Practical Tips for Running on SUMMIT

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OUTLINE

- Talk is a collection of hands on experience in readying applications for SUMMIT.
- Lightweight MPI profiler.
- Useful jsrun/MPI flags.
- LSF+jsrun example submission scripts
  - 1 rank per socket, core, or GPU example scripts.
  - Using multiple ranks per GPU with MPS.
- Profiling of 1 rank with nvprof at scale.
- Checking on job submission
  - Useful lsf commands.
  - ssh to compute node, get stack traces, nvidia smi.

BEST PRACTICE: LIGHTWEIGHT MPI TRACING

A lightweight MPI tracing library can easily be linked against at runtime[1].

- No performance penalty–we ran this library with all CORAL benchmarks during acceptance.
- Very useful in identifying node imbalance at scale.
- How to use it
  - Official version shipped with SMPI:

```
export OMPI_LD_PRELOAD_POSTPEND=$OLCF_SPECTRUM_MPI_ROOT/lib/libmpitrace.so
```

  - Most up to date version (on SUMMIT):

```
export OMPI_LD_PRELOAD_POSTPEND=/ccs/home/walkup/mpitrace/spectrum_mpi/libmpitrace.so
```

It writes several profile files with format of mpi_profile.jobid.rank

[1] Vampire is another available profiling tool

USING THE MPI PROFILER

Can see where time is spent, calculate achieved communication bandwidth, average message size, etc.

MPI Routine	calls	avg. bytes	time(sec)
MPI_Comm_rank	320850	0.0	0.010
MPI_Comm_size	4	0.0	0.000
MPI_Isend	84	540688.0	0.036
MPI_Send_init	168	8404992.0	0.000
MPI_Recv_init	168	8404992.0	0.000
MPI_Irecv	84	540688.0	0.001
MPI_Wait	3672	0.0	18.112
MPI_Waitall	42	0.0	0.007
MPI_Start	3588	0.0	0.038
MPI_Bcast	24	37.2	0.000
MPI_Barrier	411	0.0	34.302
MPI_Reduce	1	4.0	0.001
MPI_Allreduce	696	20.0	8.602
MPI_Gather	1	4.0	0.000
MPI_Gatherv	2	288.0	0.000

total communication time = 61.108 seconds.
total elapsed time = 239.719 seconds.
user cpu time = 2211.329 seconds.
system time = 372.080 seconds.
max resident set size = 37583.938 MBytes.

IDENTIFYING WORK IMBALANCE

Ranks taking the most time in computation spend the **least** amount of time in MPI calls because all other ranks have been waiting for them. Example rank 0 output info:

Histogram of time−bin	times spent in MPI ranks	
30.231	1	<= Rank deserving closer look
32.611	0	
34.991	0	
37.371	0	
39.751	1	
42.131	1	
44.511	1	
46.891	6	
49.271	55	
51.651	261	
54.030	264	
56.410	188	
58.790	67	
61.170	15	
63.550	4	

Histogram of time−bin	times spent in MPI (Balanced Run) ranks
18.413	1
19.261	1
20.110	1
20.958	9
21.807	28
22.655	38
23.504	30
24.352	48
25.201	39
26.049	26
26.898	17
27.746	11
28.595	3
29.444	3
30.292	1

USING THE MPI PROFILER

Rank 0 summary file also provides rank to node correlation:

MPI timing summary for all ranks:

taskid	hostname	cpu	comm(s)
...			
290	sierra3358	88	52.04
291	sierra3358	128	52.29
292	sierra3800	0	43.48
293	sierra3800	40	30.23
294	sierra3800	88	54.34
295	sierra3800	128	51.69
...			

USEFUL JSRUN FLAGS

- Send kill signal to processes on a MPI failure (helps kill your job instead of hanging it).

```
jsrun -X 1 <further commands>
```

- Prepend the rank id to the output

```
jsrun --stdio_mode prepended
```

- If Spectrum MPI arguments are needed (e.g. async argument when using 1-sided communication)

```
jsrun --smpiarg="-async"
```

Example Submission Scripts

- ORNL training material is very good (link + visualizer).
- Using scripts for lsf job submission and jsrun configuration allows repeatable experiments.
- See talk by Chris Fuson for detailed explanation of lsf and jsrun.
- Key to jsrun is deciding what a resource set will represent (e.g. 1 rs per socket, or per GPU).
- The following are some examples of common use cases. Links to full submission scripts are on each page.

1 RANK PER CORE (CLICKABLE LINK)

```
nodes=1
gpus_per_socket=3 # number of gpus to use per socket
application_cores=21 # cores available to the application per socket
threads_per_core=4 # Each core can go up to smt4 for 4 hardware threads.
# user sets rank_per_socket, calculate other quantities from this:
ranks_per_socket=21 # needs to be evenly divisible by gpus_per_socket (if using GPUs)

# calculated from input:
let num_sockets=2*$nodes
let cores_per_rank=$application_cores/$ranks_per_socket # avail cores divided into the ranks.
let cores_per_socket=$cores_per_rank*$ranks_per_socket # this is used cores per socket (not
necessarily equal to application cores
let threads_per_rank=$threads_per_core*$cores_per_rank

... LSF submission stuff ...

jsrun --stdio_mode=prepend -D CUDA_VISIBLE_DEVICES \
-E OMP_NUM_THREADS=${threads_per_rank} \
--nrs ${num_sockets} \
--tasks_per_rs ${ranks_per_socket} \
--cpu_per_rs ${cores_per_socket} \
--gpu_per_rs ${gpus_per_socket} \
--bind=proportional-packed:${cores_per_rank} \
-d plane:${ranks_per_socket} \
./print-affinity.sh
```

1 RANK PER GPU (CLICKABLE LINK)

```
nodes=1
gpus_per_socket=3 # number of gpus to use per socket ( 3 for summit, 2 for sierra )
gpus_per_rs=1 # 1 res set per GPU (one to one gpu to rs mapping).
threads_per_core=2 # Each core can go up to smt4 for 4 hardware threads.
ranks_per_rs=1 # If using more than 1 rank per gpu, need to enable mps through lsf.

# derived quantities :
let rs_per_socket=$gpus_per_socket/$gpus_per_rs
let ranks_per_socket=$ranks_per_rs*$rs_per_socket
# There are 21 (of 22) cores available to the application per socket (on Summit)
let cores_per_rank=21/$ranks_per_socket # 21 avail cores divided into the ranks.
let cores_per_rs=$cores_per_rank*$ranks_per_rs
let nrs=2*$rs_per_socket*$nodes # total number of resource sets :
let threads_per_rank=$threads_per_core*$cores_per_rank

... LSF submission stuff ...

jsrun --stdio_mode=prepend -D CUDA_VISIBLE_DEVICES \
      -E OMP_NUM_THREADS=${threads_per_rank} \
      --nrs ${nrs} --tasks_per_rs ${ranks_per_rs} \
      --cpu_per_rs ${cores_per_rs} \
      --gpu_per_rs ${gpus_per_rs} \
      --bind=proportional-packed:${cores_per_rank} \
      -d plane:${ranks_per_rs} \
      ./ print - affinity.sh
```

SHARING GPU AMONG 2 RANKS CLICK FOR FULL EXAMPLE

One resource set per GPU, multiple tasks per resource set.

```
gpus_per_socket=3 # number of gpus to use per socket ( 3 for summit, 2 for sierra )
gpus_per_rs=1 # 1 res set per GPU (one to one gpu to rs mapping).
threads_per_core=4 # Each core can go up to smt4 for 4 hardware threads.
ranks_per_rs=2 # If using more than 1 rank per gpu, need to enable mps through lsf.

# derived quantities :
let rs_per_socket=$gpus_per_socket/$gpus_per_rs
let ranks_per_socket=$ranks_per_rs*$rs_per_socket
# There are 21 (of 22) cores available to the application per socket (on Summit)
let cores_per_rank=21/$ranks_per_socket # 21 avail cores divided into the ranks.
let cores_per_rs=$cores_per_rank*$ranks_per_rs
let nrs=2*$rs_per_socket*$nodes # total number of resource sets :
let threads_per_rank=$threads_per_core*$cores_per_rank
```

Must enable MPS in lsf submission[2]:

```
#BSUB -alloc_flags gpumps
```

```
jsrun --stdio_mode=prepend -D
      CUDA_VISIBLE_DEVICES \
   -E OMP_NUM_THREADS=${threads_per_rank} \
   --nrs ${nrs} \
   --tasks_per_rs ${ranks_per_rs} \
   --cpu_per_rs ${cores_per_rs} \
   --gpu_per_rs ${gpus_per_rs} \
   --bind=proportional-packed:${cores_per_rank} \
   -d plane:${ranks_per_rs}  \
   ./ print - affinity.sh
```

[2] If specifying multiple flags, must do it in one line. e.g. #BSUB -alloc_flags “smt2 gpumps“

CHECKING ON YOUR SUBMISSION

- *bjobs* will show a list of your current jobs and their status.
- To check pending reason of a specific job, *bjobs -p <jobid>*
- Is the que busy/open? *bqueues*

```
[dappelh@login5.summit]$ bqueues
QUEUE_NAME  PRIO STATUS          MAX JL/U JL/P JL/H NJOBS PEND RUN SUSP
test           5 Open:Inact      45    -    -    -     0    0   0    0
storage        4 Open:Inact       -    -    -    -     0    0   0    0
tested         3 Open:Active      -    -    -    -     0    0   0    0
new            2 Open:Inact       -    -    -    -    43   43   0    0
batch          1 Open:Active      -    -    -    -    85    0  85    0
```

- What jobs are scheduled on the machine? *bjobs -u all*

```
[dappelh@login1.summit]$ bjobs -u all
JOBID   USER    STAT  SLOTS  QUEUE      START_TIME    FINISH_TIME   JOB_NAME
220841  bykov   RUN   86017  batch      Nov 28 14:15  Nov 29 02:15  lsdalton
220932  jaharris RUN  43     batch      Nov 28 17:37  Nov 28 18:07  Not_Specified
220933  ngawande RUN  2017   batch      Nov 28 17:40  Nov 28 19:40  d48_c
220908  chochia PEND  -      tested     -             -             Not_Specified
220926  chochia PEND  -      tested     -             -             Not_Specified
```

CHECKING ON A RUNNING JOB

- *bpeek* will show you tail of standard out and standard error (jobid is optional):

```
bpeek <jobid> | less
```

- Something seems wrong, can I check into a job further?

```
bjobs -WP <jobid> | less
```

```
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME %COMPLETE
220933  ngawand RUN   batch      login1      batch1      d48_c      Nov 28 17:40  32.62% L
                                              g36n12
                                              g36n12
                                               ...
```

- Can ssh to a compute node (only while job is running)

```
ssh g36n12
```

TROUBLESHOOTING A JOB ON A COMPUTE NODE

- Use gstack to get call stack of each thread (use top to get pid)

```
gstack <pid>
```

- See if the GPUs have something currently running:

```
nvidia−smi
```

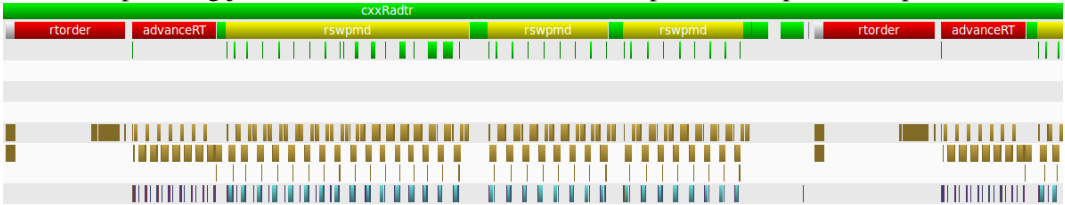
Example idle GPUs:

```
 +-----------------------------------------------------------------------------+
| NVIDIA-SMI 396.58                 Driver Version: 396.58                    |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Tesla V100-SXM2...  On   | 00000004:04:00.0 Off |                    0 |
| N/A   34C    P0    36W / 300W |      0MiB / 16128MiB |      0%   E. Process |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

PROFILING AT SCALE

- Running nvprof on every rank of a large scale job will slow to a crawl.
- However, profiling just one of the ranks at scale with nvprof/visual profiler is possible.



- See talk later this week on detailed usage of nvprof and visual profiler as well as Score-P/Vampire.

SCRIPT FOR 1 RANK TO LAUNCH NVPROF

Have jsrun launch this script which executes profiler+application if rank matches profile rank, otherwise just launches application without profiling:

```
export PROFILE_RANK=1
export PROFILE_PATH="/gpfs/path_to_your_directory"
jsrun <flags> profile_helper.sh a.out
```

Contents of profile_helper.sh:

```
#!/bin/bash
if [ $PMIX_RANK == $PROFILE_RANK ]; then
    nvprof -f -o $PROFILE_PATH "$@"
else
    "$@"
fi
```

Closing Remarks

Hopefully you have learned how to

- Use the lightweight mpi profiler even if not focusing on MPI performance.
- Use scripts for lsf/jsrun submissions.
- Check on your job submission after submitting.
- Launching a profiler at scale on a single MPI rank.

Questions?

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Github script location: `https://github.com/dappelha/summit-scripts`