/d/1p6d9F12EtykmI2-7MnHkg0U15UAtaCvWz8Ip92ZEsWo

From the documentation of OSU (https://mvapich.cse.ohio-state.edu/benchmarks/):

```
osu_latency - Latency Test
The latency tests are carried out in a ping-pong fashion. The sender sends a message with a
    certain data size to the receiver and waits for a reply from the receiver. The receiver
    receives the message from the sender and sends back a reply with the same data size.
    Many iterations of this ping-pong test are carried out and average one-way latency
    numbers are obtained. Blocking version of MPI functions (MPI_Send and MPI_Recv) are used
     in the tests.

osu_bw - Bandwidth Test
The bandwidth tests are carried out by having the sender sending out a fixed number (equal
    to the window size) of back-to-back messages to the receiver and then waiting for a
    reply from the receiver. The receiver sends the reply only after receiving all these
    messages. This process is repeated for several iterations and the bandwidth is
    calculated based on the elapsed time (from the time sender sends the first message until
     the time it receives the reply back from the receiver) and the number of bytes sent by
    the sender. The objective of this bandwidth test is to determine the maximum sustained
    date rate that can be achieved at the network level. Thus, non-blocking version of MPI
    functions (MPI_Isend and MPI_Irecv) are used in the test.
```

For building we first have to load all required modules (gcc and openmpi) then we can use configure with the flags CC=mpicc CXX=mpic++ and a proper –prefix=path where we have access to. Then we can build and install with `make && make install`. After that the compiled binaries should be located in our specified path.

```bash
#!/bin/bash

#SBATCH --partition=lva
#SBATCH --job-name ps1.1
#SBATCH --output=output1.log

#SBATCH --ntasks=2
#SBATCH --nodes=1

#SBATCH --exclusive

# load all required modules
module purge
module load openmpi/3.1.6-gcc-12.2.0-d2gmn55

# executing
for i in {1..5}; do
echo $i
mpiexec --display-map --bind-to core --map-by core /home/cb76/cb761014/exercise1/osu-micro-
    benchmarks-5.8/executables/libexec/osu-micro-benchmarks/mpi/pt2pt/osu_latency
done
for i in {1..5}; do
echo $i
```

```
mpiexec --display-map --bind-to core --map-by core /home/cb76/cb761014/exercise1/osu-micro-
    benchmarks-5.8/executables/libexec/osu-micro-benchmarks/mpi/pt2pt/osu_bw
done
```

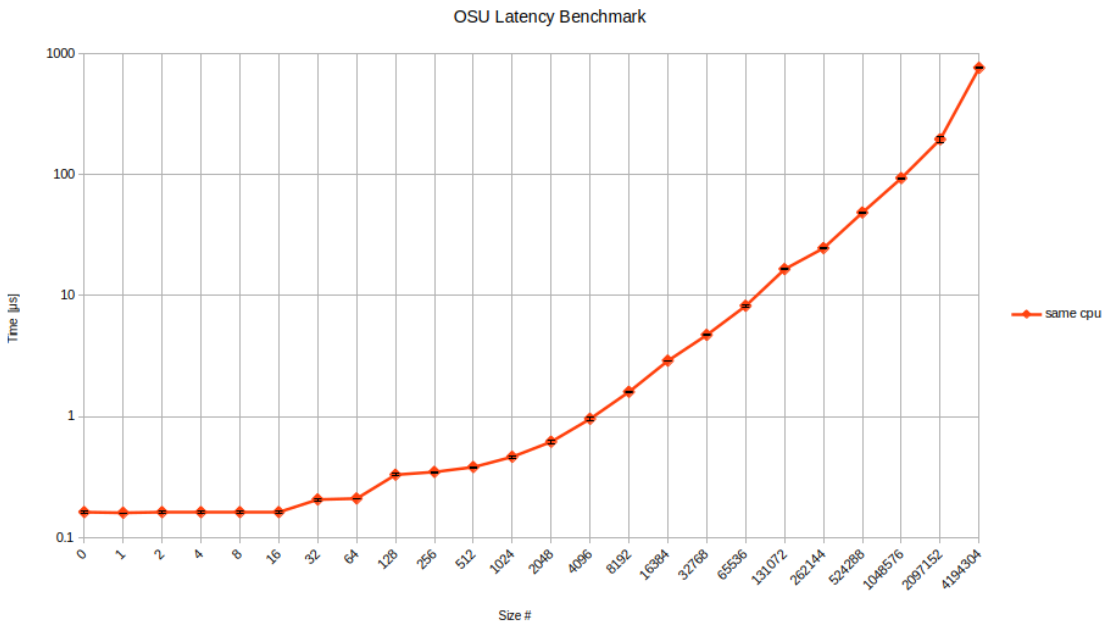


Figure 1: OSU latency plot only cpu.

In the above Fig. 2 we can observe the latency remains constant until about a size of 16-32 (kB) which would correspond to the L1d cache, after that a slow incline can be seen until about 256-512 (kB) which again would fit the L2 cache after that we can see a steep increase in latency which could be the jump to L3 and later on after about 12MB, to main memory.

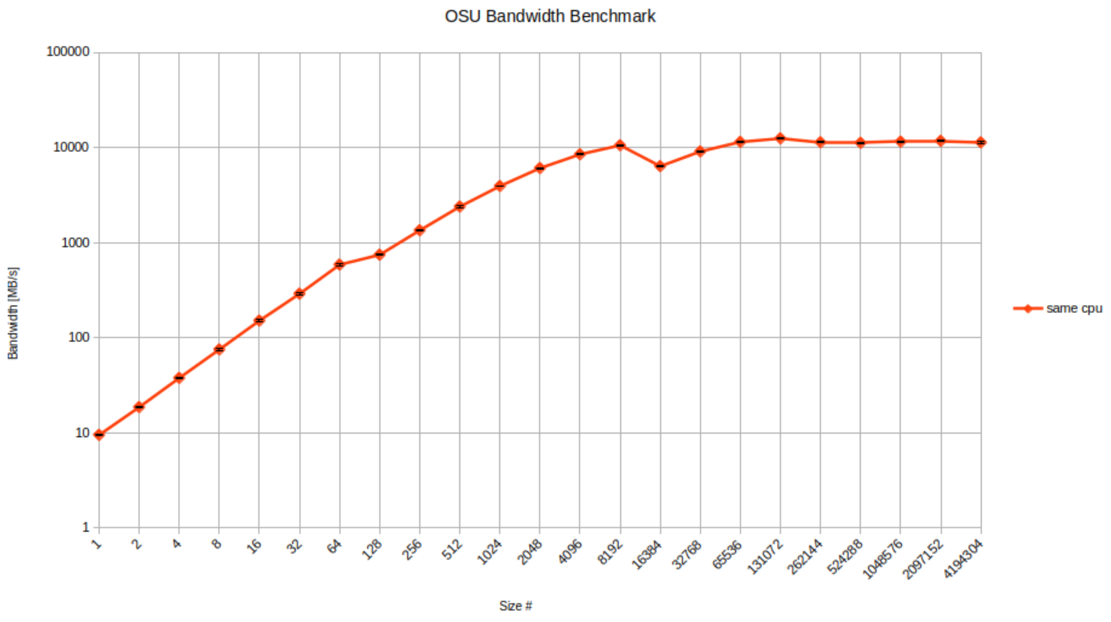
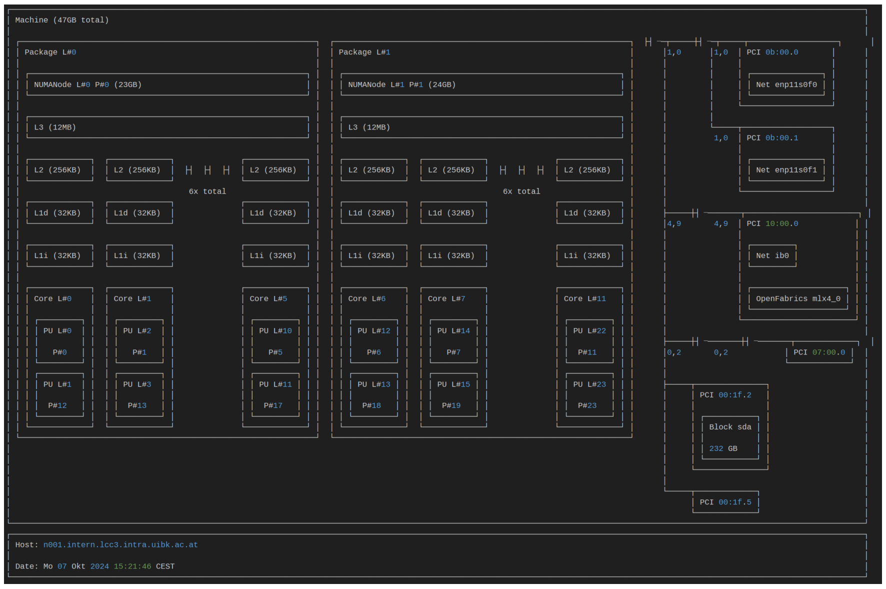


Figure 2: OSU bandwidth plot only cpu.

Here in Fig. 2 we can observe something similar we have a nice linear relationship until 64 (kB?) after that it slowly tapers off. Interestingly at a size of 8192 (kB) it reached its peak and remains at a rate of about 10GB/s.

Size	Avg latency μs	Avg bandwidth MB/s
0	0.162	
1	0.16	9.514
2	0.162	18.632
4	0.162	37.798
8	0.162	75.33
16	0.162	151.436
32	0.206	290.404
64	0.21	587.482
128	0.33	746.458
256	0.348	1349.638
512	0.382	2396.042
1024	0.464	3939.186
2048	0.618	6083.762
4096	0.956	8495.482
8192	1.598	10568.65
16384	2.888	6370.756
32768	4.714	9105.146
65536	8.21	11464.932
131072	16.492	12488.038
262144	24.61	11369.246
524288	48.462	11217.328
1048576	93.19	11540.738
2097152	195.026	11746.71
4194304	759.64	11330.14



```
Machine (47GB total)

  Package L#0                                          Package L#1
    NUMANode L#0 P#0 (23GB)                              NUMANode L#1 P#1 (24GB)
    L3 (12MB)                                            L3 (12MB)
    L2 (256KB)   L2 (256KB)   6x total  L2 (256KB)       L2 (256KB)   L2 (256KB)   6x total  L2 (256KB)
    L1d (32KB)   L1d (32KB)             L1d (32KB)       L1d (32KB)   L1d (32KB)             L1d (32KB)
    L1i (32KB)   L1i (32KB)             L1i (32KB)       L1i (32KB)   L1i (32KB)             L1i (32KB)
    Core L#0     Core L#1               Core L#5         Core L#6     Core L#7               Core L#11
      PU L#0       PU L#2                 PU L#10          PU L#12      PU L#14                PU L#22
        P#0          P#1                    P#5              P#6          P#7                    P#11
      PU L#1       PU L#3                 PU L#11          PU L#13      PU L#15                PU L#23
        P#12         P#13                   P#17             P#18         P#19                   P#23

  1,0   1,0  PCI 0b:00.0
               Net enp11s0f0
        1,0  PCI 0b:00.1
               Net enp11s0f1
  4,9   4,9  PCI 10:00.0
               Net ib0
               OpenFabrics mlx4_0
  0,2   0,2        PCI 07:00.0
     PCI 00:1f.2
       Block sda
       232 GB
     PCI 00:1f.5

Host: n001.intern.lcc3.intra.uibk.ac.at
Date: Mo 07 Okt 2024 15:21:46 CEST
```

Figure 3: lstopo output.

From the lstopo output we can infer that a node consists of 2 NUMA nodes (i.e. has 2 CPU sockets) with 23GB and 24GB of main memory. They both have the same cache architecture with 12MB of L3 cache. 256KB L2 per core cache and 32KB L1d and L1i caches. And we can see that a core consists of two processing units (hw core and hyperthreading/SMT). The nodes are interconnected using OpenFabrics interconnect (InfiniBand) and have two ethernet interfaces. (The login node has compared to the other nodes 32GB of memory per socket.)

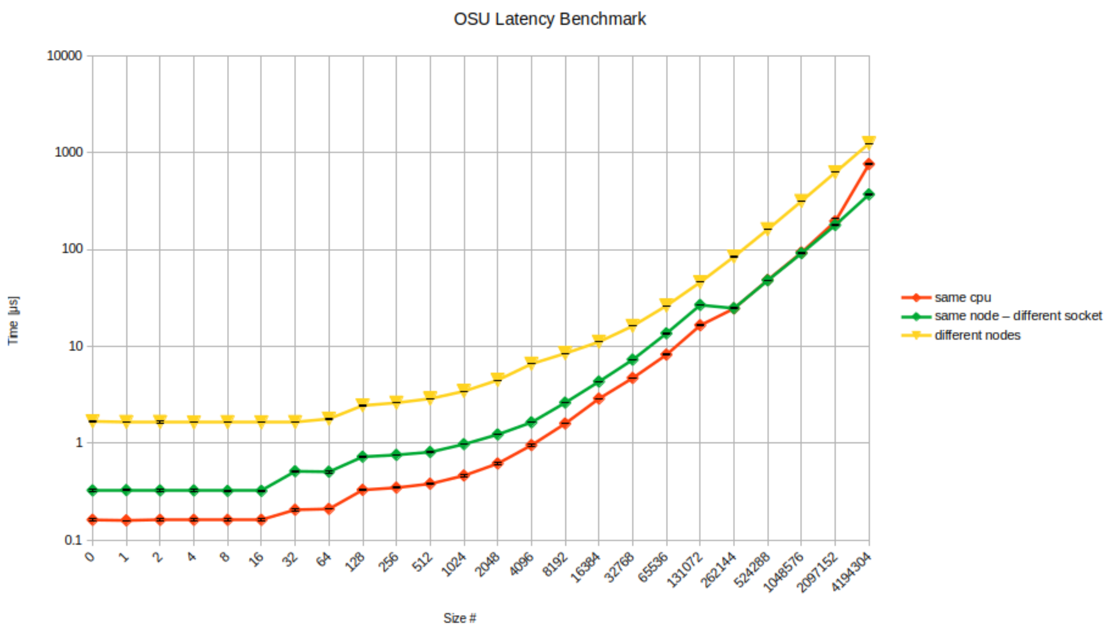


Figure 4: Plot of OSU latency benchmark output.

From the latency benchmark Fig. 4 a large difference between the CPU vs. rest can be seen. The relative difference is at first larger (up to ×10) and gets smaller. Something unexpected is that the latency of the

CPU bench gets larger than the different socket benchmark. Would be interesting to get to know the reason behind this.

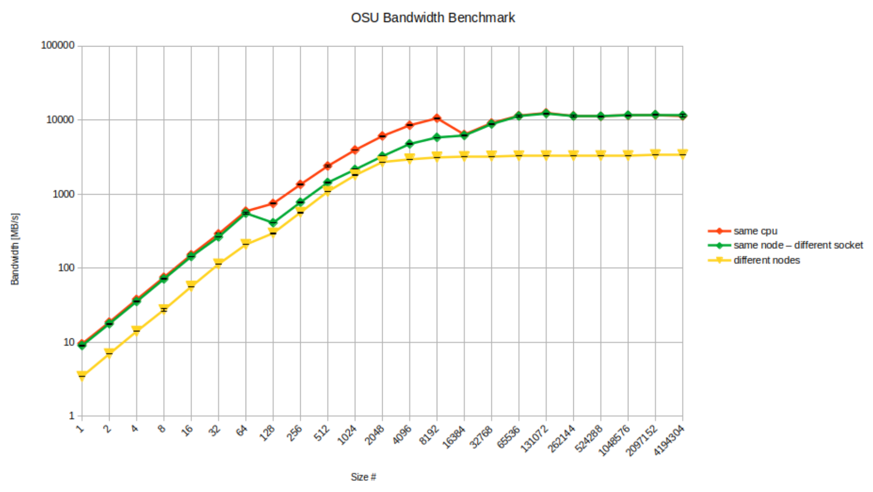


Figure 5: Plot of OSU bandwidth benchmark output.

For the bandwidth benchmark (Fig. 5) we can observe that the throughput of the CPU and socket benchmark are quite similar. Both taper off to about 11 GB/s while the benchmark distributed on 2 separate nodes tapers off at about 3.4 GB/s which is considerably less. So we could conclude that distance in distributed systems is a very relevant metric and if possible message passing should be kept to a minimum size and maximum time distance if possible. And to try and keep the tasks/jobs as close as possible to another (especially if they have to communicate a lot). Otherwise we decrease computational efficiency and extend the runtime of the program by multiple times.

To verify rank placement we can utilize `mpiexec --display-map` (display-map - mpiexec man page) in our job script. This displays the location of the tasks on the hardware.

```
# different CPU cores
 Data for node: n001  Num slots: 2  Max slots: 0  Num procs: 2
Process OMPI jobid: [4154,1] App: 0 Process rank: 0 Bound: socket 0[core 0[hwt 0-1]]:[BB
    /../../../../..][../../../../../..]
Process OMPI jobid: [4154,1] App: 0 Process rank: 1 Bound: socket 0[core 1[hwt 0-1]]:[../BB
    /../../../..][../../../../../..]

# different Sockets
Data for node: n001 Num slots: 2  Max slots: 0  Num procs: 2
Process OMPI jobid: [8583,1] App: 0 Process rank: 0 Bound: socket 0[core 0[hwt 0-1]]:[BB
    /../../../../..][../../../../../..]
Process OMPI jobid: [8583,1] App: 0 Process rank: 1 Bound: socket 1[core 6[hwt
    0-1]]:[../../../../../..][BB/../../../../..]



# Different Nodes (interestingly mpiexec is unable to display the "Bound" on the second node
    )
 Data for node: n002  Num slots: 1  Max slots: 0  Num procs: 1
Process OMPI jobid: [28289,1] App: 0 Process rank: 0 Bound: socket 0[core 0[hwt 0-1]]:[BB
    /../../../../..][../../../../../..]

Data for node: n003 Num slots: 1  Max slots: 0  Num procs: 1
Process OMPI jobid: [28289,1] App: 0 Process rank: 1 Bound: N/A
```

The measurements were all conducted 5 times and looking at the table/plots we can say the measurements are stable within $1-2\%$ with one exception where the standard deviation is 6% of the average which is not that much to invalidate the measurement.

Measurements all in μs.

Size	μ Lat. CPU	σ Lat. CPU	μ Lat. Socket	σ Lat. Socket	μ Lat. Nodes	σ Lat. Nodes
0	0.162	0.004	0.326	0.005	1.684	0.005
1	0.16	0	0.328	0.004	1.654	0.008
2	0.162	0.004	0.326	0.005	1.656	0.026
4	0.162	0.004	0.326	0.005	1.638	0.004
8	0.162	0.004	0.322	0.004	1.648	0.004
16	0.162	0.004	0.322	0.004	1.642	0.004
32	0.206	0.005	0.514	0.005	1.65	0.007
64	0.21	0	0.508	0.010	1.786	0.005
128	0.33	0.007	0.726	0.008	2.454	0.008
256	0.348	0.004	0.758	0.004	2.614	0.011
512	0.382	0.004	0.812	0.004	2.888	0.008
1024	0.464	0.011	0.978	0.008	3.444	0.005
2048	0.618	0.017	1.232	0.004	4.484	0.008
4096	0.956	0.034	1.644	0.005	6.6	0.014
8192	1.598	0.008	2.624	0.005	8.466	0.011
16384	2.888	0.021	4.33	0.014	11.12	0.007
32768	4.714	0.034	7.286	0.015	16.236	0.011
65536	8.21	0.165	13.626	0.068	26.314	0.037
131072	16.492	0.260	26.744	0.140	45.936	0.027
262144	24.61	0.273	24.748	0.333	84.4	0.411
524288	48.462	0.771	47.968	0.385	161.268	0.029
1048576	93.19	0.932	91.462	0.687	315.738	0.019
2097152	195.026	12.984	178.528	1.06	624.568	0.070
4194304	759.64	5.819	370.196	3.98	1243.174	0.287

Measurements all in MB/s.

Size	μ Bw. CPU	σ Bw. CPU	μ Bw. Socket	σ Bw. Socket	μ Bw. Nodes	σ Bw. Nodes
0						
1	9.514	0.110	9.022	0.118	3.444	0.008
2	18.632	0.354	17.77	0.256	6.974	0.023
4	37.798	0.663	35.458	0.454	14.03	0.045
8	75.33	1.248	71.428	1.078	27.404	1.051
16	151.436	3.124	143.618	0.631	56.314	0.544
32	290.404	7.547	264.164	2.439	113.484	0.251
64	587.482	14.886	551.892	10.357	208.796	0.528
128	746.458	5.328	410.014	3.271	297.122	4.872
256	1349.638	25.323	774.53	5.609	566.312	8.173
512	2396.042	43.719	1431.542	16.969	1083.606	10.124
1024	3939.186	36.755	2145.924	23.387	1799.9	15.884
2048	6083.762	63.182	3246.95	17.027	2712.14	6.580
4096	8495.482	110.107	4760.958	27.490	2946.168	4.597
8192	10568.65	62.968	5825.58	16.604	3128.782	5.183
16384	6370.756	113.711	6188.69	90.301	3203.914	4.412
32768	9105.146	119.976	8823.432	225.554	3245.912	1.133
65536	11464.932	227.476	11327.316	190.221	3270.642	0.987
131072	12488.038	262.564	12231.7	303.271	3282.504	0.866
262144	11369.246	166.984	11306.872	177.802	3286.506	4.150
524288	11217.328	124.078	11243.862	130.569	3294.292	0.497
1048576	11540.738	123.555	11611.17	149.700	3296.104	0.779
2097152	11746.71	106.510	11809.352	214.741	3395.628	0.069
4194304	11330.14	260.713	11494.262	418.389	3396.388	0.014