

Introduction to Parallel Performance Engineering with Score-P

Marc-André Hermanns Jülich Supercomputing Centre

(with content used with permission from tutorials by Bernd Mohr/JSC and Luiz DeRose/Cray)



Performance factors of parallel applications

- Sequential performance factors
 - Computation
 - Choose right algorithm, use optimizing compiler
 - Cache and memory
 - Tough! Only limited tool support, hope compiler gets it right
 - Input / output
 - Often not given enough attention
- Parallel performance factors
 - Partitioning / decomposition
 - Communication (i.e., message passing)
 - Multithreading
 - Synchronization / locking
 - More or less understood, good tool support

VIRTUAL INSTITUTE - HIGH PRODUCTIVITY SUPERCOMPUTING

Performance engineering workflow



The 80/20 rule

- Programs typically spend 80% of their time in 20% of the code
- Programmers typically spend 20% of their effort to get 80% of the total speedup possible for the application
 - Know when to stop!
- Don't optimize what does not matter
 - Make the common case fast!

Metrics of performance

- What can be measured?
 - A count of how often an event occurs
 - E.g., the number of MPI point-to-point messages sent
 - The **duration** of some interval
 - E.g., the time spent these send calls
 - The **size** of some parameter
 - E.g., the number of bytes transmitted by these calls
- Derived metrics
 - E.g., rates / throughput
 - Needed for normalization

Example metrics

- Execution time
- Number of function calls
- CPI
 - CPU cycles per instruction
- FLOPS
 - Floating-point operations executed per second

"math" Operations? HW Operations? HW Instructions? 32-/64-bit? ...

Execution time

- Wall-clock time
 - Includes waiting time: I/O, memory, other system activities
 - In time-sharing environments also the time consumed by other applications
- CPU time
 - Time spent by the CPU to execute the application
 - Does not include time the program was context-switched out
 - Problem: Does not include inherent waiting time (e.g., I/O)
 - Problem: Portability? What is user, what is system time?
- Problem: Execution time is non-deterministic
 - Use mean or minimum of several runs

Inclusive vs. Exclusive values

- Inclusive
 - Information of all sub-elements aggregated into single value
- Exclusive
 - Information cannot be subdivided further



Classification of measurement techniques

- How are performance measurements triggered?
 - Sampling
 - Code instrumentation
- How is performance data recorded?
 - Profiling / Runtime summarization
 - Tracing

Sampling



Instrumentation



Large relative overheads for small functions

Critical issues

Accuracy

- Intrusion overhead
 - Measurement itself needs time and thus lowers performance
- Perturbation
 - Measurement alters program behaviour
 - E.g., memory access pattern
- Accuracy of timers & counters
- Granularity
 - How many measurements?
 - How much information / processing during each measurement?
- *Tradeoff: Accuracy vs. Expressiveness of data*

Classification of measurement techniques

- How are performance measurements triggered?
 - Sampling
 - Code instrumentation
- How is performance data recorded?
 - Profiling / Runtime summarization
 - Tracing

Profiling / Runtime summarization

- Recording of aggregated information
 - Total, maximum, minimum, ...
- For measurements
 - Time
 - Counts
 - Function calls
 - Bytes transferred
 - Hardware counters
- Over program and system entities
 - Functions, call sites, basic blocks, loops, ...
 - Processes, threads

Profile = summarization of events over execution interval

Types of profiles

- Flat profile
 - Shows distribution of metrics per routine / instrumented region
 - Calling context is not taken into account
- Call-path profile
 - Shows distribution of metrics per executed call path
 - Sometimes only distinguished by partial calling context (e.g., two levels)
- Special-purpose profiles
 - Focus on specific aspects, e.g., MPI calls or OpenMP constructs
 - Comparing processes/threads

Tracing

- Recording detailed information about significant points (events) during execution of the program
 - Enter / leave of a region (function, loop, ...)
 - Send / receive a message, ...
- Save information in event record
 - Timestamp, location, event type
 - Plus event-specific information (e.g., communicator, sender / receiver, ...)
- Abstract execution model on level of defined events
- Sevent trace = Chronologically ordered sequence of event records

Tracing Pros & Cons

- Tracing advantages
 - Event traces preserve the temporal and spatial relationships among individual events (@ context)
 - Allows reconstruction of **dynamic** application behaviour on any required level of abstraction
 - Most general measurement technique
 - Profile data can be reconstructed from event traces
- Disadvantages
 - Traces can very quickly become extremely large
 - Writing events to file at runtime may causes perturbation

Typical performance analysis procedure

- Do I have a performance problem at all?
 - Time / speedup / scalability measurements
- What is the key bottleneck (computation / communication)?
 - MPI / OpenMP / flat profiling
- Where is the key bottleneck?
 - Call-path profiling, detailed basic block profiling
- Why is it there?
 - Hardware counter analysis, trace selected parts to keep trace size manageable
- Does the code have scalability problems?
 - Load imbalance analysis, compare profiles at various sizes function-by-function

Score-P functionality

- Provide typical functionality for HPC performance tools
- Support all fundamental concepts of partner's tools
- Instrumentation (various methods)
- Flexible measurement without re-compilation:
 - Basic and advanced profile generation
 - Event trace recording
 - Online access to profiling data
- MPI/SHMEM, OpenMP/Pthreads, and hybrid parallelism (and serial)
- Enhanced functionality (CUDA, OpenCL, OpenACC, highly scalable I/O)

VIRTUAL INSTITUTE – HIGH PRODUCTIVITY SUPERCOMPUTING

NPB-MZ-MPI / BT instrumentation

```
# The Fortran compiler used for MPI programs
MPIF77 = mpif77
# Alternative variants to perform instrumentation
MPIF77 = scorep --user mpif77
. . .
\#MPIF77 = \$(PREP) mpif77
# This links MPI Fortran programs; usually the same as ${MPIF
        = $(MPIF77)
FITNK
. . .
```

- Edit config/make.def to adjust build configuration
 - Modify specification of compiler/linker: MPIF77

Uncomment the compiler wrapper specification

NPB-MZ-MPI / BT instrumented build

% make clean

```
% make bt-mz CLASS=C NPROCS=8
cd BT-MZ; make CLASS=C NPROCS=8 VERSION=
make: Entering directory 'BT-MZ'
cd ../sys; cc -o setparams setparams.c -lm
../sys/setparams bt-mz 8 B
scorep --user mpif77 -c -O3 -fopenmp bt.f
[...]
cd ../common; scorep --user mpif77 -c -O3 -qopenmp timers.f
scorep --user mpif77 -O3 -qopenmp -o ../bin.scorep/bt-mz_C.8 \
bt.o initialize.o exact_solution.o exact_rhs.o set_constants.o \
adi.o rhs.o zone_setup.o x_solve.o y_solve.o exch_qbc.o \
solve_subs.o z_solve.o add.o error.o verify.o mpi_setup.o \
../common/print_results.o ../common/timers.o
Built executable ../bin.scorep/bt-mz_C.8
make: Leaving directory 'BT-MZ'
```

- Return to root directory and clean-up
- Re-build executable using Score-P compiler wrapper

Summary measurement collection



- Change to the directory containing the new executable before running it with the desired configuration
- Check settings

Leave other lines commented out for the moment

Submit job

Summary measurement collection

```
% less mzmpibt scorep.<job_id>
NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP \
>Benchmark
Number of zones: 16 x 16
Iterations: 200 dt: 0.000100
Number of active processes: 8
Use the default load factors with threads
Total number of threads: 48 ( 6.0 threads/process)
Calculated speedup = 47.97
Time step
           1
 [... More application output ...]
```

 Check the output of the application run

BT-MZ summary analysis report examination



- Creates experiment directory including
 - A record of the measurement configuration (scorep.cfg)
 - The analysis report that was collated after measurement (profile.cubex)
- Interactive exploration with Cube

Congratulations!?

- If you made it this far, you successfully used Score-P to
 - instrument the application
 - analyze its execution with a summary measurement, and
 - examine it with one the interactive analysis report explorer GUIs
- In revealing the call-path profile annotated with
 - the "Time" metric
 - Visit counts
 - MPI message statistics (bytes sent/received)
- ... but how good was the measurement?
 - The measured execution produced the desired valid result
 - however, the execution took rather longer than expected!
 - even when ignoring measurement start-up/completion, therefore
 - it was probably dilated by instrumentation/measurement overhead

BT-MZ summary analysis result scoring



BT-MZ summary analysis report breakdown



BT-MZ summary analysis score

- Summary measurement analysis score reveals
 - Total size of event trace would be ${\sim}160~\text{GB}$
 - Maximum trace buffer size would be ~21 GB per rank
 - smaller buffer would require flushes to disk during measurement resulting in substantial perturbation
 - 99.9% of the trace requirements are for USR regions
 - purely computational routines never found on COM call-paths common to communication routines or OpenMP parallel regions
 - These USR regions contribute around 39% of total time
 - however, much of that is very likely to be measurement overhead for frequently-executed small routines
- Advisable to tune measurement configuration
 - Specify an adequate trace buffer size
 - Specify a filter file listing (USR) regions not to be measured

BT-MZ summary analysis report filtering



BT-MZ summary analysis report filtering

<pre>% scorep-score -r -f/config/scorep.filt \</pre>							
<pre>scorep_bt-mz_sum/profile.cubex</pre>							
flt	type	max_buf[B]	visits	time[s]	time[%]	time/visit[us]	region
-	ALL	21,476,892,880	6,583,834,153	2537.82	100.0	0.39	ALL
-	USR	21,431,996,118	6,574,793,529	1222.38	48.2	0.19	USR
-	OMP	42,257,056	8,283,136	1270.45	50.1	153.38	OMP
-	COM	2,351,570	723,560	2.99	0.1	4.13	COM
-	MPI	288,136	33,928	42.00	1.7	1237.91	MPI
*	ALL	44,928,768	9,050,465	1315.44	51.8	145.35	ALL-FLT
+	FLT	21,431,964,112	6,574,783,688	1222.37	48.2	0.19	FLT
-	OMP	42,257,056	8,283,136	1270.45	50.1	153.38	OMP-FLT
*	COM	2,351,570	723,560	2.99	0.1	4.13	COM-FLT
-	MPI	288,136	33,928	42.00	1.7	1237.91	MPI-FLT
*	USR	32,006	9,841	0.00	0.0	0.31	USR-FLT
+	USR	6,883,222,086	2,110,313,472	513.22	20.2	0.24	binvcrhs Filtered
+	USR	6,883,222,086	2,110,313,472	381.01	15.0	0.18	matmul_sub routines
+	USR	6,883,222,086	2,110,313,472	284.34	11.2	0.13	matvec_sub_ marked with
+	USR	293,617,584	87,475,200	20.34	0.8	0.23	lhsinit_ `+'
+	USR	293,617,584	87,475,200	14.82	0.6	0.17	binvrhs_
+	USR	224,028,792	68,892,672	8.64	0.3	0.13	exact_solution_
-	OMP	3,357,504	308,736	0.09	0.0	0.31	!\$omp parallel @exch_qbc.f:244

BT-MZ filtered summary measurement

```
% vi scorep.lsf
[...]
export SCOREP_EXPERIMENT_DIRECTORY=scorep_bt-mz_sum filter
export SCOREP FILTERING FILE=../config/scorep.filt
[...]
% bsub < scorep.lsf</pre>
```

 Set new experiment directory and re-run measurement with new filter configuration

```
    Submit job
```



Analysis report examination with Cube

Marc-André Hermanns Jülich Supercomputing Centre





Cube (Performance Report Browser & Tools)

- Parallel program analysis report exploration tools
 - Libraries for XML+binary report reading & writing
 - Algebra utilities for report processing
 - GUI for interactive analysis exploration
 - Requires Qt4 \geq 4.6 or Qt 5
- Originally developed as part of the Scalasca toolset
- Now available as a separate component
 - Can be installed independently of Score-P, e.g., on laptop or desktop
 - Latest release: Cube 4.3.4 (April 2016)

VIRTUAL INSTITUTE - HIGH PRODUCTIVITY SUPERCOMPUTING

Analysis presentation and exploration

- Representation of values (severity matrix) on three hierarchical axes
 - Performance property (metric)
 - Call path (program location)
 - System location (process/thread)
- Three coupled tree browsers
- Cube displays severities
 - As value: for precise comparison
 - As color: for easy identification of hotspots
 - Inclusive value when closed & exclusive value when expanded
 - Customizable via display modes





Inclusive vs. exclusive values

- Inclusive
 - Information of all sub-elements aggregated into single value
- Exclusive
 - Information cannot be subdivided further



VIRTUAL INSTITUTE - HIGH PRODUCTIVITY SUPERCOMPUTING

Analysis presentation





Automatic trace analysis with the Scalasca Trace Tools

Brian Wylie Jülich Supercomputing Centre

scalasca 🗖



Automatic trace analysis using Scalasca

Idea

- Automatic search for patterns of inefficient behaviour
- Classification of behaviour & quantification of significance
- Identification of delays as root causes of inefficiencies



- Guaranteed to cover the entire event trace
- Quicker than manual/visual trace analysis
- Parallel replay analysis exploits available memory & processors to deliver scalability

Example: "Late Sender" wait state



time

- Waiting time caused by a blocking receive operation posted earlier than the corresponding send
- Applies to blocking as well as non-blocking communication

VI-HPS

Scalasca workflow



Local setup (CLAIX)

- Load environment modules
 - Required for each shell session

```
% module load UNITE
% module load cube/4.3.4-gnu
% module load scorep/3.1-openmpi-intel-papi
% module load scalasca/2.3.1-openmpi-intel-papi
```

- Important:
 - Some Scalasca commands have a run-time dependency on Score-P & CUBE
 - Therefore also have those modules loaded when using Scalasca
 - Scalasca may need the same MPI and compiler modules as applications instrumented with Score-P

VIRTUAL INSTITUTE – HIGH PRODUCTIVITY SUPERCOMPUTING

scalasca command – One command for (almost) everything

```
<sup>9</sup> scalasca
Scalasca 2.3.1
Toolset for scalable performance analysis of large-scale parallel applications
usage: scalasca [OPTION]... ACTION <argument>...
    1. prepare application objects and executable for measurement:
       scalasca -instrument <compile-or-link-command> # skin (using scorep)
    2. run application under control of measurement system:
       scalasca -analyze <application-launch-command> # scan
    3. interactively explore measurement analysis report:
       scalasca -examine <experiment-archive report> # square
Options:
   -c, --show-config
                         show configuration summary and exit
   -h, --help
                         show this help and exit
   -n, --dry-run
                         show actions without taking them
                         show quick reference quide and exit
       --quickref
       --remap-specfile
                         show path to remapper specification file and exit
   -v, --verbose
                         enable verbose commentary
                         show version information and exit
   -V, --version
```

• The `scalasca -instrument' command is deprecated and only provided for backwards compatibility with Scalasca 1.x., recommended: use Score-P instrumenter directly

Scalasca convenience command: scan / scalasca -analyze

<pre>% scan</pre>							
Scalasca 2.3.1: measurement collection & analysis nexus							
usage: scan {options} [launchcmd [launchargs]] target [targetargs]							
where {options} may include:							
-h Help: show this brief usage message and exit.							
-v Verbose: increase verbosity.							
-n Preview: show command(s) to be launched but don't execute.							
-q Quiescent: execution with neither summarization nor tracing.							
-s Summary: enable runtime summarization. [Default]							
-t Tracing: enable trace collection and analysis.							
-a Analyze: skip measurement to (re-)analyze an existing trace.							
-e exptdir : Experiment archive to generate and/or analyze.							
(overrides default experiment archive title)							
-f filtfile : File specifying measurement filter.							
-l lockfile : File that blocks start of measurement.							
-m metrics : Metric specification for measurement.							

Scalasca measurement collection & analysis nexus

Scalasca convenience command: square / scalasca -examine

```
% square
Scalasca 2.3.1: analysis report explorer
usage: square [-v] [-s] [-f filtfile] [-F] <experiment archive | cube file>
-c <none | quick | full> : Level of sanity checks for newly created reports
-F : Force remapping of already existing reports
-f filtfile : Use specified filter file when doing scoring
-s : Skip display and output textual score report
-v : Enable verbose mode
-n : Do not include idle thread metric
```

Scalasca analysis report explorer (Cube)

Automatic measurement configuration

scan configures Score-P measurement by automatically setting some environment variables and exporting them

- E.g., experiment title, profiling/tracing mode, filter file, ...
- Precedence order:
 - Command-line arguments
 - Environment variables already set
 - Automatically determined values
- Also, scan includes consistency checks and prevents corrupting existing experiment directories
- For tracing experiments, after trace collection completes then automatic parallel trace analysis is initiated
 - Uses identical launch configuration to that used for measurement (i.e., the same allocated compute resources)

BT-MZ summary measurement collection...

```
% cd bin.scorep
```

- % cp ../jobscript/claix/scalasca.lsf .
- % vim scalasca.lsf

[...]

```
export SCOREP_FILTERING_FILE=scorep.filt
#export SCOREP_TOTAL_MEMORY=100M
#export SCOREP_METRIC_PAPI=PAPI_TOT_INS,PAPI_TOT_CYC
```

```
# Scalasca configuration
export SCAN_ANALYZE_OPTS="--time-correct"
```

```
scalasca -analyze $MPIEXEC [...] ./bt-mz_C.8
```

 Change to directory with the executable and edit the job script

Submit the job

```
% bsub < scalasca.lsf</pre>
```

BT-MZ summary analysis report examination

Score summary analysis report

% square -s scorep_bt-mz_C_8x6_sum
INFO: Post-processing runtime summarization result...
INFO: Score report written to ./scorep bt-mz C 8x6 sum/scorep.score

Post-processing and interactive exploration with Cube

% square scorep_bt-mz_C_8x6_sum INFO: Displaying ./scorep_bt-mz_C_8x6_sum/summary.cubex...

[GUI showing summary analysis report]

 The post-processing derives additional metrics and generates a structured metric hierarchy

Post-processed summary analysis report



BT-MZ trace measurement collection...

```
% cd bin.scorep
% cp ../jobscript/claix/scalasca.lsf .
% vim scalasca.lsf
[...]
export SCOREP FILTERING FILE=scorep.filt
export SCOREP TOTAL MEMORY=100M
#export SCOREP METRIC PAPI=PAPI TOT INS, PAPI TOT CYC
# Scalasca configuration
export SCAN ANALYZE OPTS="--time-correct"
scalasca -analyze -t mpiexec -np 8 ./bt-mz C.8
```

% bsub < scalasca.lsf</pre>

- Change to directory with the executable and edit the job script
- Add "-t" to the scalasca -analyze command

Set/uncomment
 scorep_тотаL_мемоку
 when more than
 16MB per process

Submit the job

BT-MZ trace measurement ... analysis



BT-MZ trace analysis report exploration

 Produces trace analysis report in the experiment directory containing trace-based wait-state metrics

% square scorep_bt-mz_C_8x6_trace INFO: Post-processing runtime summarization result... INFO: Post-processing trace analysis report... INFO: Displaying ./scorep_bt-mz_C_8x6_trace/trace.cubex...

Post-processed trace analysis report



Scalasca Trace Tools: Further information

- Collection of trace-based performance tools
 - Specifically designed for large-scale systems
 - Features an automatic trace analyzer providing wait-state, critical-path, and delay analysis
 - Supports MPI, OpenMP, POSIX threads, and hybrid MPI+OpenMP/Pthreads
- Available under 3-clause BSD open-source license
- Documentation & sources:
 - http://www.scalasca.org
- Contact:
 - mailto: scalasca@fz-juelich.de

