Gaining Insight into Parallel Program Performance using HPCToolkit

John Mellor-Crummey
Department of Computer Science
Rice University

http://hpctoolkit.org
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    – Laksono Adhianto, Mark Krentel, Scott Warren, Doug Moore
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Challenges for Computational Scientists

• Rapidly evolving platforms and applications
  — architecture
    – rapidly changing designs for compute nodes
    – significant architectural diversity
      multicore, manycore, accelerators
    – increasing parallelism within nodes
  — applications
    – exploit threaded parallelism in addition to MPI
    – leverage vector parallelism
    – augment computational capabilities

• Computational scientists need to
  — adapt codes to changes in emerging architectures
  — improve code scalability within and across nodes
  — assess weaknesses in algorithms and their implementations

Performance tools can play an important role as a guide
Performance Analysis Challenges

• Complex node architectures are hard to use efficiently
  — multi-level parallelism: multiple cores, ILP, SIMD, accelerators
  — multi-level memory hierarchy
  — result: gap between typical and peak performance is huge

• Complex applications present challenges
  — measurement and analysis
  — understanding behaviors and tuning performance

• Supercomputer platforms compound the complexity
  — unique hardware & microkernel-based operating systems
  — multifaceted performance concerns
    – computation
    – data movement
    – communication
    – I/O
What Users Want

• Multi-platform, programming model independent tools

• Accurate measurement of complex parallel codes
  — large, multi-lingual programs
  — (heterogeneous) parallelism within and across nodes
  — optimized code: loop optimization, templates, inlining
  — binary-only libraries, sometimes partially stripped
  — complex execution environments
    – dynamic binaries on clusters; static binaries on supercomputers
    – batch jobs

• Effective performance analysis
  — insightful analysis that pinpoints and explains problems
    – correlate measurements with code for actionable results
    – support analysis at the desired level
      intuitive enough for application scientists and engineers
detailed enough for library developers and compiler writers

• Scalable to petascale and beyond
Outline

- Overview of Rice’s HPCToolkit
- Pinpointing scalability bottlenecks
  - scalability bottlenecks on large-scale parallel systems
  - scaling on multicore processors
- Understanding temporal behavior
- Assessing process variability
- Understanding OpenMP performance
  - blame shifting
  - assessing variability across threads and ranks
- Other capabilities
- Today and the future
Rice University’s HPCToolkit

• Employs binary-level measurement and analysis
  — observe fully optimized, dynamically linked executions
  — support multi-lingual codes with external binary-only libraries

• Uses sampling-based measurement (avoid instrumentation)
  — controllable overhead
  — minimize systematic error and avoid blind spots
  — enable data collection for large-scale parallelism

• Collects and correlates multiple derived performance metrics
  — diagnosis often requires more than one species of metric

• Associates metrics with both static and dynamic context
  — loop nests, procedures, inlined code, calling context

• Supports top-down performance analysis
  — identify costs of interest and drill down to causes
    – up and down call chains
    – over time
HPCToolkit Workflow

source code → optimized binary

compile & link

profile execution [hpcrun]

call path profile

binary analysis [hpcstruct]

program structure

interpret profile correlate w/ source [hpcprof/hpcprof-mpi]

database

presentation [hpcviewer/hpctraceviewer]
HPCToolkit Workflow

- For dynamically-linked executables, e.g., Linux clusters
  - compile and link as you usually do: nothing special needed
- For statically-linked executables, e.g., Cray, Blue Gene/Q
  - add monitoring by using `hpclink` as prefix to your link line
Measure execution unobtrusively

— launch optimized application binaries
  — dynamically-linked: launch with `hpcrun`, arguments control monitoring
  — statically-linked: environment variables control monitoring

— collect statistical call path profiles of events of interest
Call Path Profiling

Measure and attribute costs in context
- sample timer or hardware counter overflows
- gather calling context using stack unwinding

Call path sample
- return address
- return address
- return address
- instruction pointer

Calling context tree

Overhead proportional to sampling frequency...
...not call frequency
HPCToolkit Workflow

- Analyze binary with **hpcstruct**: recover program structure
  - analyze machine code, line map, debugging information
  - extract loop nests & identify inlined procedures
  - map transformed loops and procedures to source

- Presentation
  - [hpcviewer/hpctraceviewer]

- Database
  - [hpcprof/hpcprof-mpi]

- Interpret profile correlate w/ source
  - [hpcprof/hpcprof-mpi]
HPCToolkit Workflow

- Combine multiple profiles
  - multiple threads; multiple processes; multiple executions
- Correlate metrics to static & dynamic program structure

presentation
  [hpcviewer/hpctraceviewer]

interpret profile correlate w/ source
  [hpcprof/hpcprof-mpi]

database

profile execution
  [hpcrun]

binary analysis
  [hpcstruct]

call path profile

program structure

compile & link

source code

optimized binary
• Presentation
  — explore performance data from multiple perspectives
    – rank order by metrics to focus on what’s important
    – compute derived metrics to help gain insight
      e.g. scalability losses, waste, CPI, bandwidth
  — graph thread-level metrics for contexts
  — explore evolution of behavior over time
Code-centric Analysis with hpcviewer

- function calls in full context
- inlined procedures
- inlined templates
- outlined OpenMP loops
- loops
The Problem of Scaling

Note: higher is better
Goal: Automatic Scalability Analysis

• Pinpoint scalability bottlenecks
• Guide user to problems
• Quantify the magnitude of each problem
• Diagnose the nature of the problem
Challenges for Pinpointing Scalability Bottlenecks

• Parallel applications
  — modern software uses layers of libraries
  — performance is often context dependent

Example climate code skeleton

• Monitoring
  — bottleneck nature: computation, data movement, synchronization?
  — 2 pragmatic constraints
    – acceptable data volume
    – low perturbation for use in production runs
Performance Analysis with Expectations

• You have performance expectations for your parallel code
  — strong scaling: linear speedup
  — weak scaling: constant execution time

• Put your expectations to work
  — measure performance under different conditions
    – e.g. different levels of parallelism or different inputs
  — express your expectations as an equation
  — compute the deviation from expectations for each calling context
    – for both inclusive and exclusive costs
  — correlate the metrics with the source code
  — explore the annotated call tree interactively
Pinpointing and Quantifying Scalability Bottlenecks

\[ \frac{1}{Q} \times Q - \frac{1}{P} \times P = \] coefficients for analysis of weak scaling

600K

400K

200K
scalability analysis demo

code:
university of chicago flash

simulation:
white dwarf detonation

platform:
blue gene/p

experiment:
8192 vs. 256 processors

scaling type:
weak

figures courtesy of flash team, university of chicago
Scalability Analysis of Flash (Demo)
Scalability Analysis

- Difference call path profile from two executions
  - different number of nodes
  - different number of threads
- Pinpoint and quantify scalability bottlenecks within and across nodes

significant scaling losses caused by passing data around a ring of processors
Improved Flash Scaling of AMR Setup

Graph courtesy of Anshu Dubey, U Chicago
• Profiling compresses out the temporal dimension
  — temporal patterns, e.g. serialization, are invisible in profiles

• What can we do? Trace call path samples
  — sketch:
    – N times per second, take a call path sample of each thread
    – organize the samples for each thread along a time line
    – view how the execution evolves left to right
    – what do we view?
      assign each procedure a color; view a depth slice of an execution
hpctraceviewer: detail of FLASH@256PE

Time-centric analysis: load imbalance among threads appears as different lengths of colored bands along the x axis
OpenMP: A Challenge for Tools

- Large gap between threaded programming models and their implementations

- Runtime support is necessary for tools to bridge the gap

User-level calling context for code in OpenMP parallel regions and tasks executed by worker threads is not readily available.
Challenges for OpenMP Node Programs

• Tools provide implementation-level view of OpenMP threads
  — asymmetric threads
    – master thread
    – worker thread
  — run-time frames are interspersed with user code

• Hard to understand causes of idleness
  — long serial sections
  — load imbalance in parallel regions
  — waiting for critical sections or locks
OMPT: An OpenMP Tools API

- **Goal:** a standardized tool interface for OpenMP
  - prerequisite for portable tools
  - missing piece of the OpenMP language standard

- **Design objectives**
  - enable tools to measure and attribute costs to application source and runtime system
    - support low-overhead tools based on asynchronous sampling
    - attribute to user-level calling contexts
    - associate a thread’s activity at any point with a descriptive state
  - minimize overhead if OMPT interface is not in use
    - features that may increase overhead are optional
  - define interface for trace-based performance tools
  - don’t impose an unreasonable development burden
    - runtime implementers
    - tool developers
Integrated View of MPI+OpenMP with OMPT
LLNL’s luleshMPI_OMP (8 MPI x 3 OMP), 30, REALTIME@1000

source view

thread view

metric view
Case Study: AMG2006

2 18-core Haswell
4 MPI ranks
6+3 threads per rank
<table>
<thead>
<tr>
<th>Blame-shifting: Analyze Thread Performance</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Problem</th>
<th>Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Undirected Blame Shifting</strong>&lt;sup&gt;1,3&lt;/sup&gt;</td>
<td>A thread is idle waiting for work</td>
</tr>
<tr>
<td><strong>Directed Blame Shifting</strong>&lt;sup&gt;2,3&lt;/sup&gt;</td>
<td>A thread is idle waiting for a mutex</td>
</tr>
</tbody>
</table>

<sup>1</sup>Tallent & Mellor-Crummey: PPoPP 2009

<sup>2</sup>Tallent, Mellor-Crummey, Porterfield: PPoPP 2010

<sup>3</sup>Liu, Mellor-Crummey, Fagan: ICS 2013
Blame-shifting Metrics for OpenMP

- **OMP_IDLE**
  - attribute idleness to insufficiently-parallel code being executed by other threads

- **OMP_MUTEX**
  - attribute waiting for locks to code holding the lock
    - attribute to the lock release as a proxy

- Measuring these metrics requires sampling using a time-based sample source
  - REALTIME, CPUTIME, cycles, PAPI_TOT_CYC
Blame Shifting: Idleness in AMG2006
OpenMP Tool API Status

• HPCToolkit supports OMPT interface based on OpenMP TR4

• OMPT prototype implementations
  — LLVM (emerging: OpenMP 5 TR7)
    – interoperable with GNU, Intel compilers
  — IBM LOMP (currently targets OpenMP 4.5)

• Ongoing work
  — refining OpenMP 5.0 OMPT support in LLVM
  — refining HPCToolkit to match emerging OpenMP 5 standard
Other Capabilities

- Measure hardware counters using Linux perf_events
  - available events can be listed with
    - hpcrun -L
    - launching a binary created by hpclink with environment setting
      \texttt{HPRUN\_EVENT\_LIST\_LIST}
  - frequency based sampling: 300/s per thread or machine max
    - no need to set periods or frequencies unless you want precise control
  - hardware event multiplexing
    - measure more events than hardware counters

- Kernel sampling
  - measure activity in the Linux kernel in addition to your program
    - e.g., allocating and clearing memory pages
  - not available on BG/Q
  - measurement and attribution subject to system permissions
    - detailed attribution not available on NERSC or ANL systems
Ongoing Work and Future Plans

• Ongoing work
  — compliance with emerging OpenMP 5.0 standard
    – updates to HPCToolkit, LLVM OpenMP, vendor OpenMP implementations
    – support for measurement and attribution of GPU accelerated code
  — improving support for measuring GPU-accelerated nodes
    – sampling-based measurement and analysis of CUDA and OpenMP 5
  — data-centric analysis: associate costs with variables
    – analysis and attribution of performance to optimized code
  — automated analysis to deliver performance insights

• Future plans
  — scale measurement and analysis for exascale
  — support top-down analysis methods using hardware counters
  — resource-centric performance analysis
    – within and across nodes
HPCToolkit at ALCF

• ALCF systems (vesta, cetus)
  — in your .soft file, add the following line below
    – +hpctoolkit-devel
      (this package is always the most up-to-date)
  — on theta, add the following at the head of your path
    – /projects/Tools/hpctoolkit/pkgs-theta/hpctoolkit/bin

• Man pages
  — automatically added to MANPATH by the aforementioned softenv command

• ALCF guide to HPCToolkit
  — http://www.alcf.anl.gov/user-guides/hpctoolkit

• Download binary packages for HPCToolkit’s user interfaces on your laptop
  — http://hpctoolkit.org/download/hpcviewer
Detailed HPCToolkit Documentation

http://hpctoolkit.org/documentation.html

• Comprehensive user manual:
  — Quick start guide
    – essential overview that almost fits on one page
  — Using HPCToolkit with statically linked programs
    – a guide for using hpctoolkit on BG/Q and Cray platforms
  — The hpcviewer and hpctraceviewer user interfaces
  — Effective strategies for analyzing program performance with HPCToolkit
    – analyzing scalability, waste, multicore performance ...
  — HPCToolkit and MPI
  — HPCToolkit Troubleshooting
    – why don’t I have any source code in the viewer?
    – hpcviewer isn’t working well over the network ... what can I do?

• Installation guide
An Example

- git clone https://github.com/jmellorcrummey/hpctoolkit-examples
- The repository contains the AMG2006 application benchmark
- The Makefile in the top level will build it on cetus, vesta, or theta
- The executable ‘amg2006’ is generated in the test directory with HPCToolkit’s measurement library linked in
- To launch and monitor amg2006 using HPCToolkit, use one of the provided scripts ./bgq-trace or ./theta-trace (as appropriate)
- Run a script once without arguments and the script will prompt you to add arguments, which are self-explanatory
- To analyze your measurement data
  - on theta, use the provided scripts ./theta-analyze to analyze your data in parallel
  - (for now) on BG/Q, analyze your data serially using hpcprof
Exercises

• Start with the trace
  • use the summary view to get a rough quantitative measure of OpenMP idle time
  • notice that the master and worker thread have consistent call stacks
  • look at the depth view for a MPI thread (thread 0 of an MPI process)
• Move to the profile view
  • use the flame button to see where the application spends its time
  • use the OMP_IDLE column to pinpoint where threads are idle because there is insufficient parallelism
  • graph the OMP_WORK across threads for the outermost context using the “bar chart” icon
• Additional measurements and analysis
  • use hpcprof (the sequential version of hpcprof-mpi) to analyze profiles for a single MPI rank by specifying only its measurement files as an argument to hpcprof instead of the entire measurement directory
    • e.g. hpcprof -S amg2006.hpcstruct <meas-dir>/amg2006-00000-*.*
  • use hpctoolkit to measure amg2006 using a different number of OpenMP threads and try a scaling study
• Download HPCToolkit GUIs for use on your laptop from hpctoolkit.org
Advice for Using HPCToolkit
Using HPCToolkit

- Add hpctoolkit’s bin directory to your path using softenv
- Adjust your compiler flags (if you want full attribution to src)
  - add -g flag after any optimization flags
- Add hpclink as a prefix to your Makefile’s link line
  - e.g. hpclink mpixlf -o myapp foo.o ... lib.a -lm ...
- See what sampling triggers are available on BG/Q
  - use hpclink to link your executable
  - launch executable with environment variable
    HPCRUN_EVENT_LIST=LIST
    - you can launch this on 1 core of 1 node
    - no need to provide arguments or input files for your program
    - they will be ignored
Collecting Performance Data on BG/Q

- Collecting traces on BG/Q
  - set environment variable HPCRUN_TRACE=1
  - use WALLCLOCK or PAPI_TOT_CYC as one of your sample sources when collecting a trace

- Launching your job on BG/Q using hpctoolkit
  - qsub -A ... -t 10 -n 1024 --mode c1 --proccount 16384 \ 
    --cwd `pwd` \ 
    --env OMP_NUM_THREADS=2:\ 
    HPCRUN_EVENT_LIST=WALLCLOCK@5000:\ 
    HPCRUN_TRACE=1\ 
  your_executable
Monitoring Large Executions

- Collecting performance data on every node is typically not necessary.
- Can improve scalability of data collection by recording data for only a fraction of processes.
  - Set environment variable `HPCRUN_PROCESS_FRACTION`.
  - E.g., collect data for 10% of your processes.
    - Set environment variable `HPCRUN_PROCESS_FRACTION=0.10`.
Digesting your Performance Data

• Use hpcstruct to reconstruct program structure
  — e.g. hpcstruct your_app
    – creates your_app.hpcstruct

• Correlate measurements to source code with hpcprof and hpcprof-mpi
  — run hpcprof on the front-end to analyze data from small runs
  — run hpcprof-mpi on the compute nodes to analyze data from lots of nodes/threads in parallel
    – notes
      much faster to do this on an x86_64 vis cluster (cooley) than on BG/Q
      avoid expensive per-thread profiles with --metric-db no

• Digesting performance data in parallel with hpcprof-mpi
  — qsub -A ... -t 20 -n 32 --mode c1 --proccount 32 --cwd `pwd` \ /projects/Tools/hpctoolkit/pkgs-vesta/hpctoolkit/bin/hpcprof-mpi \ -S your_app.hpcstruct \ -l /path/to/your_app/src/+ \ hpctoolkit-your_app-measurements.jobid

• Hint: you can run hpcprof-mpi on the x86_64 vis cluster (cooley)
Analysis and Visualization

• Use hpcviewer to open resulting database
  — warning: first time you graph any data, it will pause to combine info from all threads into one file

• Use hpctraceviewer to explore traces
  — warning: first time you open a trace database, the viewer will pause to combine info from all threads into one file

• Try our our user interfaces before collecting your own data
  — example performance data
    http://hpctoolkit.org/examples.html
Installing HPCToolkit GUls on your Laptop

- See http://hpctoolkit.org/download/hpcviewer
- Download the latest for your laptop (Linux, Mac, Windows)
  - hpctraceviewer
  - hpcviewer

A Note for Mac Users
When installing HPCToolkit GUls on your Mac laptop, don’t simply download and double click on the zip file and have Finder unpack them. Follow the Terminal-based installation directions on the website to avoid interference by Mac Security.
L2Unit measurement capabilities
- e.g., counts load/store activity
- node-wide counting; not thread-centric
- global or per slice counting
- supports threshold-based sampling
  - samples delivered late: about 800 cycles after threshold reached
  - each sample delivered to ALL threads/cores

HPCToolkit approach
- attribute a share of L2Unit activity to each thread context for each sample
  - e.g., when using a threshold of 1M loads and T threads, attribute 1M/T events to the active context in each thread when each sample event occurs
- best effort attribution
  - strength: correlate L2Unit activity with regions of your code
  - weakness: some threads may get blamed for activity of others
Troubleshooting Deadlock or SEGV on BG/Q

• Sadly, IBM’s PAMI (the implementation layer below MPI) and IBM’s XL OpenMP implementations have race conditions that can cause them to fail

• Measuring applications with sampling-based performance tools can increase the likelihood that the race conditions will resolve the wrong way, causing deadlock (PAMI) or failure (XL OpenMP)

• If you run into problems, the following environment variable settings can disable buggy optimizations in IBM’s software
  • PAMID_COLLECTIVES=0
  • ATOMICS_OPT_LEVEL=0

• If you don’t run into problems, don’t use these settings as they reduce performance