Best Practice Guides

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Outline

- Profilers
- Examples of profiling in real applications
- Best Practice Guides
- Hands On on supplied codes or your own code
- Discussion

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- Profiler is software that gets metrics on source execution, without addition of timers in source code.
- Serial Profilers
  - One can find detailed time spent in code procedures, i.e. How many times a procedure was called, average time per call, total time spent in procedure, from which point in source was called etc.
  - Standard Unix profiler gprof and its variants, for example sprof.
  - Compiler specific profilers, like vtune for Intel compilers or pgprof for PGI.

- MPI
  - mpiP : Traces MPI calls and gives performance indicators, possible bottlenecks etc. OpenSource, Works with any compiler and MPI implementation.
  - MPI implementations profilers, for example OpeMPI VampirTrace.
- Hybrid MPI/OpenMP/Threads Profilers
  - scalasca : Traces MPI calls, as well as OpenMP calls, provides detailed information timing information per thread, task, node, code line. Graphical Interface to explore profile information.
  - Other mainly commercial profilers/debuggers, for example DDT

In Practice

- Serial Applications : gprof
  - At Compile time use the flags : -pg
  - It is suggested to use -O0 for optimization to avoid any inlining that may result to missing functions timing.
  - Example : `00_profiling1.f` : Matrix Matrix Maltiplication.

```
module load binutils
gcc 00_profiling1.f -pg -O0 -o 00_profiling1.x
./00_profiling1.x
gprof 00_profiling1.x
```

  - You'll se something like

```
  %   cumulative   self              self     total
 time   seconds   seconds    calls   s/call   s/call  name
100.30     10.82    10.82        1    10.82    10.82  mymm_
  0.09     10.83     0.01        1     0.01     0.01  initializearrays_
  0.00     10.83     0.00        1     0.00    10.83  MAIN__
```

- In Brief :
  - mymm is executed 1 times, need 10.82 seconds for each call, it is the main time consuming procedure.
  - initializearrays is executed 1 times, need 0.01 secs per call.
  - Main is executed 1 times, it needs less than 0.005 seconds to complete.
  - We have a good estimation where the execution time is spent. In real serial applications output is more interesting.

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In Practice

- Pure MPI Applications : mpiP
- If you compile your application using : mpif90 mycode.f -o mycode.x
  do

```
module load mpiP
mpif90 mycode.f -g -L$MPIPROOT/lib -lmpiP -lbfd -lunwind -o mycode.x
```

- -g (debug) flag is needed to include source code information in executable.
- If (that is usually the case) you have a makefile to compile, use in the linking stage mpiP, example :

```
$LD $(OBJECTFILES) -g -L$MPIPROOT/lib -lmpiP -lbfd -lunwind -o mycode.x
```

- Run it : srun mycode.x in slurm

- or mpiexec.hydra -n 8 mycode.x (interactively on login node with 8 procs)
- After completion you'll find a report file called mycode.x.NPROCS.PID.mpiP
- Have a look in the provided information.
- You'll se something like

```
@ mpiP
@ Command : ./06.x
@ Version                    : 3.4.1
@ MPIP Build date            : Sep  7 2015, 16:33:51
@ Start time                 : 2017 11 29 21:45:28
@ Stop time                  : 2017 11 29 21:45:31
@ Timer Used                 : PMPI_Wtime
@ MPIP env var               : [null]
@ Collector Rank             : 0
@ Collector PID              : 29284
@ Final Output Dir           : .
@ Report generation          : Collective
@ MPI Task Assignment        : 0 login01
```

```
......
@--- MPI Time (seconds) ---------------------------------------------
---------------------------------------------------------------------
Task    AppTime    MPITime     MPI%
   0       2.72        0.7    25.69
   1       2.72       1.16    42.52
   2       2.72       1.07    39.11
   3       2.72       1.06    38.98
   4       2.72       1.04    38.24
   5       2.72       1.32    48.29
.....
 31       2.72       1.13    41.51
  *       87.1       34.9    40.05
......
@--- Callsites: 11 --------------------------------------------------
---------------------------------------------------------------------
 ID Lev File/Address                 Line Parent_Funct           MPI_Call
  1   0 06_md_inhomegeneous_reduce.f  115 md                     Bcast
  2   0 06_md_inhomegeneous_reduce.f  137 md                     Bcast
  3   0 06_md_inhomegeneous_reduce.f  202 md                     Reduce
.....
@--- Aggregate Time (top twenty, descending, milliseconds) ----------
---------------------------------------------------------------------
Call                     Site       Time    App%    MPI%     COV
Reduce                      4   1.27e+04   14.57   36.37    0.94
```

```
Barrier                  8   1.03e+04   11.78   29.41    1.09
Bcast                    6    8.8e+03   10.10   25.22    0.18
......
@--- Aggregate Sent Message Size (top twenty, descending, bytes) ----------
---------------------------------------------------------------------------
Call                 Site       Count       Total       Avrg  Sent%
Reduce                  3          32     3.2e+07      1e+06  11.11
Reduce                  4          32     3.2e+07      1e+06  11.11
Reduce                  9          32     3.2e+07      1e+06  11.11
Bcast                  11          32     3.2e+07      1e+06  11.11
......
@--- Callsite Time statistics (all, milliseconds): 352 --------------------
---------------------------------------------------------------------------
Name              Site Rank  Count      Max     Mean      Min   App%   MPI%
Barrier              8    0      1    0.048    0.048    0.048   0.00   0.01
Barrier              8    1      1      774      774      774  28.42  66.83
Barrier              8    2      1      769      769      769  28.23  72.17
```

....

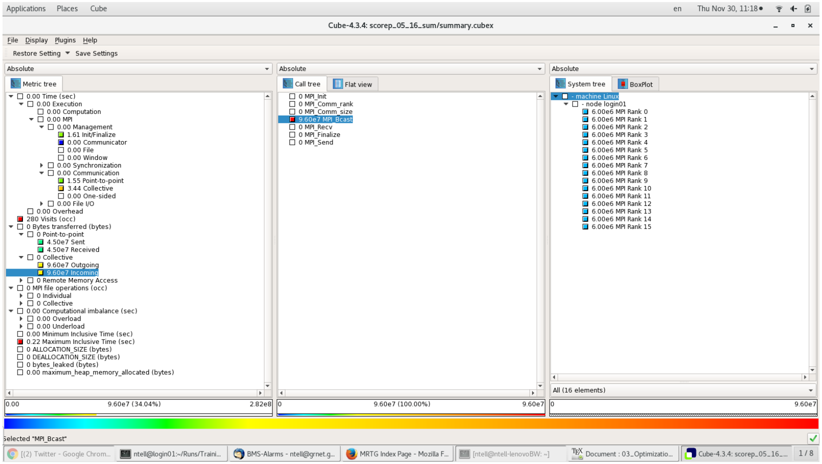
and more.

In Practice

- Hybrid Applications : Scalasca
- If you compile your application using : mpif90 mycode.f -o mycode.x
  do

```
module load binutils qt/5.6.0 cuda/7.5.18
scalasca -instrument mpif90 mycode.f -o mycode.x
scalasca -analyze mpiexec.hydra -n 8 ./mycode.x
scalasca -examine scorep_mycode.x_8_sum
```

- You'll see something like (You need X11 at your Desktop)
- https://sourceforge.net/projects/xming/
- If not X11 available, instead of scalasca -examine use : square -s `scorep_mycode.x_8_sum`. A report will be in `scorep_mycode.x_8_sum/scorep.score` text file.



Cube-4.3.4: scorep_05_16_sum/summary.cubex

```
0.00 Time (sec)
  0.00 Execution
    0.00 Computation
    0.00 MPI
      0.00 Management
        1.61 Init/Finalize
        0.00 Communicator
        0.00 File
        0.00 Window
      0.00 Synchronization
      0.00 Communication
        1.55 Point-to-point
        3.44 Collective
        0.00 One-sided
      0.00 File I/O
  0.00 Overhead
280 Visits (occ)
0 Bytes transferred (bytes)
  0 Point-to-point
    4.50e7 Sent
    4.50e7 Received
  0 Collective
    9.60e7 Outgoing
    9.60e7 Incoming
  0 Remote Memory Access
0 MPI file operations (occ)
  0 Individual
  0 Collective
0.00 Computational imbalance (sec)
  0.00 Overload
  0.00 Underload
0.00 Minimum Inclusive Time (sec)
0.22 Maximum Inclusive Time (sec)
0 ALLOCATION_SIZE (bytes)
0 DEALLOCATION_SIZE (bytes)
0 bytes_leaked (bytes)
0.00 maximum_heap_memory_allocated (bytes)
```

```
0 MPI_Init
0 MPI_Comm_rank
0 MPI_Comm_size
9.60e7 MPI_Bcast
0 MPI_Recv
0 MPI_Finalize
0 MPI_Send
```

```
- machine Linux
  - node login01
    6.00e6 MPI Rank 0
    6.00e6 MPI Rank 1
    6.00e6 MPI Rank 2
    6.00e6 MPI Rank 3
    6.00e6 MPI Rank 4
    6.00e6 MPI Rank 5
    6.00e6 MPI Rank 6
    6.00e6 MPI Rank 7
    6.00e6 MPI Rank 8
    6.00e6 MPI Rank 9
    6.00e6 MPI Rank 10
    6.00e6 MPI Rank 11
    6.00e6 MPI Rank 12
    6.00e6 MPI Rank 13
    6.00e6 MPI Rank 14
    6.00e6 MPI Rank 15
```

```
0.00    9.60e7 (34.04%)    2.82e8
0    9.60e7 (100.00%)    9.60e7
0    9.60e7
```

Selected "MPI_Bcast"

[(2) Twitter - Google Chrom...
ntell@login01:~/Runs/Traini...
BMS-Alarms - ntell@grnet.g...
MRTG Index Page - Mozilla F...
[ntell@ntell-lenovoBW: ~]
Document : 03_Optimizatio...
Cube-4.3.4: scorep_05_16_...
1 / 8

Efficient use I

- ARIS compute nodes have 20 or 40 cores. Use if possible full nodes, i.e. 20/40 cores/node.
- If it is not the case, limit the required nodes.

cores	Nodes	tasks/node	Unused cores
64	4	20	16 on 1 node
128	7	20	12 on 1 node
256	13	20	4 on 1 node
512	26	20	8 on 1 node

Efficient use II

- Common mistake

cores	Nodes	tasks/node	Unused cores
64	8	8	12 cores/node on 8 nodes=96
64	4	16	4 cores/node on 4 nodes = 16
90	6	15	5 cores/node on 6 nodes = 30
128	8	16	4 cores/node on 8 nodes = 32
480	40	12	8 cores/node on 40 nodes = 320
512	32	16	4 cores/node on 32 nodes = 128

- Do not use mpirun/mpiexec nor typical desktop arguments like -np. It happens to forget to change the really needed resources, for example :

Efficient use III

```
#SBATCH --nodes=10
#SBATCH --ntasks=200
mpirun -np 8
or
srun -n 8
```

You allocate (and charged for) 200 cores while you use only 8.

- Try to use the correct combination of tasks and threads with Hybrid applications. Check that the `OMP_NUM_THREADS` is set. In SLURM script template there is code that checks for this.

Efficient use IV

- Surprisingly, this piece of code is frequently removed.

Efficient use I

- Explore the capabilities of your application. With some options in input file(s) you may see much better performance.

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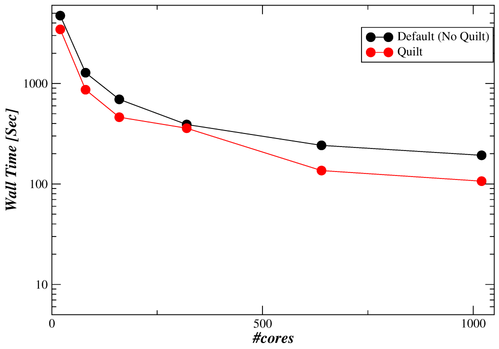
Efficient use II

- Example : WRF quilting

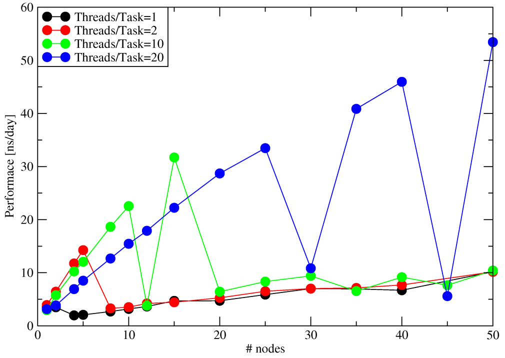


Efficient use

- It depends on the algorithm
- ..and mainly on data
- The same algorithm may exhibit diffierent efficiency with different data
- There are ”gold” rules for algorithms, but :
- Measure performance with your data before decision

Efficient use

- Example : MD of an inhomogeneous system



Efficient use I

- If you can use save/restart and need very long time, use it. Instead of a job of 10 days, use 10 jobs of 1 day (propability of a HW failure in 10 days much higher - especially with multinode runs).
- Request from the Resource Manager wall time slightly higher than the expected. NOT the typical 2 days.
- Example : Submit 100 jobs requesting 2 days each. Scheduler will arrange to run them in $\sim$ 1 week. If each run takes 5 minutes, requesting 6 minutes, all runs will finish in $\sim$ 1 hour instead of $\sim$ 1 week.

Efficient use II

- Even better, submit few jobs with multiple srun, for example 10 jobs with 10 srun.
- Stats : Sept. 2017
  65% of jobs took up to 5% of requested time
  9% between 5 and 10%.
  11% more than 50%

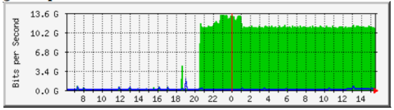
Efficient use III

- Avoid to use .bashrc. Especially when more than 1 versions of package are available. Use modules instead. For example, OpenFOAM :
  `module load openfoam/3.0.1`
  `source $FOAM_BASHRC` instead of put in `.bashrc` all OpenFOAM variables, specific to a certain version.
- Avoid no necessary parameters in input, especially those that affect load balance, grids, methods etc. if it is possible to specify them at runtime, for example, `NPROC_X/Y` in WRF, `processors` or `pair_style lj/cut/gpu` vs `pair_style lj/cut` and `-sf gpu` with LAMMPS.

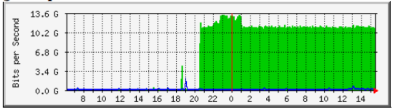
Efficient use IV

- Heavy use of scratch : Read from files with rate 12.6 GBytes/sec for 2 days = 2.12 PBytes for a 100 cores job!!.

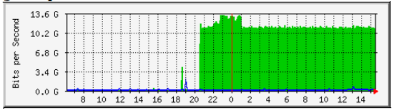
gss01-port1



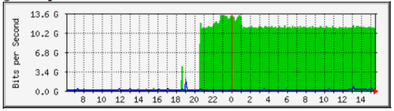
gss01-port2



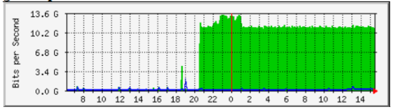
gss01-port3



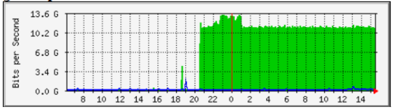
gss01-port4



gss02-port1



gss02-port2



Hands On

- Profile Serial, MPI, Hybrid MPI/OpenMP applications with gprof, mpiP, scalasca.
- For those who have their own Code, try to profile your own code.
- Those who are familiar with vtune, try also vtune, especially with OpenMP only codes.
- Discuss Findings, Suggestions to improve performance.

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