Performance Tuning Workshop

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Workshop Set up

- Workshop – set up account at `my.osc.edu`
  - If you already have an OSC account, sign in to `my.osc.edu`
  - Go to Project
  - Project access request
  - PROJECT CODE = PZS0724
- Slides are on event page: osc.edu/events
- Workshop website: `https://www.osc.edu/~skhuvis/opt19`

Outline

- Introduction
- Debugging
- Hardware overview
- Performance measurement and analysis
- Help from the compiler
- Code tuning/optimization
- Parallel computing

Introduction

Workshop Philosophy

- Aim for “reasonably good” performance
- Discuss performance tuning techniques common to most HPC architectures
  - Compiler options
  - Code modification
- Focus on serial performance
  - Reduce time spent accessing memory
- Parallel processing
  - Multithreading
  - MPI

Hands-on Code

During this workshop, we will be using a code based on the HPCCG miniapp from Mantevo.

- Performs Conjugate Gradient (CG) method on a 3D chimney domain.
- CG is an iterative algorithm to numerically approximate the solution to a system of linear equations.
- Run code with `mpiexec -np <numprocs> ./test_HPCCG nx ny nz`, where `nx`, `ny`, and `nz` are the number of nodes in the x, y, and z dimension on each processor.
- Download with `git clone git@code.osu.edu:khuvis.1/performance2019_handson.git`
- Make sure that the following modules are loaded: `intel/18.0.3 mvapich2/2.3`

More important than Performance!

- Correctness of results
- Code readability/maintainability
- Portability - future systems
- Time to solution vs execution time

Factors Affecting Performance

- Effective use of processor features
  - High degree of internal concurrency in a single core
- Memory access pattern
  - Memory access is slow compared to computation
- File I/O
  - Use an appropriate file system
- Scalable algorithms
- Compiler optimizations
  - Modern compilers are amazing!
- Explicit parallelism

Debugging

What can a debugger do for you?

- Debuggers let you
  - execute your program one line at a time (“step”)
  - inspect variable values
  - stop your program at a particular line (“breakpoint”)
  - open a “core” file (after program crashes)
- HPC debuggers
  - support multithreaded code
  - support MPI code
  - support GPU code
  - provide a nice GUI

Compilation flags for debugging

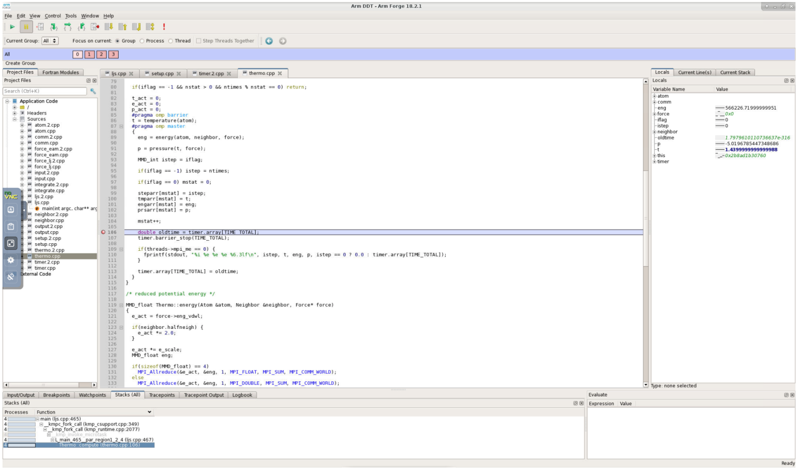
For debugging:

- Use -g flag
- Remove optimization or set to -O0
- Examples:
  - `icc -g -o mycode mycode.c`
  - `gcc -g -O0 -o mycode mycode.c`
- Use `icc -help diag` to see what compiler warnings and diagnostic options are available for the Intel compiler
- Diagnostic options can also be found by reading the `man` page of `gcc` with `man gcc`

ARM DDT

- Available on all OSC clusters
  - `module load arm-ddt`
- To run a non-MPI program from the command line:
  - `ddt --offline --no-mpi ./mycode [args]`
- To run a MPI program from the command line:
  - `ddt --offline -np num_procs ./mycode [args]`

ARM DDT



Current Group: All   Focus on current: [✓ Group] Process Thread

All 0 1 2 3

Project Files

```
Application Code
  /
  Headers
  Sources
    atom.2.cpp
    atom.cpp
    comm.2.cpp
    comm.cpp
    force_eam.2.cpp
    force_eam.cpp
    force_lj.2.cpp
    force_lj.cpp
    input.2.cpp
    input.cpp
    integrate.2.cpp
    integrate.cpp
    ljs.2.cpp
    ljs.cpp
      main(int argc, char** arg
    neighbor.2.cpp
    neighbor.cpp
    output.2.cpp
    output.cpp
    setup.2.cpp
    setup.cpp
    thermo.2.cpp
    thermo.cpp
    timer.2.cpp
    timer.cpp
External Code
```

```cpp
  if(iflag == -1 && nstat > 0 && ntimes % nstat == 0) return;

  t_act = 0;
  e_act = 0;
  p_act = 0;
  #pragma omp barrier
  t = temperature(atom);
  #pragma omp master
  {
    eng = energy(atom, neighbor, force);

    p = pressure(t, force);

    MMD_int istep = iflag;

    if(iflag == -1) istep = ntimes;

    if(iflag == 0) mstat = 0;

    steparr[mstat] = istep;
    tmparr[mstat] = t;
    engarr[mstat] = eng;
    prsarr[mstat] = p;

    mstat++;

    double oldtime = timer.array[TIME_TOTAL];
    timer.barrier_stop(TIME_TOTAL);

    if(threads->mpi_me == 0) {
      fprintf(stdout, "%i %e %e %e %6.3lf\n", istep, t, eng, p, istep == 0 ? 0.0 : timer.array[TIME_TOTAL]);
    }

    timer.array[TIME_TOTAL] = oldtime;
  }
}

/* reduced potential energy */

MMD_float Thermo::energy(Atom &atom, Neighbor &neighbor, Force* force)
{
  e_act = force->eng_vdwl;

  if(neighbor.halfneigh) {
    e_act *= 2.0;
  }

  e_act *= e_scale;
  MMD_float eng;

  if(sizeof(MMD_float) == 4)
    MPI_Allreduce(&e_act, &eng, 1, MPI_FLOAT, MPI_SUM, MPI_COMM_WORLD);
  else
    MPI_Allreduce(&e_act, &eng, 1, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);
```

Locals | Current Line(s) | Current Stack

Variable Name	Value
atom	
comm	
eng	566226.71999999951
force	0x0
iflag	0
istep	0
neighbor	
oldtime	1.7979610110736637e-316
p	-5.0196785447348686
t	1.4399999999999988
this	0x2b8ad1b30760
timer	

Stacks (All)

```
Processes  Function
4          main (ljs.cpp:465)
4            __kmpc_fork_call (kmp_csupport.cpp:349)
4              __kmp_fork_call (kmp_runtime.cpp:2077)
4                __kmp_invoke_microtask
4                  L_main_465__par_region1_2_4 (ljs.cpp:467)
4                    Thermo::compute (thermo.cpp:106)
```

Hands-on - Debugging with DDT

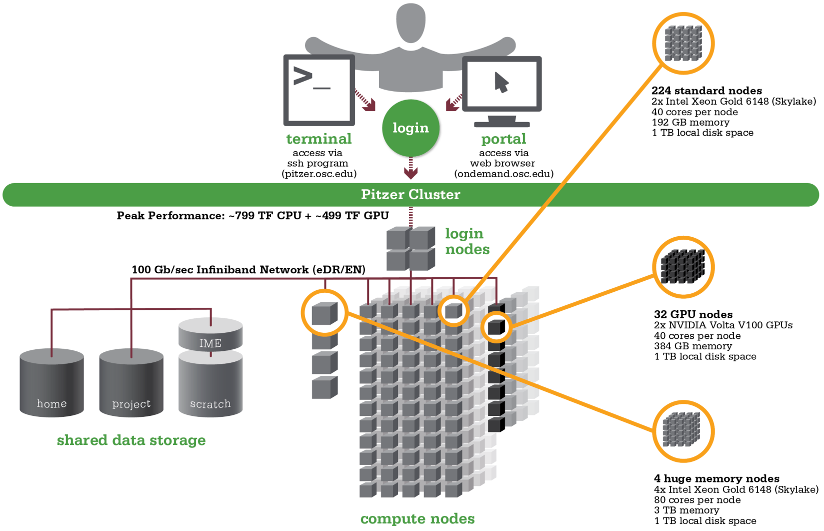
- Compile and run the code:

```
make
mpiexec -np 2 ./test_hpccg 150 150 150
```

- Debug any issues with ARM DDT:
  - Set compiler flags to `-O0 -g` (`CPP_OPT_FLAGS` in Makefile), then recompile
  - `make clean; make`
  - `module load arm-ddt`
  - `ddt -np 2 ./test_hpcg 150 150 150`

Hardware Overview

Pitzer Cluster Specification



224 standard nodes
2x Intel Xeon Gold 6148 (Skylake)
40 cores per node
192 GB memory
1 TB local disk space

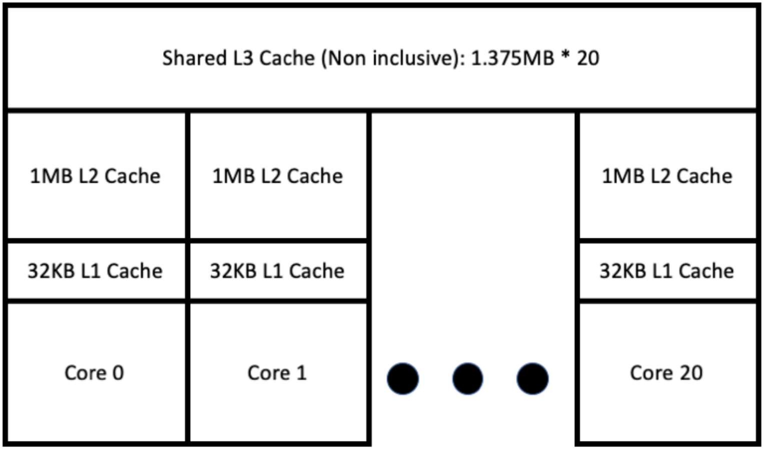
32 GPU nodes
2x NVIDIA Volta V100 GPUs
40 cores per node
384 GB memory
1 TB local disk space

4 huge memory nodes
4x Intel Xeon Gold 6148 (Skylake)
80 cores per node
3 TB memory
1 TB local disk space

Pitzer Cache Statistics

Cache level	Size (KB)	Latency (cycles)	Max BW (bytes/cycle)	Sustained BW (bytes/cycle)
L1 DCU	32	4–6	192	133
L2 MLC	1024	14	64	52
L3 LLC	28160	50–70	16	15

Pitzer Cache Structure



- L3 cache bandwidth is $\sim 5x$ bandwidth of main memory
- L2 cache bandwidth is $\sim 20x$ bandwidth of main memory
- L1 cache bandwidth is $\sim 60x$ bandwidth of main memory

Some Processor Features

- 40 cores per node
  - 20 cores per socket * 2 sockets per node
- Vector unit
  - Supports AVX512
  - Vector length 8 double or 16 single precision values
  - Fused multiply-add
- Hyperthreading
  - Hardware support for 4 threads per core
  - Not currently enabled on OSC systems

Keep data close to the processor - file systems

- **NEVER DO HEAVY I/O IN YOUR HOME DIRECTORY!**
  - Home directories are for long-term storage, not scratch files
  - One user's heavy I/O load can affect all users
- For I/O-intensive jobs
  - Local disk on compute node (not shared)
    - Stage files to and from home directory into $TMPDIR using the `pbsdcp` command (i.e. `pbsdcp file1 file2 $TMPDIR`)
    - Execute program in $TMPDIR
  - Scratch file system
    - /fs/scratch/username or $PFSDIR
    - Faster than other file systems
    - Good for parallel jobs
    - May be faster than local disk
  - For more information about OSC's filesystem see osc.edu/supercomputing/storage-environment-at-osc/available-file-systems
  - For example batch scripts showing use of $TMPDIR and $PFSDIR see osc.edu/supercomputing/batch-processing-at-osc/job-scripts

Performance measurement and analysis

What is good performance

- FLOPS
  - Floating Point OPerations per Second
- Peak performance
  - Theoretical maximum (all cores fully utilized)
  - Pitzer - 720 trillion FLOPS (720 teraflops)
- Sustained performance
  - LINPACK benchmark
    - Solves a dense system of linear equations
    - Pitzer - 543 teraflops
  - STREAM benchmark
    - Measures sustainable memory bandwidth (in MB/s) and the corresponding computation rate for vector kernels.
    - Applications are often memory-bound, meaning performance is limited by memory bandwidth of the system
    - Pitzer - Copy: 299095.01 MB/s, scale: 298741.01 MB/s, add: 331719.18 MB/s, triad: 331712.19 MB/s
- Application performance is typically much less

Performance Measurement and Analysis

- Wallclock time
  - How long the program takes to run
- Performance reports
  - Easy, brief summary
- Profiling
  - Detailed information, more involved

Timing - command line

- Time a program
  - `/usr/bin/time` command

```
/usr/bin/time j3
5415.03user 13.75system 1:30:29elapsed 99%CPU \
(0avgtext+0avgdata 0maxresident)k \
0inputs+0outputs (255major+509333minor)pagefaults 0 swaps
```

  - Note: Hardcode the path - less information otherwise
- `/usr/bin/time` gives results for
  - user time (CPU time spent running your program)
  - system time (CPU time spent by your program in system calls)
  - elapsed time (wallclock)
- % CPU = (user+system)/elapsed
- memory, pagefault, and swap statistics
- I/O statistics

Timing routines embedded in code

- Time portions of your code
  - C/C++
    - Wallclock: time(2), difftime(3), getrusage(2)
    - CPU: times(2)
  - Fortran 77/90
    - Wallclock: SYSTEM_CLOCK(3)
    - CPU: DTIME(3), ETIME(3)
  - MPI (C/C++/Fortran)
    - Wallclock: MPI_Wtime(3)

Profiling Tools Available at OSC

- Profiling tools
  - ARM Performance Reports
  - ARM MAP
  - Intel VTune
  - Intel Trace Analyzer and Collector (ITAC)
  - Intel Advisor
  - TAU Commander
  - HPCToolkit

What can a profiler show you?

- Whether code is
  - compute-bound
  - memory-bound
  - communication-bound
- How well the code uses available resources
  - Multiple cores
  - Vectorization
- How much time is spent in different parts of the code

Compilation flags for profiling

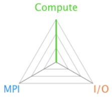
- For profiling
  - Use –g flag
  - Explicitly specify optimization level -On
  - Example: `icc -g -O3 -o mycode mycode.c`
- Use the same level of optimization you normally do
  - Bad example: `icc -g -o mycode mycode.c`
    - Equivalent to `-O0`

ARM Performance Reports

- Easy to use
  - "-g" flag not needed - works on precompiled binaries
- Gives a summary of your code's performance
  - view report with browser
- For a non-MPI program:
  - `module load arm-pr`
  - `perf-report --no-mpi ./mycode [args]`
- For an MPI program:
  - `perf-report -np num_procs ./mycode [args]`

arm PERFORMANCE REPORTS

Command:	/fs/project/PZS0720/skhuvis/SETSM/setsm dataset/WV01_15MAY080613301-P1BS-102001003C02A600.tif dataset/WV01_15MAY080614188-P1BS-102001003EA5DA00.tif out -outres 8 -projection ps
Resources:	1 node (40 physical, 40 logical cores per node)
Tasks:	1 process, OMP_NUM_THREADS was 28
Machine:	p0165.ten.osc.edu
Start time:	Fri Dec 28 2018 14:13:20 (UTC-05)
Total time:	372 seconds (about 6 minutes)
Full path:	/fs/project/PZS0720/skhuvis/SETSM



Summary: setsm is Compute-bound in this configuration

Compute	99.3%	Time spent running application code. High values are usually good. This is **very high**; check the CPU performance section for advice
MPI	0.0%	Time spent in MPI calls. High values are usually bad. This is **very low**; this code may benefit from a higher process count
I/O	0.7%	Time spent in filesystem I/O. High values are usually bad. This is **very low**; however single-process I/O may cause MPI wait times

This application run was Compute-bound. A breakdown of this time and advice for investigating further is in the CPU section below.

As very little time is spent in MPI calls, this code may also benefit from running at larger scales.

CPU

A breakdown of the 99.3% CPU time:

Single-core code	44.5%
OpenMP regions	55.5%
Scalar numeric ops	21.8%
Vector numeric ops	4.4%
Memory accesses	43.7%

The per-core performance is memory-bound. Use a profiler to identify time-consuming loops and check their cache performance.

Little time is spent in vectorized instructions. Check the compiler's vectorization advice to see why key loops could not be vectorized.

MPI

A breakdown of the 0.0% MPI time:

Time in collective calls	0.0%
Time in point-to-point calls	0.0%
Effective process collective rate	0.00 bytes/s
Effective process point-to-point rate	0.00 bytes/s

No time is spent in MPI operations. There's nothing to optimize here!

I/O

A breakdown of the 0.7% I/O time:

Time in reads	71.4%
Time in writes	28.6%
Effective process read rate	2.88 GB/s
Effective process write rate	3.23 GB/s

Most of the time is spent in read operations with a high effective transfer rate. It may be possible to achieve faster effective transfer rates using asynchronous file operations.

OpenMP

A breakdown of the 55.5% time in OpenMP regions:

Computation	78.5%
Synchronization	21.5%
Physical core utilization	70.0%
System load	57.9%

OpenMP thread performance looks good. Check the CPU breakdown for advice on improving code efficiency.

Memory

Per-process memory usage may also affect scaling:

Mean process memory usage	1.16 GiB
Peak process memory usage	3.70 GiB
Peak node memory usage	8.0%

The peak node memory usage is very low. Larger problem sets can be run before scaling to multiple nodes.

Energy

A breakdown of how the 19.1 Wh was used:

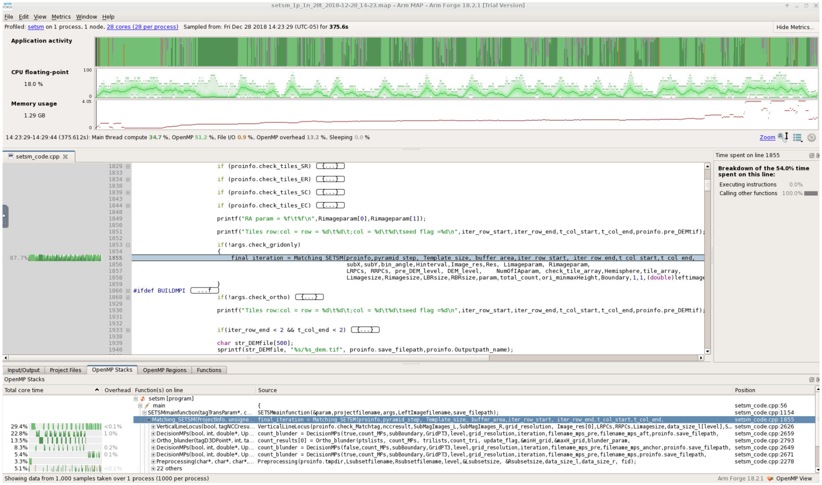
CPU	100.0%
System	not supported %
Mean node power	not supported W
Peak node power	0.00 W

The whole system energy has been calculated using the CPU energy usage.

System power metrics: No Arm IPMI Energy Agent config file found in /var/spool/ipmi-energy-agent. Did you start the Arm IPMI Energy Agent?

ARM MAP

- Interpretation of profile requires some expertise
- Gives details about your code's performance
- For a non-MPI program:
  - module load arm-map
  - `map --profile --no-mpi ./mycode [args]`
- For an MPI program:
  - `map --profile -np num_procs ./mycode [args]`
- View and explore resulting profile using ARM client


setsm_1p_1n_28t_2018-12-28_14-23.map - Arm MAP - Arm Forge 18.2.1 [Trial Version]
File Edit View Metrics Window Help
Hide Metrics...
Zoom
setsm_code.cpp
Input/Output
Project Files
OpenMP Stacks
OpenMP Regions
Functions

Profiled: setsm on 1 process, 1 node, 28 cores (28 per process) Sampled from: Fri Dec 28 2018 14:23:29 (UTC-05) for **375.6s**

Application activity

CPU floating-point 18.0 %

Memory usage 1.29 GB

14:23:29-14:29:44 (375.612s): Main thread compute 34.7 %, OpenMP 51.2 %, File I/O 0.9 %, OpenMP overhead 13.2 %, Sleeping 0.0 %

```
1829         if (proinfo.check_tiles_SR) {...}
1833
1834         if (proinfo.check_tiles_ER) {...}
1838
1839         if (proinfo.check_tiles_SC) {...}
1843
1844         if (proinfo.check_tiles_EC) {...}
1848
1849         printf("RA param = %f\t%f\n",Rimageparam[0],Rimageparam[1]);
1850
1851         printf("Tiles row:col = row = %d\t%d\t;col = %d\t%d\tseed flag =%d\n",iter_row_start,iter_row_end,t_col_start,t_col_end,proinfo.pre_DEMtif);
1852
1853         if(!args.check_gridonly)
1854         {
1855 87.7%       final_iteration = Matching_SETSM(proinfo,pyramid_step, Template_size, buffer_area,iter_row_start, iter_row_end,t_col_start,t_col_end,
1856                                     subX,subY,bin_angle,Hinterval,Image_res,Res, Limageparam, Rimageparam,
1857                                     LRPCs, RRPCs, pre_DEM_level, DEM_level,    NumOfIAparam, check_tile_array,Hemisphere,tile_array,
1858                                     Limagesize,Rimagesize,LBRsize,RBRsize,param,total_count,ori_minmaxHeight,Boundary,1,1,(double)leftimage
1859         }
1860 #ifdef BUILDMPI ...f
1868         if(!args.check_ortho) {...}
1929
1930         printf("Tiles row:col = row = %d\t%d\t;col = %d\t%d\tseed flag =%d\n",iter_row_start,iter_row_end,t_col_start,t_col_end,proinfo.pre_DEMtif);
1931
1932
1933         if(iter_row_end < 2 && t_col_end < 2) {...}
1938
1939         char str_DEMfile[500];
1940         sprintf(str_DEMfile, "%s/%s_dem.tif", proinfo.save_filepath,proinfo.Outputpath_name);
```

Time spent on line 1855

Breakdown of the 54.0% time spent on this line:

Executing instructions	0.0%
Calling other functions	100.0%

OpenMP Stacks

Total core time	Overhead	Function(s) on line	Source	Position
		setsm [program]		
		main	{	setsm_code.cpp:56
		SETSMmainfunction(tagTransParam*, c...	SETSMmainfunction(&param,projectfilename,args,LeftImagefilename,save_filepath);	setsm_code.cpp:1154
		Matching_SETSM(ProjectInfo, unsigne...	final_iteration = Matching_SETSM(proinfo,pyramid_step, Template_size, buffer_area,iter_row_start, iter_row_end,t_col_start,t_col_end,	setsm_code.cpp:1855
29.4%	<0.1%	VerticalLineLocus(bool, tagNCCresu...	VerticalLineLocus(proinfo.check_Matchtag,nccresult,SubMagImages_L,SubMagImages_R,grid_resolution, Image_res[0],LRPCs,RRPCs,Limagesize,data_size_l[level],S...	setsm_code.cpp:2626
22.8%	1.0%	DecisionMPs(bool, int, double*, Up...	count_blunder = DecisionMPs(true,count_MPs,subBoundary,GridPT3,level,grid_resolution,iteration,filename_mps_pre,filename_mps_aft,proinfo.save_filepath,	setsm_code.cpp:2659
13.5%		Ortho_blunder(tagD3DPoint*, int, ta...	count_results[0] = Ortho_blunder(ptslists, count_MPs, trilists,count_tri, update_flag,&minH_grid,&maxH_grid,blunder_param,	setsm_code.cpp:2793
8.3%	0.2%	DecisionMPs(bool, int, double*, Up...	count_blunder = DecisionMPs(false,count_MPs,subBoundary,GridPT3,level,grid_resolution,iteration,filename_mps_pre,filename_mps_anchor,proinfo.save_filepath,	setsm_code.cpp:2649
5.4%	0.1%	DecisionMPs(bool, int, double*, Up...	count_blunder = DecisionMPs(true,count_MPs,subBoundary,GridPT3,level,grid_resolution,iteration,filename_mps_pre,filename_mps,proinfo.save_filepath,	setsm_code.cpp:2671
3.3%		Preprocessing(char*, char*, char*,...	Preprocessing(proinfo.tmpdir,Lsubsetfilename,Rsubsetfilename,level,&Lsubsetsize, &Rsubsetsize,data_size_l,data_size_r, fid);	setsm_code.cpp:2278
5.1%	<0.1%	22 others		

Showing data from 1,000 samples taken over 1 process (1000 per process)

Arm Forge 18.2.1 OpenMP View

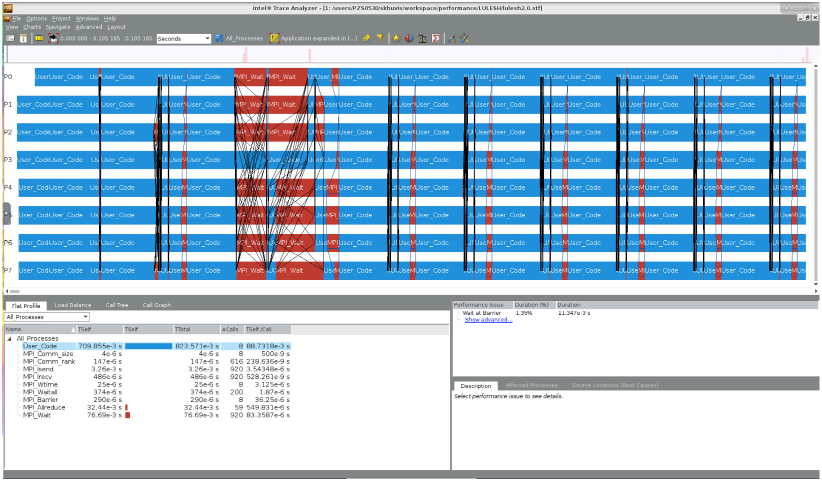
More information about ARM Tools

- www.osc.edu/resources/available_software/software_list/ARM
- www.arm.com

Intel Trace Analyzer and Collector (ITAC)

- Graphical tool for profiling MPI code (Intel MPI)
- To use:
  - `module load intelmpi # then compile (-g) code`
  - `mpiexec -trace ./mycode`
- View and explore existing results using GUI with `traceanalyzer`:
  - `traceanalyzer <mycode>.stf`

ITAC GUI


Intel® Trace Analyzer - [1: /users/PZS0530/skhuvis/workspace/performance/LULESH/lulesh2.0.stf]
File Options Project Windows Help
View Charts Navigate Advanced Layout
0.000 000 - 0.105 165 : 0.105 165
Seconds
All_Processes
Application expanded in (...)
P0
P1
P2
P3
P4
P5
P6
P7
User_Code
MPI_Wait
Flat Profile
Load Balance
Call Tree
Call Graph
All_Processes
Description
Affected Processes
Source Locations (Root Causes)

Name	TSelf	TSelf	TTotal	#Calls	TSelf /Call
All_Processes					
User_Code	709.855e-3 s		823.571e-3 s	8	88.7318e-3 s
MPI_Comm_size	4e-6 s		4e-6 s	8	500e-9 s
MPI_Comm_rank	147e-6 s		147e-6 s	616	238.636e-9 s
MPI_Isend	3.26e-3 s		3.26e-3 s	920	3.54348e-6 s
MPI_Irecv	486e-6 s		486e-6 s	920	528.261e-9 s
MPI_Wtime	25e-6 s		25e-6 s	8	3.125e-6 s
MPI_Waitall	374e-6 s		374e-6 s	200	1.87e-6 s
MPI_Barrier	290e-6 s		290e-6 s	8	36.25e-6 s
MPI_Allreduce	32.44e-3 s		32.44e-3 s	59	549.831e-6 s
MPI_Wait	76.69e-3 s		76.69e-3 s	920	83.3587e-6 s

Performance Issue	Duration (%)	Duration
Wait at Barrier	1.35%	11.347e-3 s
Show advanced...		

Select performance issue to see details.

Profiling - What to look for?

- Hot spots - where most of the time is spent
  - This is where we'll focus our optimization effort
- Excessive number of calls to short functions
  - Use inlining! (compiler flags)
- Memory usage
  - Swapping, thrashing - not allowed at OSC (job gets killed)
- CPU time vs wall time (% CPU)
  - Low CPU utilization may mean excessive I/O delays

Help from the compiler

Compiler and Language Choice

- HPC software traditionally written in Fortran or C/C++
- OSC supports several compiler families
  - Intel (icc, icpc, ifort)
    - Usually gives fastest code on Intel architecture
  - Portland Group (PGI - pgcc, pgc++, pgf90)
    - Good for GPU programming, OpenACC
  - GNU (gcc, g++, gfortran)
    - Open source, universally available

Compiler Options for Performance Tuning

- Why use compiler options?
  - Processors have a high degree of internal concurrency
  - Compilers do an amazing job at optimization
  - Easy to use - Let the compiler do the work!
  - Reasonably portable performance
- Optimization options
  - Let you control aspects of the optimization
- Warning:
  - Different compilers have different default values for options

Compiler Optimization

- Function inlining
  - Eliminate function calls
- Interprocedural optimization/analysis (ipo/ipa)
  - Same file or multiple files
- Loop transformations
  - Unrolling, interchange, splitting, tiling
- Vectorization
  - Operate on arrays of operands
- Automatic parallelization of loops
  - Very conservative multithreading

What compiler flags to try first?

- General optimization flags (-O2, -O3, -fast)
- Fast math
- Interprocedural optimization/analysis

- Profile again, look for changes
- Look for new problems/opportunities

Floating Point Speed vs. Accuracy

- Faster operations are sometimes less accurate
- Some algorithms are okay, some quite sensititive
- Intel compilers
  - Fast math by default with -O2 and -O3
  - Use `-fp-model precise` if you have a problem (slower)
- GNU compilers
  - Precise math by default with -O2 and -O3 (slower)
  - Use `-ffast-math` for faster performance

Interprocedural Optimization/Inlining

- Inlining
  - Replace a subroutine or function call with the actual body of the subprogram
- Advantages
  - Overhead of calling the subprogram is eliminated
  - More loop optimizations are possible if calls are eliminated
- One source file
  - Typically automatic with -O2 and -O3
- Multiple source files compiled separately
  - Use compiler option for compile and link phases

Optimization Compiler Options - Intel compilers

`-fast`	Common optimizations
`-On`	Set optimization level (0,1,2,3)
`-ipo`	Interprocedural optimization, multiple files
`-O3`	Loop transforms
`-xHost`	Use highest instruction set available
`-parallel`	Loop auto-parallelization

- Don't use **-fast** for MPI programs with Intel compilers
- Use same compiler command to link for **-ipo** with separate compilation
- Many other optimization options are available
- See **man** pages for details
- Recommended options: `-O3 -xHost`
- Example: `ifort -O3 program.f90`

Optimization Compiler Options - PGI compilers

`-fast`	Common optimizations
`-On`	Set optimization level (0,1,2,3,4)
`-Mipa`	Interprocedural analysis
`-Mconcur`	Loop auto-parallelization

- Many other optimization options are available
- Use same compiler command to link for -**Mipa** with separate compilation
- See **man** pages for details
- Recommended options: `-fast`
- Example: `pgf90 -fast program.f90`

Optimization Compiler Options - GNU compilers

`-On`	Set optimization level (0,1,2,3)
N/A for separate compilation	Interprocedural optimization
`-O3`	Loop transforms
`-ffast-math`	Potentially unsafe float pt optimizations
`-march=native`	Use highest instruction set available

- Many other optimization options are available
- See **man** pages for details
- Recommended options: `-O3 -ffast-math`
- Example:

```
gfortran -O3
program.f90
```

Hands-on – Compiler options

- Compile and run with different compiler options.

```
time mpiexec -np 2 ./test_hpcg 150 150 150
```

- Which compiler options give the best performance?

Hands-on - Performance Report

Now that you have selected the optimal compiler flags, get an overview of the bottlenecks in the code with the ARM performance report.

```
module load arm-pr
perf-report -np 2 ./test_hpcg 150 150 150
```

Open the html file in your browser to view the report. What are the bottlenecks in the code?

Compiler Optimization Reports

- Let you understand
  - how well the compiler is doing at optimizing your code
  - what parts of code need work
- Generated at compile time
  - Describe what optimizations were applied at various points in the source code
  - May tell you why optimizations could not be performed

Compiler Optimization Reports

- Intel compilers
  - `-qopt-report`
  - Output to a file
- Portland Group compilers
  - `-Minfo`
  - Output to stderr
- GNU compilers
  - `-fopt-info`
  - Output to stderr by default

Sample from an Optimization Report

```
LOOP BEGIN at laplace-good.f(10,7)
   remark #15542: loop was not vectorized: inner loop was already vectorized

   LOOP BEGIN at laplace-good.f(11,10)
   <Peeled loop for vectorization>
   LOOP END

   LOOP BEGIN at laplace-good.f(11,10)
      remark #15300: LOOP WAS VECTORIZED
   LOOP END

   LOOP BEGIN at laplace-good.f(11,10)
   <Remainder loop for vectorization>
      remark #15301: REMAINDER LOOP WAS VECTORIZED
   LOOP END

   LOOP BEGIN at laplace-good.f(11,10)
   <Remainder loop for vectorization>
   LOOP END
LOOP END
```

Hands-on - Optimization Report

Add the `-qopt-report=5` compiler flag and recompile to view an optimization report.

A word about algorithms

- Problem-dependent - can't generalize
- Scalability is important
  - How computational time increases with problem size
- Replace with an equivalent algorithm of lower complexity
- Replace home-grown algorithm with call to optimized library

Code tuning and optimization

Code modifications for Optimization

- Memory optimizations
  - Unit stride memory access
  - Efficient cache usage
- Vectorization
  - Vectorizable loops
  - Vectorization inhibitors

Unit Stride Memory Access

- Often the most important factor in your code's performance!!!
- Loops that work with arrays should use a stride of one whenever possible
- C, C++ are ***row-major***, in a 2D array, they store elements consecutively by row:
  - First array index should be outermost loop
  - Last array index should be innermost loop
- Fortran is ***column-major***, so the reverse is true:
  - Last array index should be outermost loop
  - First array index should be innermost loop
- Avoid arrays of derived data types, structs, or classes (i.e. use struct of arrays (SoA) instead of arrays of structures (AoS))

Data Layout: Object-Oriented Languages

- Arrays of objects may give poor performance on HPC systems if used naively
  - C structs
  - C++ classes
  - Fortran 90 user-defined types
- Inefficient use of cache - not unit stride
  - Can often get factor of 3 or 4 speedup just by fixing it
- You can use them efficiently! Be aware of data layout
- Data layout may be the only thing modern compilers can't optimize

Efficient Cache Usage

- Cache lines
  - 8 words (64 bytes) of consecutive memory
  - Entire cache line is loaded when a piece of data is fetched
- Good example - Entire cache line used
  - 2 cache lines used for every 8 loop iterations
  - Unit stride

```
real*8 a(N), b(N)
do i=1,N
  a(i)=a(i)+b(i)
end do
```

```
2 cache lines:
a(1),a(2),a(3),...a(8)
b(1),b(2),b(3),...b(8)
```

Efficient Cache Usage - Cache Lines (cont.)

- Bad example - Unneeded data loaded
    - 1 cache line loaded for *each* loop iteration
    - 8 words loaded, only 2 words used
    - Not unit stride

```
TYPE :: node
  real*8 a, b, c, d, w, x, y, z
END TYPE node
TYPE(node) :: s(N)
do i=1,N
  s(i)%a = s(i)%a + s(i)%b
end do
```

```
cache line:
a(1),b(1),c(1),d(1),w(1),x(1),y(1),z(1)
```

Hands-on - Memory utilization

- Use ARM MAP to identify the most expensive parts of the code.

```
module load arm-map
map -np 2 ./test_HPCCG 150 150 150
```

- Look for any inefficient memory access patterns.
- Modify the code to improve memory access patterns and rerun the code. Do these changes improve performance?

Vectorization/Streaming

- Code is structured to operate on arrays of operands
  - Single Instruction, Multiple Data (SIMD)
- Vector instructions built into processor (AVX512, AVX, SSE, etc.)
  - Vector length 16 single or 8 double precision on Pitzer
- Best performance with unit stride
- Fortran 90, MATLAB have this idea built in
- A vectorizable loop:

```
do i=1,N
  a(i)=b(i)+x(i)*c(i)
end do
```

Vectorization Inhibitors

- Not unit stride
  - Loops in wrong order (column-major vs. row-major)
    - Usually fixed by the compiler
  - Loops over derived types
- Function calls
  - Sometimes fixed by inlining
  - Can split loop into two loops
- Too many conditionals
  - “if” statements
- Indexed array accesses

Hands-on - Vectorization

- Look again at the most expensive parts of the code using ARM MAP.

```
module load arm-map
map -np 2 ./test_HPCCG 150 150 150
```

- Check the optimization report previosuly generated by the compiler (with `-qopt-report=5`) to see if any of the loops in the regions of the code are not being vectorized.
- Modify the code to enable vectorization and rerun the code. Do these changes improve performance?

Optimized Mathematical Libraries

- MKL (Intel Math Kernel Library)
  - BLAS
  - LAPACK
  - FFT
  - Vectorized transcendental functions (sin, cos, exp)
- AI libraries
  - Intel MKL-DNN
  - Intel DAAL
  - CuDNN
- FFTW
- ScaLAPACK
- SuperLU
- ... and many others

Parallel computing

Parallel Computing

- Multithreading
  - Shared-memory model (single node)
  - OpenMP support in compilers
- Message Passing Interface (MPI)
  - Distributed-memory model (single or multiple nodes)
  - Several available libraries
- GPUs

What is OpenMP?

- Shared-memory, threaded parallel programming model
- Portable standard
- A set of compiler directives
- A library of support functions
- Supported by vendors' compilers
  - Intel
  - Portland Group
  - GNU
  - Cray

Parallel loop execution - Fortran

- Inner loop vectorizes
- Outer loop executes on multiple threads

```
PROGRAM omploop
INTEGER, PARAMETER :: N = 1000
INTEGER i, j
REAL, DIMENSION(N,N) :: a, b, c, x
... ! Initialize arrays
!$OMP PARALLEL DO
do j=1,N
  do i=1,N
    a(i,j)=b(i,j)+x(i,j)*c(i,j)
  end do
end do
!$OMP END PARALLEL DO
END PROGRAM omploop
```

Parallel loop execution - C

- Inner loop vectorizes
- Outer loop executes on multiple threads

```
int main()
{
  int N = 1000
  float *a, *b, *c, *x
... // Allocate and initialize arrays
#pragma omp parallel for
  for (int i=0; i<N; i++) {
    for (int j=0; j<N; j++) {
      a[i*N+j]=b[i*N+j]+x[i*N+j]*c[i*N+j]
    }
  }
}
```

Compiling a program with OpenMP

- Intel compilers
  - Add the `-qopenmp` option

```
ifort -qopenmp ompex.f90 -o ompex
```

- gnu compilers
  - Add the `-fopenmp` option

```
gcc -fopenmp ompex.c -o ompex
```

- Portland group compilers
  - Add the `-mp` option

```
pgf90 -mp ompex.f90 -o ompex
```

Running an OpenMP program

- Request multiple processors through PBS
  - Example: `nodes=1:ppn=40`
- Set the `OMP_NUM_THREADS` environment variable
  - Default: Use all available cores
- For best performance run at most one thread per core
  - Otherwise too much overhead
  - Applies to typical HPC workload, exceptions exist

Running an OpenMP program - Example

```
#PBS -N omploop
#PBS -j oe
#PBS -l nodes=1:ppn=40
#PBS -l walltime=1:00

cd $PBS_O_WORKDIR
export OMP_NUM_THREADS=40
/usr/bin/time ./omploop
```

More Information about OpenMP

- www.openmp.org
- OpenMP Application Program Interface
  - Version 4.5, November 2015
  - http://www.openmp.org/wp-content/uploads/openmp-4.5.pdf
- OSC will host an XSEDE OpenMP workshop on November 5, 2019.
- Self-paced tutorial materials available from https://portal.xsede.org/online-training

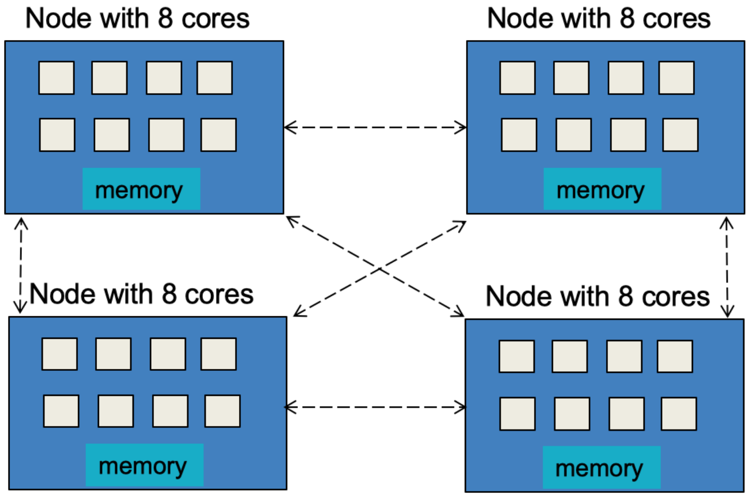
What is MPI?

- Message Passing Interface
  - Multiple processes run on one or more nodes
  - Distributed-memory model
- A message passing library
- A run-time environment
  - *mpiexec*
- Compiler wrappers
- Supported by all major parallel machine manufacturers

MPI Functions

- MPI has functions for point-to-point communication (i.e. `MPI_Send`, `MPI_Recv`)
- MPI also provides a number of functions for typical collective communication patterns, including:
  - `MPI_Bcast`: broadcasts value from root process to all other processes
  - `MPI_Reduce`: reduces values on all processes to a single value on a root process
  - `MPI_Allreduce`: reduces value on all processes to a single value and distributes the result back to all processes
  - `MPI_Gather`: gathers together values from a group of processes to a root process
  - `MPI_Alltoall`: sends data from all processes to all processes

OpenMP vs. MPI



A simple MPI program

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char *argv[])
{
    int rank,size

    MPI_Init(&argc,&argv)
    MPI_Comm_rank(MPI_COMM_WORLD,&rank)
    MPI_Comm_size(MPI_COMM_WORLD,&size)
    printf("Hello from node %d of %d\n",rank,size)
    MPI_Finalize()
    return(0)
}
```

MPI Implementations Available at OSC

- mvapich2
    - default
- Intel MPI
    - available only with Intel compilers
- OpenMPI

Compiling MPI programs

- Compile with the MPI compiler wrappers
  - `mpicc`, `mpicxx`, and `mpif90`
  - Accept the same arguments as the compilers they wrap

```
mpicc -o hello hello.c
```

- Compiler and MPI implementation depend on modules loaded

Running MPI programs

- MPI programs must run in batch only
  - Debugging runs may be done with interactive batch jobs
- ***mpiexec***
  - Automatically determines execution nodes from PBS
  - Starts the program running, 2x40=80 copies

```
#PBS -N mpi_hello
#PBS -j oe
#PBS -l nodes=2:ppn=40
#PBS -l walltime=1:00

cd $PBS_O_WORKDIR
mpiexec ./hello
```

More Information about MPI

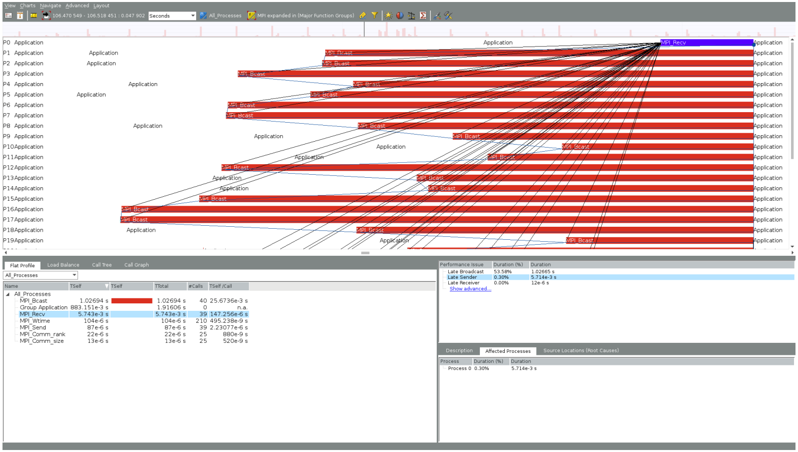
- www.mpi-forum.org
- MPI: A Message-Passing Interface Standard
  - Version 3.1, June 4, 2015
  - http://mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf
- OSC will host an XSEDE MPI workshop on September 3–4, 2019.
- Self-paced tutorial materials available from https://portal.xsede.org/online-training

Hands-on - MPI

- Use ITAC to get a timeline of the run of the code.

```
module load intelmpi
LD_PRELOAD=libVT.so \
mpiexec -trace -np 40 ./test_hpcg 150 150 150
traceanalyzer <stf_file>
```

- Look at the Event Timeline (under Charts).
- Do you see any communication patterns that could be replaced by a single MPI command?
- Do you see any performance improvement by using a single MPI command? Note: you may need to run on a larger number of nodes to see the benefits (i.e., 8 nodes).



All_Processes

Name	TSelf	TSelf	TTotal	#Calls	TSelf /Call
All_Processes					
MPI_Bcast	1.02694 s	🟥	1.02694 s	40	25.6736e-3 s
Group Application	883.151e-3 s		1.91606 s	0	n.a.
MPI_Recv	5.743e-3 s		5.743e-3 s	39	147.256e-6 s
MPI_Wtime	104e-6 s		104e-6 s	210	495.238e-9 s
MPI_Send	87e-6 s		87e-6 s	39	2.23077e-6 s
MPI_Comm_rank	22e-6 s		22e-6 s	25	880e-9 s
MPI_Comm_size	13e-6 s		13e-6 s	25	520e-9 s

Performance Issue	Duration (%)	Duration
Late Broadcast	53.58%	1.02665 s
Late Sender	0.30%	5.714e-3 s
Late Receiver	0.00%	12e-6 s

Process	Duration (%)	Duration
Process 0	0.30%	5.714e-3 s

GPU-Accelerated Computing

- GPU = Graphics Processing Unit
  - Can be used to accelerate computation
- OSC clusters have some nodes with NVIDIA GPUs
- Many-core processors
  - more cores than multi-core
- Can be programmed with CUDA
  - low level
- PGI and GNU compilers support OpenACC
  - easier than CUDA
  - similar to OpenMP

Summary: What should you do with your code?

- Experiment with compiler optimization flags
- Profile it
- Read optimization reports
- Analyze data layout, memory access patterns
- Examine algorithms
  - Complexity
  - Availability of optimized version
- Look for potential parallelism and any inhibitors to parallelism
  - Improve vectorization

Resources to get your questions answered

FAQs: osc.edu/resources/getting_started/supercomputing_faq
HOW TOs: osc.edu/resources/getting_started/howto

Performance Collection Guide:
osc.edu/resources/getting_started/howto/howto_collect_performance_data_for_your_program

Office Hours:
go.osu.edu/rc-osc Tuesdays 1-3 p.m. or Weekdays 4-5 at Pomerene Hall

System updates:

- Read Message of the Day on login
- Follow @HPCNotices on Twitter

Other Sources of Information

- Online manuals
  - `man ifort`
  - `man pgc++`
  - `man gcc`
- Related workshop courses
  - www.osc.edu/supercomputing/training
- Online tutorials from Cornell
  - https://cvw.cac.cornell.edu/
- oschelp@osc.edu

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