PDC Summer School: Introduction to High-Performance Computing August 19-30, 2013 - KTH, Stockholm, Sweden

Performance Engineering

Pekka Manninen, Ph.D. Cray Inc. manninen@cray.com

Certain parts of the material Cray Inc proprietary do not reuse or redistribute without permission, please

Performance engineering

We want to get the most science and engineering through a supercomputing system as possible

90

The more efficient codes are the more productive scientists and engineers can be

Performance analysis

To optimise code we must know what is taking the time



Performance Engineering module overview

	Tuesday		Wednesday
11.15-12.00	D Introduction to performance engineering	8.30-9.00	Interim summary, Q&A
		11.15-12.00	Improving parallel
12.00-13.15	Lunch		scalability
13.15-14.00	Application performance analysis	12.00-13.15	Lunch
		13.15-15.00	Lab session
14.00-14.15	Break		
14.15-15.00	Lab session		
15.00-15.15	Coffee break		
15.15-17.00	Lab session		

Part I: Introduction to performance engineering

- About code optimization in general
- Not going to touch the source code?
- Data locality
- Why does scaling end?
- Application optimization flow chart

Code optimization

Obvious benefits

- Better throughput => more science
- Cheaper than new hardware
- Save energy, compute quota etc.

..and some non-obvious ones

- Collaboration opportunities
- Potential for cross-disciplinary research
- Deeper understanding of application

Several trends making code optimization even more important

- More and more cores
- CPU's vector units getting wider
- The gap between CPU and memory speed ever increasing
- Datasets growing rapidly but disk I/O performance lags behind

Code optimization

- Adapting the problem to the underlying hardware
- Combination of many aspects
 - Effective algorithms
 - Implementation: Processor utilization & efficient memory use
 - Parallel scalability
- Important to understand interactions
 - Algorithm code compiler libraries hardware
- Performance is not portable!

Not going to touch the source code?

- Find the *compiler* and its *compiler flags* that yield the best performance
- Employ *tuned libraries* wherever possible
- Find suitable settings for *environment parameters*
- Mind the I/O
 - Do not checkpoint too often
 - Do not ask for the output you do not need

Keep your friends close and data even closer



Why does scaling end?

- Amount of data per process small computation takes little time compared to communication
- Amdahl's law in general
 - E.g., single-writer or stderr I/O
- Load imbalance
- Communication that scales badly with N_{proc}





Part II: Application performance analysis

Tools for performance analysis

- Eight-stage procedure for identifying performance bottlenecks
- Example: Cray Performance Analysis Toolkit

Application timing

• Most basic information: total wall clock time

- Built-in timers in the program (e.g. MPI_Wtime)
- System commands (e.g. time) or batch system statistics

Built-in timers can provide also more fine-grained information

- Have to be inserted by hand
- Typically, no information about hardware related issues e.g. cache utilization
- Information about load imbalance and communication statistics of parallel program is difficult to obtain

Performance analysis tools

Instrumentation of code

- Adding special measurement code to binary
 - Special commands, compiler/linker wrappers
 - Automatic or manual
- Normally all routines do not need to be measured

• Measurement: running the instrumented binary

- Profile: sum of events over time
- Trace: sequence of events over time

Analysis

- Text based analysis reports
- Visualization

Sampling

Advantages

- Only need to instrument main routine
- Low Overhead depends only on sampling frequency
- Smaller volumes of data
 produced

Disadvantages

- Only statistical averages available
- Limited information from performance counters

Event Tracing

Advantages

- More accurate and more detailed information
- Data collected from every traced function call not statistical averages

Disadvantages

- Increased overheads as number of function calls increases
- Huge volumes of data generated

Guided tracing = trace only program parts that consume a significant portion of the total time In Cray Performance Analysis Toolkit this is referred to as "automatic profiling analysis "(APA)

Step 1: Choose a test problem

The dataset used in the analysis should

- Make scientific sense, i.e. resemble the intended use of the code
- Be large enough for getting a good view on scalability
- Be runable in a reasonable time
- For instance, with simulation codes almost a full-blown model but run only for a few time steps

Should be run long enough that initialization/finalization stages are not exaggerated

• Alternatively, we can exclude them during the analysis

Step 2: Measure scalability

- Run the uninstrumented code with different core counts and see where the parallel scaling stops
- Usually we look at strong scaling
 - Also weak scaling is definitely of interest

here?



Step 3: Instrument the application

 Obtain first a sampling profile to find which user functions should be traced

- With a large/complex software, one should not trace them all: it causes excessive overhead
- Make an instrumented exe with tracing time-consuming user functions plus e.g. MPI, I/O and library (BLAS, FFT,...) calls
- Execute and record the first analysis with
 - The core count where the scalability is still ok
 - The core count where the scalability has ended

and identify the largest differences between these profiles

Example with CrayPAT (1/2)

• Load performance tools software

module load perftools

• Re-build application (keep .o files)

make clean
make

- Instrument application for automatic profiling analysis
 - You should get an instrumented program a.out+pat

pat_build -O apa a.out

- Run the instrumented application (...+pat) to get top time consuming routines
 - You should get a performance file ("<sdatafile>.xf") or multiple files in a directory <sdatadir>

Example with CrayPAT (2/2)

• Generate text report and an .apa instrumentation file

pat_report [<sdatafile>.xf | <sdatadir>]

- Inspect the .apa file and sampling report whether additional instrumentation is needed
 - See especially sites "Libraries to trace" and "HWPC group to collect"

Instrument application for further analysis (a.out+apa)

pat_build -O <apafile>.apa

- Run application (...+apa)
- Generate text report and visualization file (.ap2)

pat_report -o my_text_report.txt [<datafile>.xf | <datadir>]

• View report in text and/or with Cray Apprentice²

app2 <datafile>.ap2

Some important options to pat_report -O

callers **Profile by Function and Callers** callers+hwpc Profile by Function and Callers callers+src Profile by Function and Callers, with Line Numbers Profile by Function and Callers, with Line Numbers callers+src+hwpc calltree Function Calltree View heap_hiwater Heap Stats during Main Program **Program HW Performance Counter Data** hwpc Load Balance across PEs load balance program+hwpc load balance sm Load Balance with MPI Sent Message Stats loop times Loop Stats by Function (from -hprofile generate) loops Loop Stats by Inclusive Time (from -hprofile generate) MPI Message Stats by Caller mpi callers profile Profile by Function Group and Function profile+src+hwpc Profile by Group, Function, and Line samp profile **Profile by Function** samp profile+hwpc **Profile by Function** samp profile+src Profile by Group, Function, and Line

For a full list see pat_report -O help

Step 4: Assessing the big picture

• Profile = Where the most of the time is really being spent?

- See also the call-tree view
- Ignore (from the optimization point-of-view) user routines with less than 5% of the execution time
- Why does the scaling end: the major differences in these two profiles?
 - Has the MPI fraction 'blown up' in the larger run?
 - Have the load imbalances increased dramatically?
 - Has something else emerged to the profile?
 - Has the time spent for user routines decreased as it should (i.e. do they scale independently)?

Example with CrayPAT





Step 5: Analyze load imbalance

• What is causing the imbalance?

Computation

 Tasks call for computational kernels (user functions, BLAS routines,...) for varying times and/or the execution time varies depending on the input/caller

Communication

• Large MPI_Sync times

• I/O

 One or more tasks are performing I/O and the others are just waiting for them in order to proceed

Example with CrayPAT

		Min Avg and Max	6.65
Eile		Ivini, Tvg, and Iviax	Help
▼090921P+hycomBase.ap2 🗶		Values	
🕘 🗢 ਨ 🗉			,
▼Overview 🗶 🔻 Callgraph 🗶 ▼Load Balance 🗶			
PE Calls	Load Balance: mpi_waitaii_		
PE #240			
PE #232		A	
PE #213			
PE #198			
PE #006			
PE #145			
PE #233			
PE #192			
PE #144			
PE #212 PE #149		/	
PE #241			
PE #185			
PE #193			
PE #215			
PE #203			
PE #228			
PE #168			
PE #000			
PE #005			
PE #122			
PE #148			
PE #177			
PE #140			
PE #220			
PE #243			
PE #242			
PE #100			
PE #167			
PE #003			
PE #159			
PE #211			
PE #029			
8e+04	0 0 41 1.2e+02		4.3e+02 ▼
090921P+hycomBase.ap2 (605,339 events in 23.985s)			

Step 6: Analyze communication

• What communication pattern is dominating the true time spent for MPI (excluding the sync times)

- Refer to the call-tree view on Apprentice2 and the "MPI Message Stats" tables in the text reports produced by pat_report
- Note that the analysis tools may report load imbalances as "real" communication
 - Put an MPI_Barrier before the suspicious routine load imbalance will aggregate into it in when then analysis is rerun

• How does the message-size profile look like?

• Are there a lot of small messages?

Example with CrayPAT

Т	ab	le 4: MPI	Message St	ats by Cal	ler
		MPI Msg M Bytes 	PI Msg Count 	MsgSz 4 <16B M Count <	KB<= Function sgSz Caller 64KB PE[mmm] ount
1	15	138076.0	4099.4	411.6 36	87.8 Total
ļ	1-	5138028.0	4093.4	405.6 3	687.8 MPI_ISEND
 3	İ	8080500.0	2062.5	93.8	1968.8 calc2_ MAIN_
4		8216000.	 0 3000.0) 1000.0	2000.0 pe.0
4 4	İİ	8208000.	0 2000.0 0 2000 0)) 500.0	2000.0 pe.9
ļ	ļİ				
 3	I.	6285250.0	1050.2	125.0	
 4		8216000.	0 3000.0	0 1000.0	2000.0 pe.0
4 4		6156000. 6156000.	0 1500.0 0 1500.0))	1500.0 pe.3 1500.0 pe.5
		======================================			

Step 7: Analyze I/O

- Trace POSIX I/O calls (fwrite, fread, write, read,...)
- How much I/O?
 - Do the I/O operations take a significant amount of time?
- Are some of the load imbalances or communication bottlenecks in fact due to I/O?
 - Synchronous single writer
 - Insert MPI_Barriers to investigate this

Step 8: Find single-core hotspots

- Remember: pay attention only to user routines that consume significant portion of the total time
- View the key hardware counters, for example
 - L1 and L2 cache metrics
 - use of vector (SSE/AVX) instructions
 - Computational intensity (= ratio of floating point ops / memory accesses)
- CrayPAT has mechanisms for finding "the" hotspot in a routine (e.g. in case the routine contains several and/or long loops)
 - CrayPAT API
 - Possibility to give labels to "PAT regions"
 - Loop statistics (works only with Cray compiler)
 - Compile & link with CCE using -h profile_generate
 - pat_report will generate loop statistics if the flag is being enabled

Example with CrayPAT

USER / conj_grad_.LOOPS Time% 59.5% Time 73.010370 secs Flat profile data Imb. Time 3.563452 secs Imb. Time% 4.7% 1.383 /sec 101.0 calls. Calls 183909710385 PERF COUNT HW CACHE L1D:ACCESS PERF COUNT HW CACHE L1D: PREFETCH 7706793512 PERF COUNT HW CACHE L1D:MISS 21336476999 . . . HW counter values 1961227352 SIMD FP 256: PACKED DOUBLE 189983282830 cycles 100.0% Time User time (approx) 73.042 secs CPU CLK 3.454GHz 9.3%peak(DP) HW FP Ops / User time 969.844M/sec 70839736685 ops Total DP ops 969.844M/sec 70839736685 ops Computational intensity 0.37 ops/cycle 0.33 ops/ref MFLOPS (aggregate) 124140.04M/sec TLB utilization 1058.97 refs/miss 2.068 avg uses Derived 90.0% hits D1 cache hit, miss ratios 10.0% misses metrics D1 cache utilization (misses) 9.98 refs/miss 1.248 avg hits 17.5% hits D2 cache hit, miss ratio 82.5% misses D1+D2 cache hit, miss ratio 91.7% hits 8.3% misses D1+D2 cache utilization 12.10 refs/miss 1.512 avg hits D2 to D1 bandwidth 18350.176MB/sec 1405449334558 bytes Average Time per Call 0.722875 secs

Example with CrayPAT

Loop I	Loop Incl	Loop Incl	Loop	Loop	Loop	Function=/.LOOP\.
Incl	Time	Time /	Hit	Trips	Notes	PE='HIDE'
Time /		Hit		Avg		
Total						
24.6%	0.057045	0.000570	100	64.1	novec	calc2LOOP.0.li.614
24.0%	0.055725	0.000009	6413	512.0	vector	calc2LOOP.1.li.615
18.9%	0.043875	0.000439	100	64.1	novec	<pre>calc1LOOP.0.li.442</pre>
18.3%	0.042549	0.000007	6413	512.0	vector	<pre>calc1LOOP.1.li.443</pre>
17.1%	0.039822	0.000406	98	64.1	novec	<pre>calc3LOOP.0.li.787</pre>
16.7%	0.038883	0.000006	6284	512.0	vector	<pre>calc3LOOP.1.li.788</pre>
9.7%	0.022493	0.000230	98	512.0	vector	<pre>calc3LOOP.2.li.805</pre>
4.2%	0.009837	0.000098	100	512.0	vector	calc2LOOP.2.li.640
========			========	=========		================

Scalability bottlenecks

- Review the performance measurements (between the two runs)
- Case: user routines scaling but MPI time blowing up
 - Issue: Not enough to compute in a domain
 - Weak scaling could still continue
 - Issue: Expensive (all-to-all) collectives
 - Issue: Communication increasing as a function of tasks

• Case: MPI_Sync times increasing

- Issue: Load imbalance
 - Tasks not having a balanced role in communication?
 - Tasks not having a balanced role in computation?
 - Synchronous (single-writer) I/O or stderr I/O?

Web resources

- CrayPAT documentation http://docs.cray.com
- Scalasca http://www.scalasca.org/
- Paraver http://www.bsc.es/computer-sciences/performance-tools/paraver
- Tau performance analysis utility http://www.cs.uoregon.edu/Research/tau

Lab session: Performance analysis

- The Game of Life (GoL) is a cellular automaton devised by John Horton Conway, read http://en.wikipedia.org/wiki/Conway's_Game_of_Life
- A parallel (MPI) implementation of the GoL is provided in GoL_mpi (.f90 or .c)
 Develop a 500x500 b
 - Compile and run the software make mpi aprun -n 4 ./gol 100 500 500

Develop a 500x500 board for 100 iterations Run through the batch job scheduler

- <u>To do</u>: Find out the reason(s) why the default version of the GoL code does not scale
 - Indeed it should scale, it is a simple domain decomposition with thin halos
 - You will find other implementations from the makefile as follows:
 - make nonb replaces MPI_Sendrecv by nonblocking operations
 - make pario parallelizes the disk I/O
 - make hyb hybrid MPI+OpenMP
- Alternatively (even preferably) you can analyse your own application!

Part III: Improving parallel scalability

- Load imbalance due to communication
- Many messages and/or large amount of data
- Expensive collectives
- I/O bottlenecks

Issue: Load imbalances

Identify the cause

- How to fix I/O related imbalance will be addressed later
- Unfortunately algorithmic, decomposition and data structure revisions are needed to fix load balance issues
 - Dynamic load balancing schemas
 - MPMD style programming
 - There may be still something we can try without code re-design

Consider hybridization (mixing OpenMP with MPI)

- Reduces the number of MPI tasks less pressure for load balance
- May be doable with very little effort
 - Just plug omp parallel do's/for's to the most intensive loops
- However, in many cases large portions of the code has to be hybridized to outperform flat MPI

Issue: Load imbalances

 Changing rank placement (on Cray and other MPI libraries based on MPICH2)

export MPICH_RANK_REORDER_METHOD=N

- These are the different values (N) that you can set it to:
 - 0: Round-robin placement
 - 1: (DEFAULT) SMP-style placement
 - 2: Folded rank placement
 - 3: Custom ordering. The ordering is specified in a file named MPICH_RANK_ORDER.
- So easy to experiment with that it should be tested with every application!
- The grid_order utility is used to generate a rank order list for use by an MPI application that uses communication between nearest neighbors in a grid
 - This output can then be copied or written into a file named MPICH_RANK_ORDER and used with MPICH_RANK_REORDER_METHOD=3
- CrayPAT is also able to make suggestions for optimal rank placement: pat_report -0 mpi_rank_order datafile.xf

Issue: Point-to-point communication consuming time

- Message transfer time

 Iatency + message size / bandwidth
 - Latency: Startup for message handling
 - Bandwidth: Network BW / number of messages using the same link
- Reduce latency by aggregating multiple small messages if possible
 - Do not pack manually but use MPI's user-defined datatypes

Bandwidth and latency depend on the used protocol

- Eager or rendezvous
 - Latency and bandwidth higher in rendezvous
- Rendezvous messages usually do not allow for overlap of computation and communication (see the extra slides for explanation), even when using non-blocking communication routines
- The platform will select the protocol basing on the message size, these limits can be adjusted

EAGER potentially allows overlapping



Data is pushed into an empty buffer(s) on the remote processor.

Data is copied from the buffer into the real receive destination when the wait or waitall is called.

Involves an extra memcopy, but much greater opportunity for overlap of computation and communication.

Further info

RENDEZVOUS does not usually overlap



Time

With rendezvous data transfer is often only occurs during the Wait or Waitall statement.

When the message arrives at the destination, the host CPU is busy doing computation, so is unable to do any message matching.

Control only returns to the library when MPI_Waitall occurs and does not return until all data is transferred.

There has been no overlap of computation and communication.

Further info

Issue: Point-to-point communication consuming time

- One way to improve performance is to send more messages using the eager protocol
 - This can be done by raising the value of the eager threshold, by setting environment variable: export MPICH_GNI_MAX_EAGER_MSG_SIZE=X
 - Values are in bytes, the default is 8192 bytes. Maximum size is 131072 bytes (128KB)
- Try to post MPI_Irecv calls before the MPI_Isend calls to avoid unnecessary buffer copies
- On Cray XE & XC: Asynchronous Progress Engine
 - Progresses also rendezvous messages on the background by launching an extra helper thread to each MPI task
 - Consult 'man mpi' and there the variable MPICH_NEMESIS_ASYNC_PROGRESS

Issue: Point-to-point communication consuming time

- Minimize the data to be communicated by carefully designing the partitioning of data and computation
- Example: domain decomposition of a 3D grid (n x n x n) with halos to be communicated, cyclic boundaries



1D decomposition ("slabs"): communication $\propto n^2 * w * 2$

2D decomposition ("tubes"): communication $\propto n^2 * p^{-1/2} * w * 4$

3D decomposition ("cubes"): communication $\propto n^2 * p^{-2/3} * w * 6$

w = halo width p = number of MPI tasks

Issue: Expensive collectives

- Reducing MPI tasks by mixing OpenMP is likely to help
- See if every all-to-all collective operation needs to be allto-all rather than one-to-all or all-to-one
 - Often encountered case: convergence checking
- See if you can live with the basic version of a routine instead of a vector version (MPI_Alltoallv etc)
 - May be faster even if some tasks would be receiving dummy data
- The MPI 3.0 introduces non-blocking collectives (MPI_lalltoall,...)
 - Allow for overlapping collectives with other operations, e.g. computation, I/O or other communication
 - Are faster (at least on Cray) than the blocking corresponds even without the overlap, and replacement is trivial

Issue: Expensive collectives

 Hand-written RDMA collectives may outperform those of the MPI library

- Fortran coarrays, Unified Parallel C, MPI one-sided communication
- On Cray XE and XC systems, the sc. DMAPP collectives will (usually significantly) improve the performance of the expensive collectives
 - Enabled by the variable: export MPICH_USE_DMAPP_COLL=1
 - Can be used selectively, e.g. export MPICH_USE_DMAPP_COLL=mpi_allreduce
 - Features some restrictions and requires explicit linking with the corresponding library and using sc. huge pages; consult 'man mpi'

Issue: Performance bottlenecks due to I/O

• Parallelize your I/O !

- MPI I/O, I/O libraries (HDF5, NetCDF), hand-written schmas,...
- Without parallelization, I/O will be a scalability bottleneck in every application

• Try to hide I/O (asynchronous I/O)





- Available on MPI I/O (MPI_File_iwrite/read(_at))
- One can also add dedicated "I/O servers" into code: separate MPI tasks or dedicating one I/O core per node on a hybrid MPI+OpenMP application

Issue: Performance bottlenecks due to I/O

• Tune filesystem (Lustre) parameters

- Lustre stripe counts & sizes, see "man lfs"
- Rule of thumb:
 - # files > # OSTs => Set stripe_count=1 You will reduce the lustre contention and OST file locking this way and gain performance
 - #files==1 => Set stripe_count=#OSTs Assuming you have more than 1 I/O client
 - #files<#OSTs => Select stripe_count so that you use all OSTs

• Use I/O buffering for all sequential I/O

- IOBUF is a library that intercepts standard I/O (stdio) and enables asynchronous caching and prefetching of sequential file access
- No need to modify the source code but just
 - Load the module iobuf
 - Rebuild your application

Case study: Single-writer I/O

• 32 MB per OST (32 MB – 5 GB) and 32 MB Transfer Size

- Unable to take advantage of file system parallelism
- Access to multiple disks adds overhead which hurts performance



Further info

Case study: Parallel I/O into a single file

- A particular code both reads and writes a 377 GB file, runs on 6000 cores
 - Total I/O volume (reads and writes) is 850 GB
 - Utilizes parallel HDF5 I/O library
- Default stripe settings: count =4, size=1M
 - 1800 s run time (~ 30 minutes)
- New stripe settings: count=-1, size=1M
 - 625 s run time (~ 10 minutes)



Issue: Performance bottlenecks due to I/O

- When using MPI and making non-contiguous writes/reads (e.g. multi-dimensional arrays), always define file views with suitable user-defined types and use collective I/O
 - Performance can be 100x compared to individual I/O



Decomposition for a 2D array

Concluding remarks

- Apply the scientific method to performance engineering: make hypotheses and measurements!
- Scaling up is the most important consideration in HPC
- Possible approaches for alleviating typical scalability bottlenecks
 - Find the optimal decomposition & rank placement
 - Overlap computation & communication use non-blocking communication operations for p2p and collective communication both!
 - Make more messages 'eager' and/or employ the Asynchronous Progress Engine (on Cray)
 - Hybridize (=mix MPI+OpenMP) the code to improve load balance and alleviate bottleneck collectives

• Mind your I/O!

- Use parallel I/O
- Tune filesystem parameters

- The file halo-exchange(.c|.f90) contains a simple benchmark that simulates the (2D) halo exchange procedure encountered in several domain-decomposition parallel algorithms
 - There are many ways to implement it with MPI see the following slides

• <u>To do</u>:

- Read the provided implementations such that you understand the difference between them
- Measure the obtained bandwidth on Lindgren (and on other platforms you may have an access to), run with e.g. 16x16=256 cores
- There are also other possibilities see if you can identify and implement them and measure their performance
- See if you can improve the performance with any of the suggested Cray MPI environment parameters
- Bonus exercise (no solution provided): Implement (and benchmark) or just sketch an equivalent scheme for a hybrid MPI+OpenMP application





Blocking 1
Send(to left)
Recv(from left)
Send(to right)
Recv(from right)
Send(to up)
Recv(from up)
Send(to down)
Recv(from down)

Blocking 2
Send(to left)
Recv(from right)
Send(to right)
Recv(from left)
Send(to up)
Recv(from down)
Send(to down)
Recv(from up)





Blocking 3
Sendrecv(to left, from right)
Sendrecv(to right, from left)
Sendrecv(to up, from down)
Sendrecv(to down, from up)



