Analyzing Parallel Program Performance using HPCToolkit

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http://hpctoolkit.org

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  - — Research Staff
    - – Laksono Adhianto, Mark Krentel, Scott Warren, Doug Moore
  - — Students
    - – Lai Wei
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    - – Xu Liu (William and Mary, 2014)
    - – Milind Chabbi (HP Labs, 2015)
    - – Mike Fagan (Rice)

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**

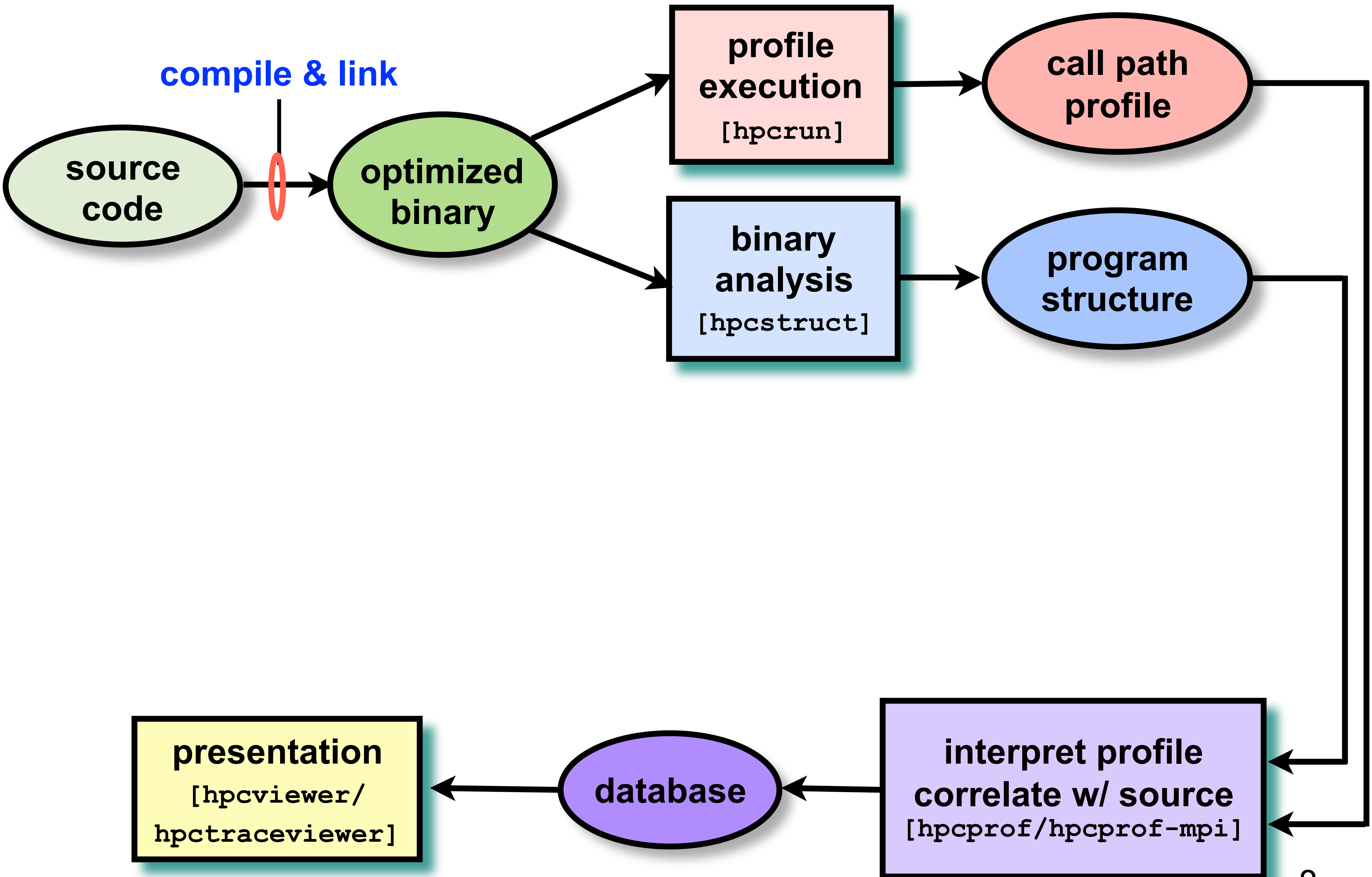
Outline

- 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 threading performance
  - blame shifting
- Today and the future

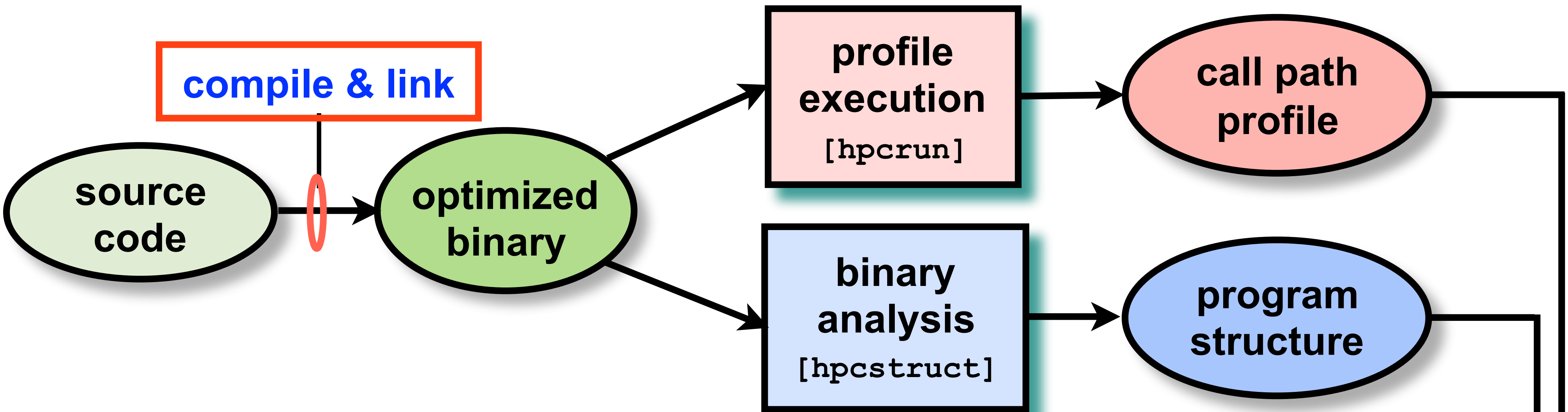
Rice University's HPCToolkit

- 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

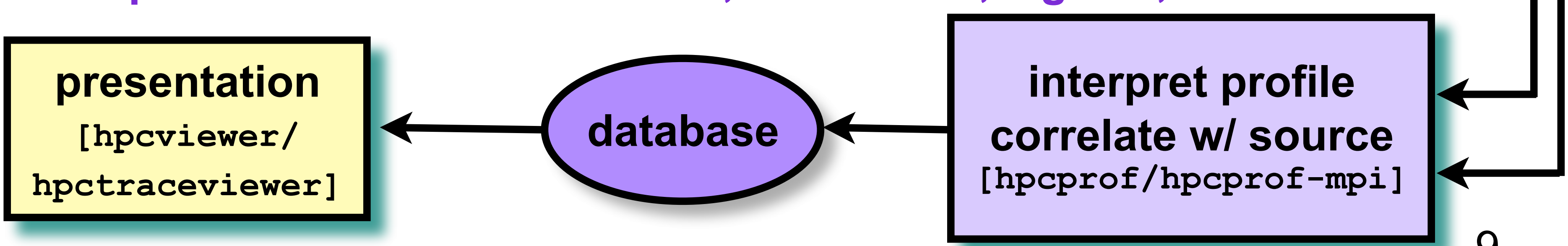
HPCToolkit Workflow



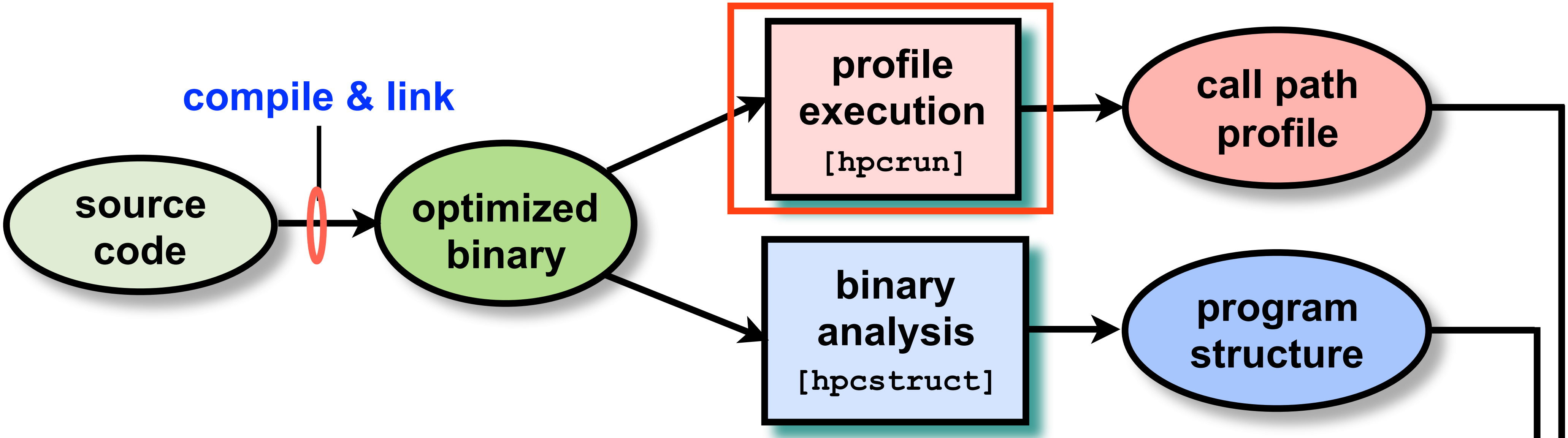
HPCToolkit Workflow



- 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
  - add monitoring by using `hpclink` as prefix to your link line
    - uses "linker wrapping" to catch "control" operations
      process and thread creation, finalization, signals, ...

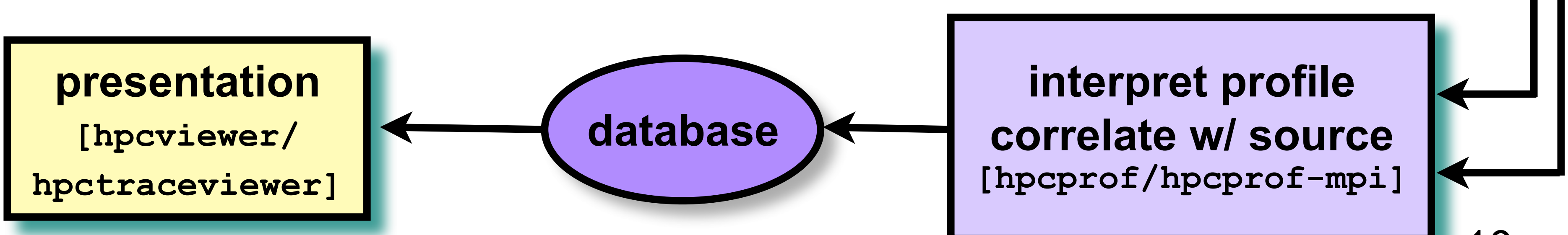


HPCToolkit Workflow



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

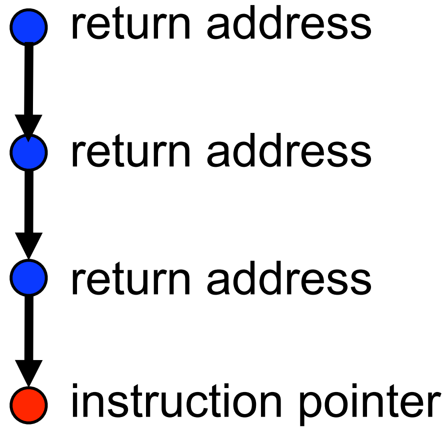


Call Path Profiling

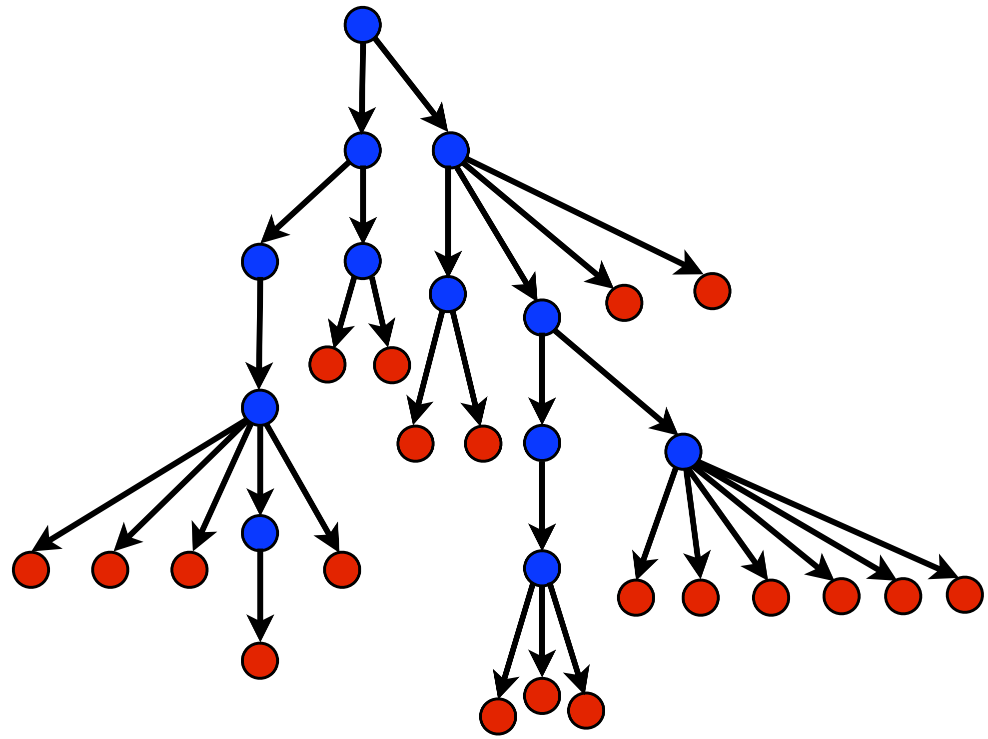
Measure and attribute costs in context

- **sample timer or hardware counter overflows**
- **gather calling context using stack unwinding**

Call path sample

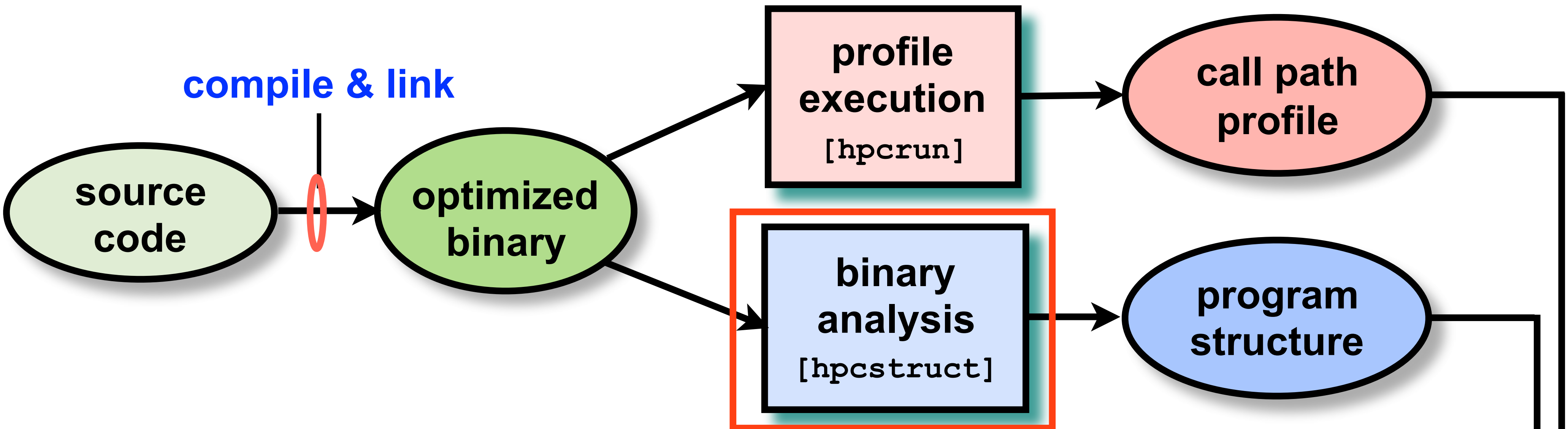


Calling context tree

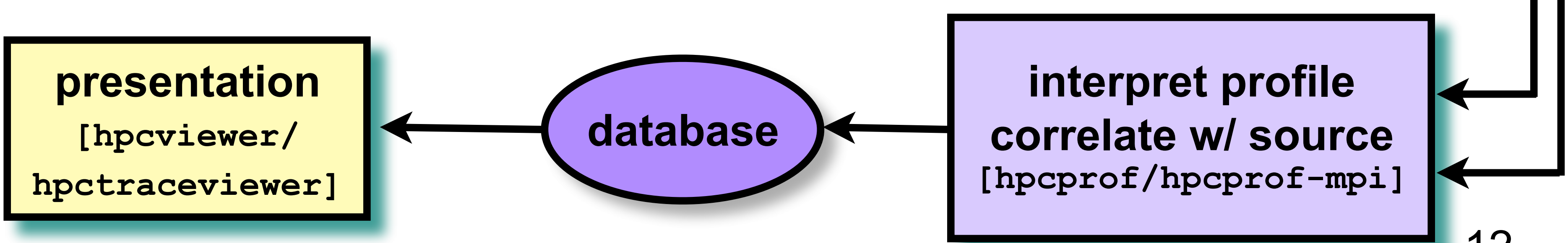


Overhead proportional to sampling frequency...
...not call frequency

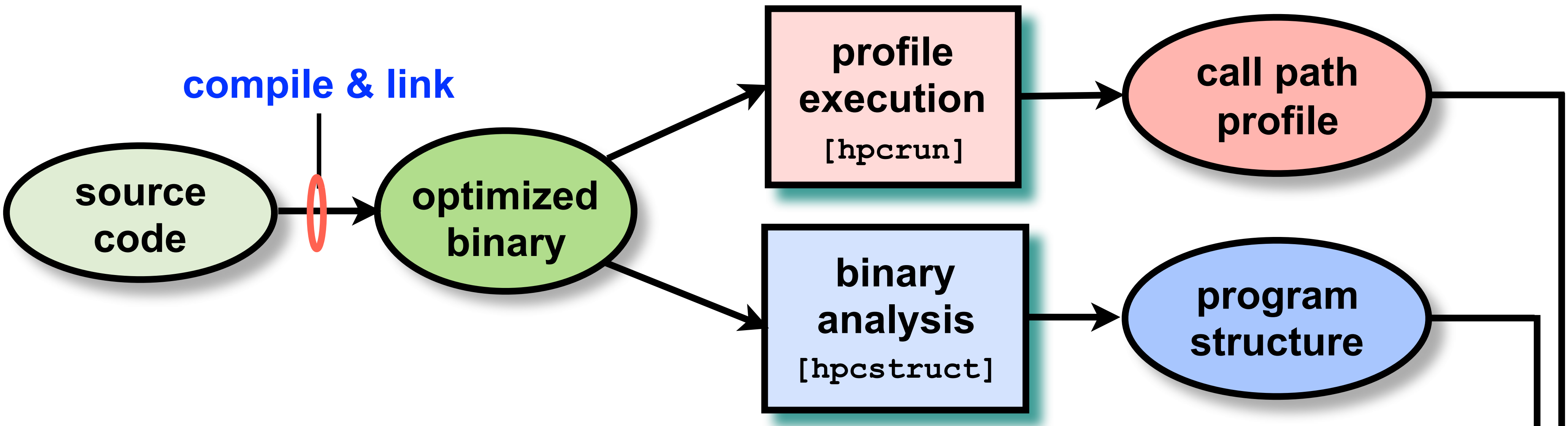
HPCToolkit Workflow



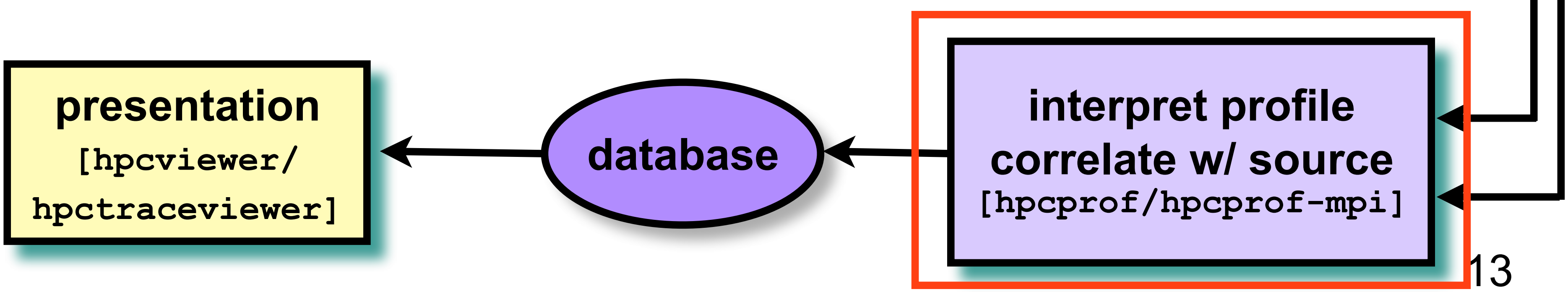
- **Analyze binary with `hpcstruct`: recover program structure**
  - — analyze machine code, line map, debugging information
  - — extract loop nests & identify inlined procedures
  - — map transformed loops and procedures to source



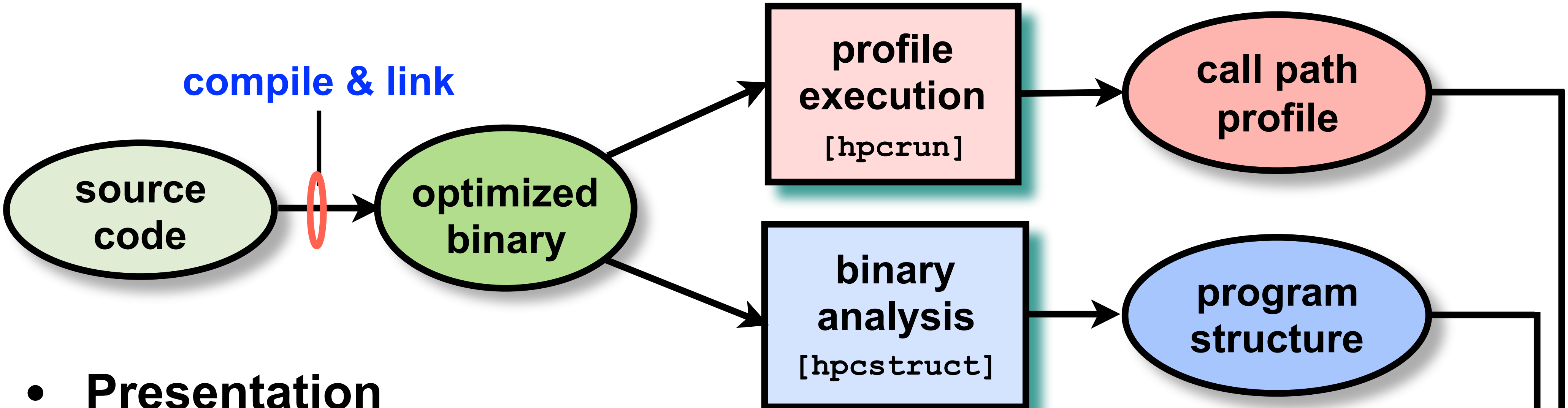
HPCToolkit Workflow



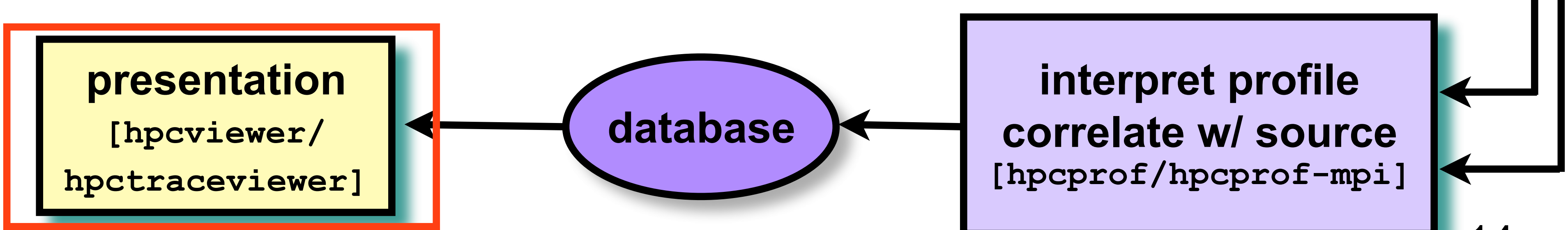
- **Combine multiple profiles**
  - multiple threads; multiple processes; multiple executions
- **Correlate metrics to static & dynamic program structure**



HPCToolkit Workflow

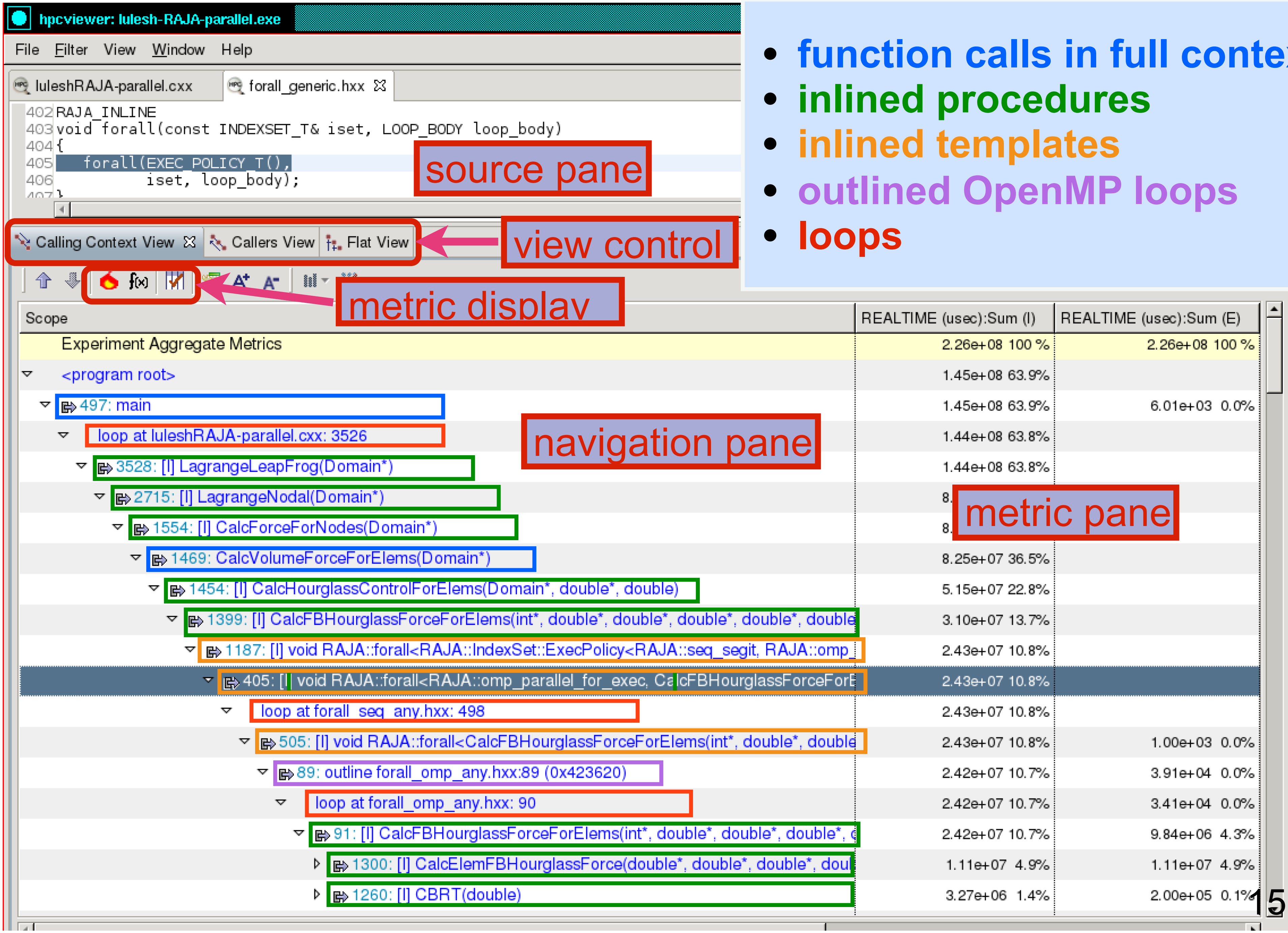


- **Presentation**
  - — explore performance data from multiple perspectives
    - – rank order by metrics to focus on what's important
    - – compute derived metrics to help gain insight
      - e.g. scalability losses, waste, CPI, bandwidth
  - — graph thread-level metrics for contexts
  - — explore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

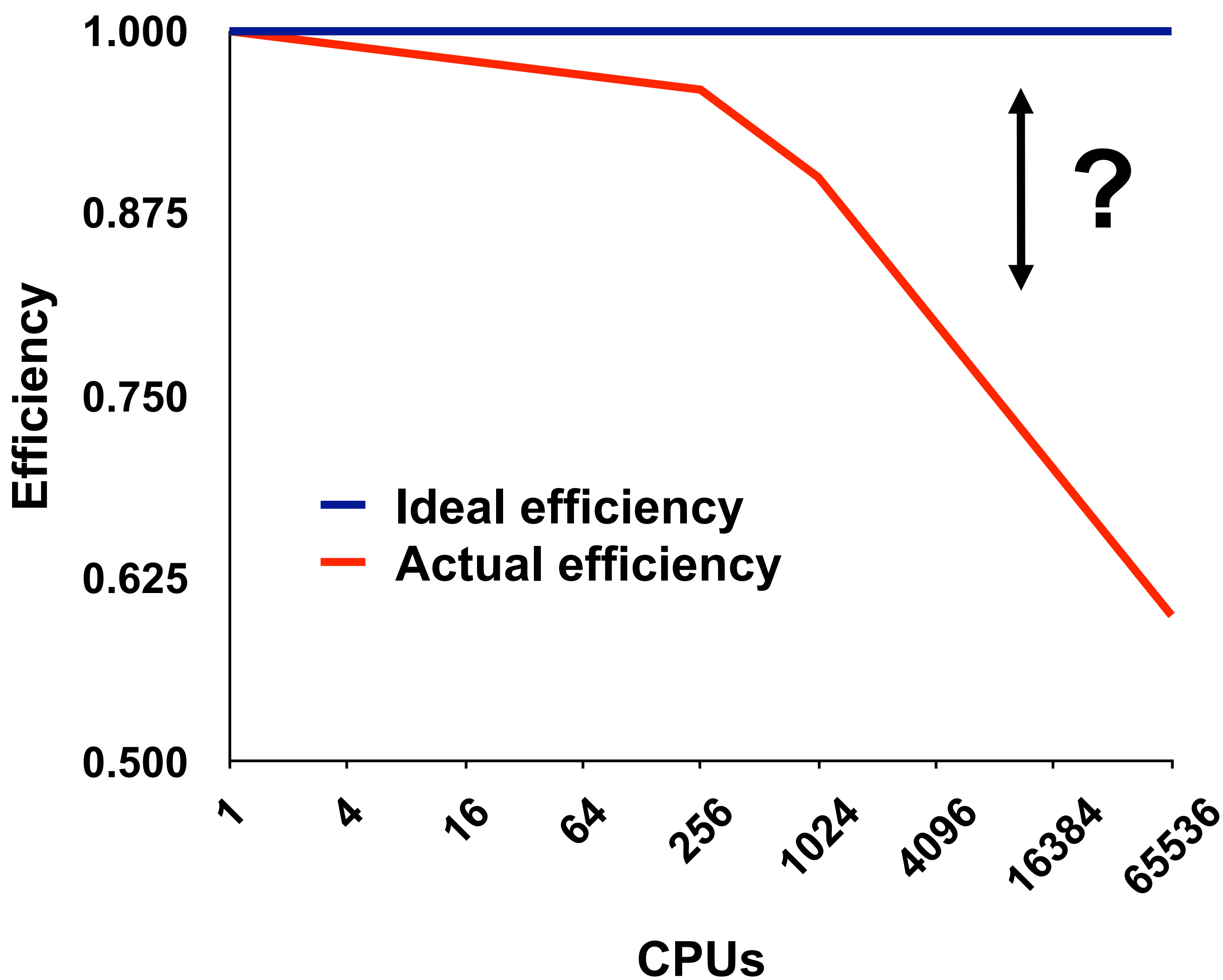


Code-centric Analysis with hpcviewer

- function calls in full context
- inlined procedures
- inlined templates
- outlined OpenMP loops
- loops



The Problem of Scaling



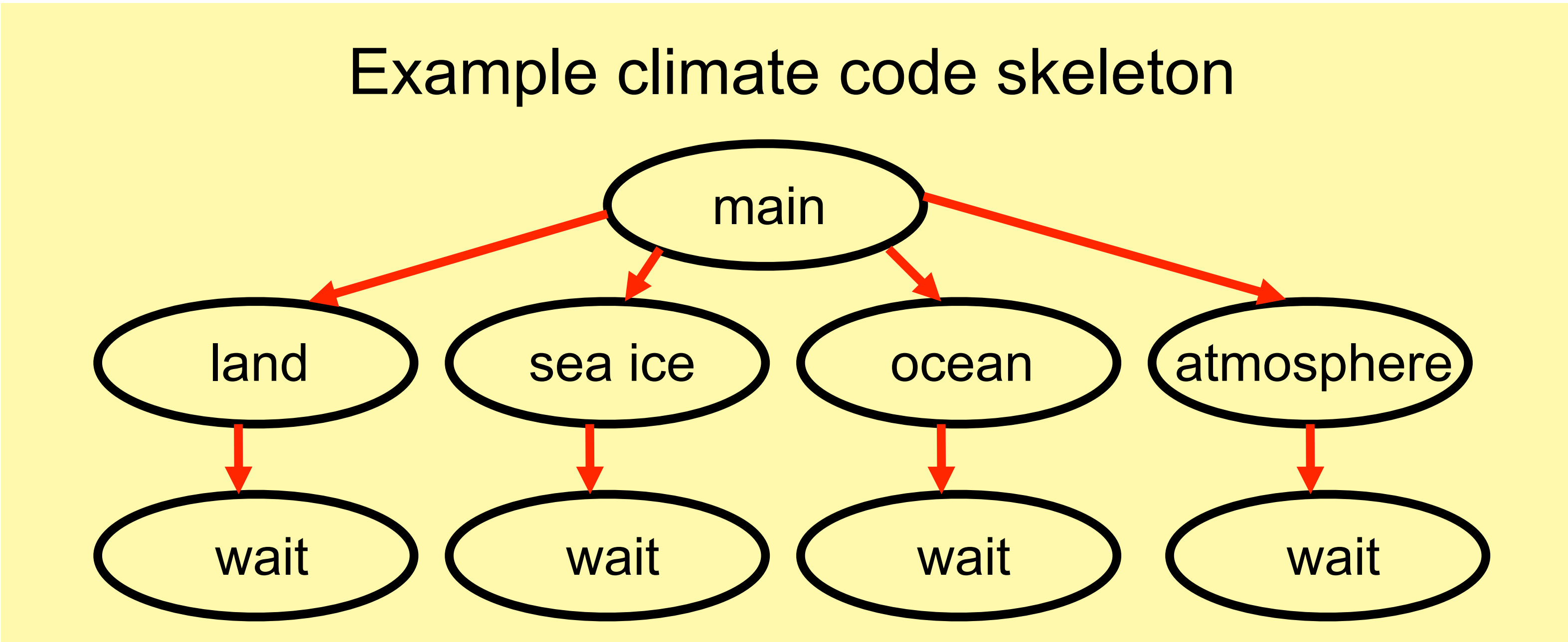
Note: higher is better

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**



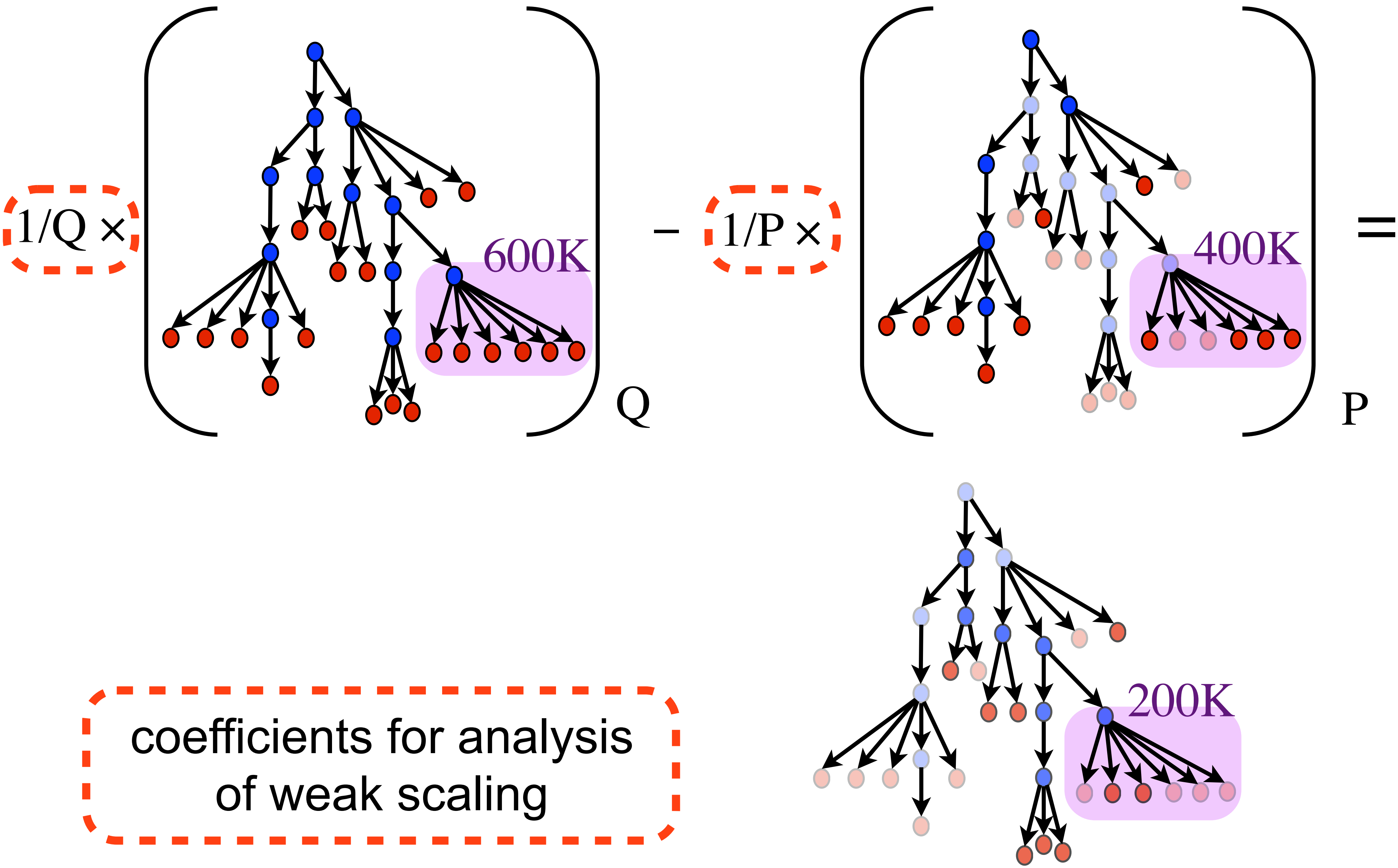
- **Monitoring**
  - — **bottleneck nature: computation, data movement, synchronization?**
  - — **2 pragmatic constraints**
    - – **acceptable data volume**
    - – **low perturbation for use in production runs**

Performance Analysis with Expectations

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

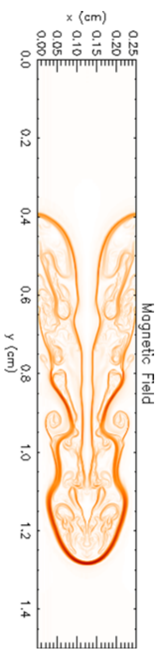
- Put your expectations to work
  - measure performance under different conditions
    - e.g. different levels of parallelism or different inputs
  - express your expectations as an equation
  - compute the deviation from expectations for each calling context
    - for both inclusive and exclusive costs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

Pinpointing and Quantifying Scalability Bottlenecks

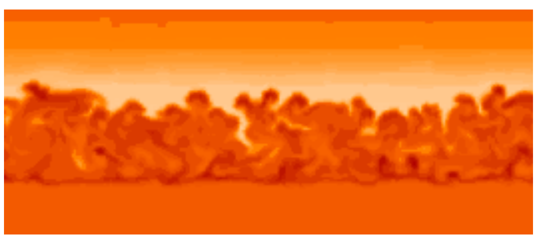


Scalability Analysis Demo

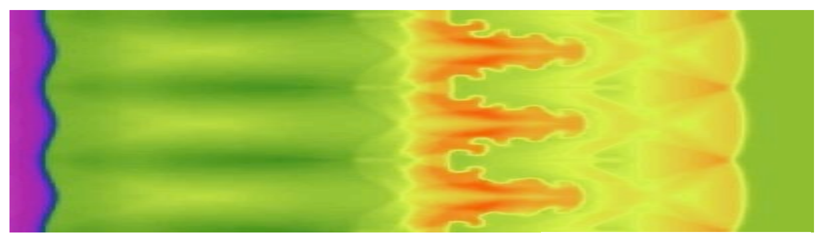
Code: University of Chicago FLASH
Simulation: white dwarf detonation
Platform: Blue Gene/P
Experiment: 8192 vs. 256 processors
Scaling type: weak



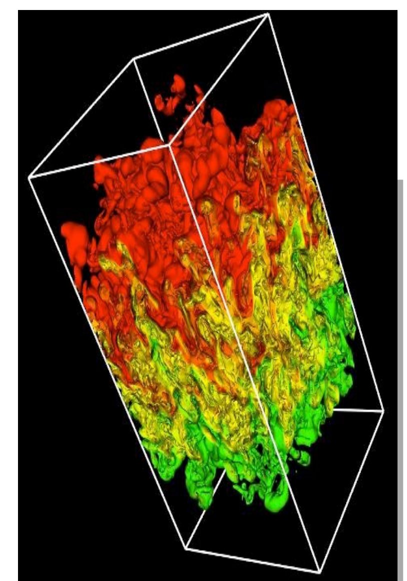
Magnetic Rayleigh-Taylor



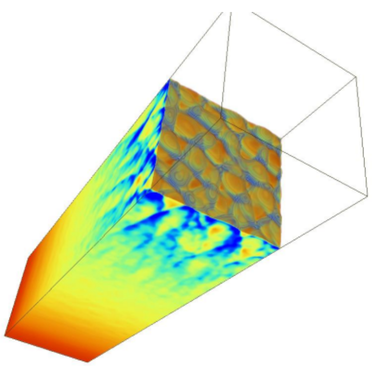
Nova outbursts on white dwarfs



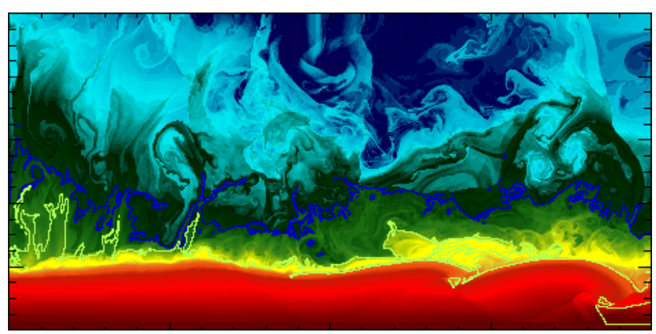
Laser-driven shock instabilities



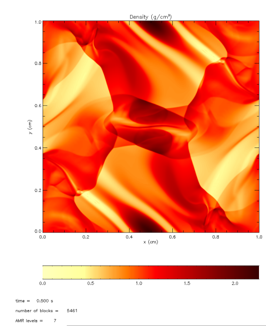
Rayleigh-Taylor instability



Cellular detonation



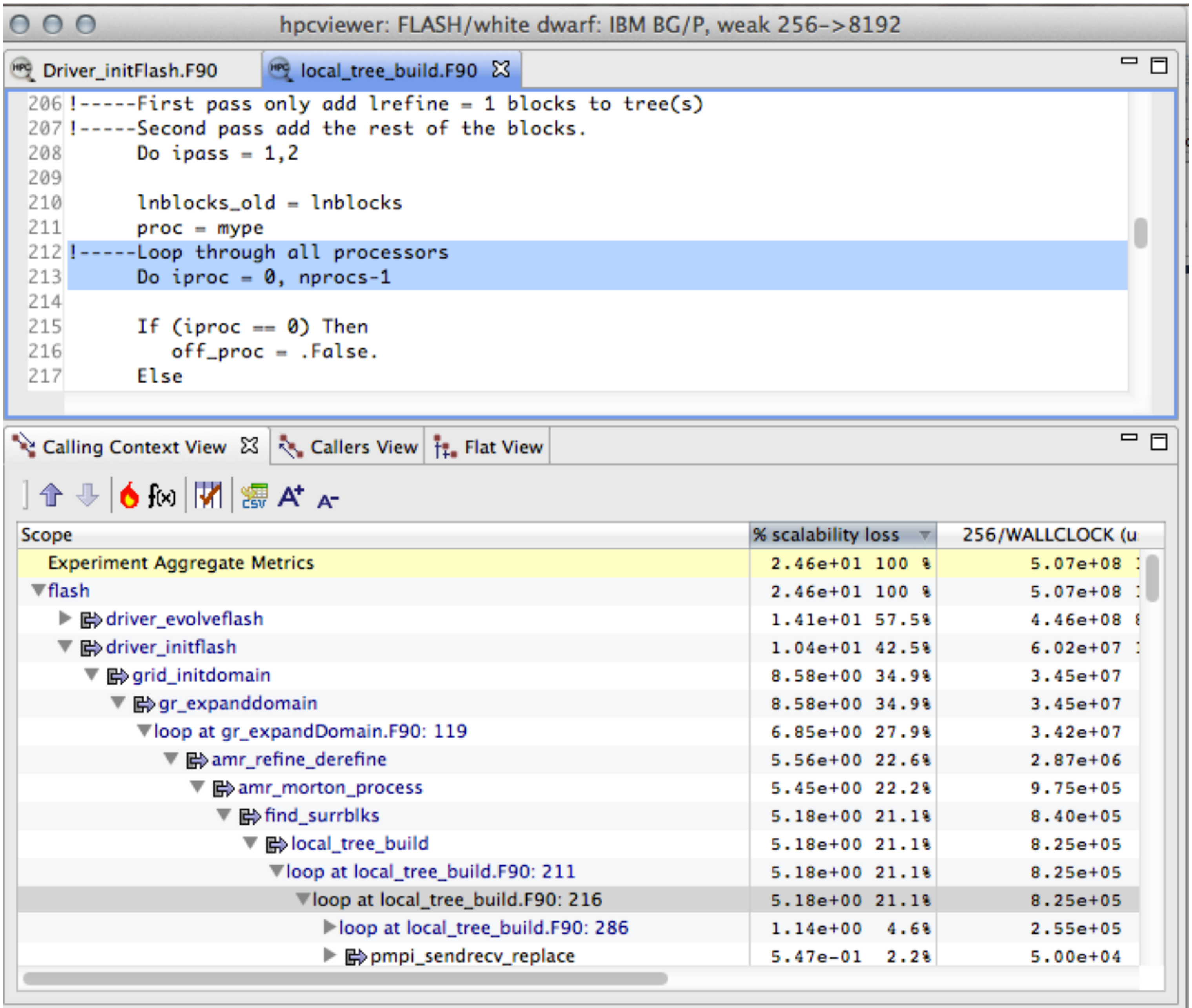
Helium burning on neutron stars



Orzag/Tang MHD vortex

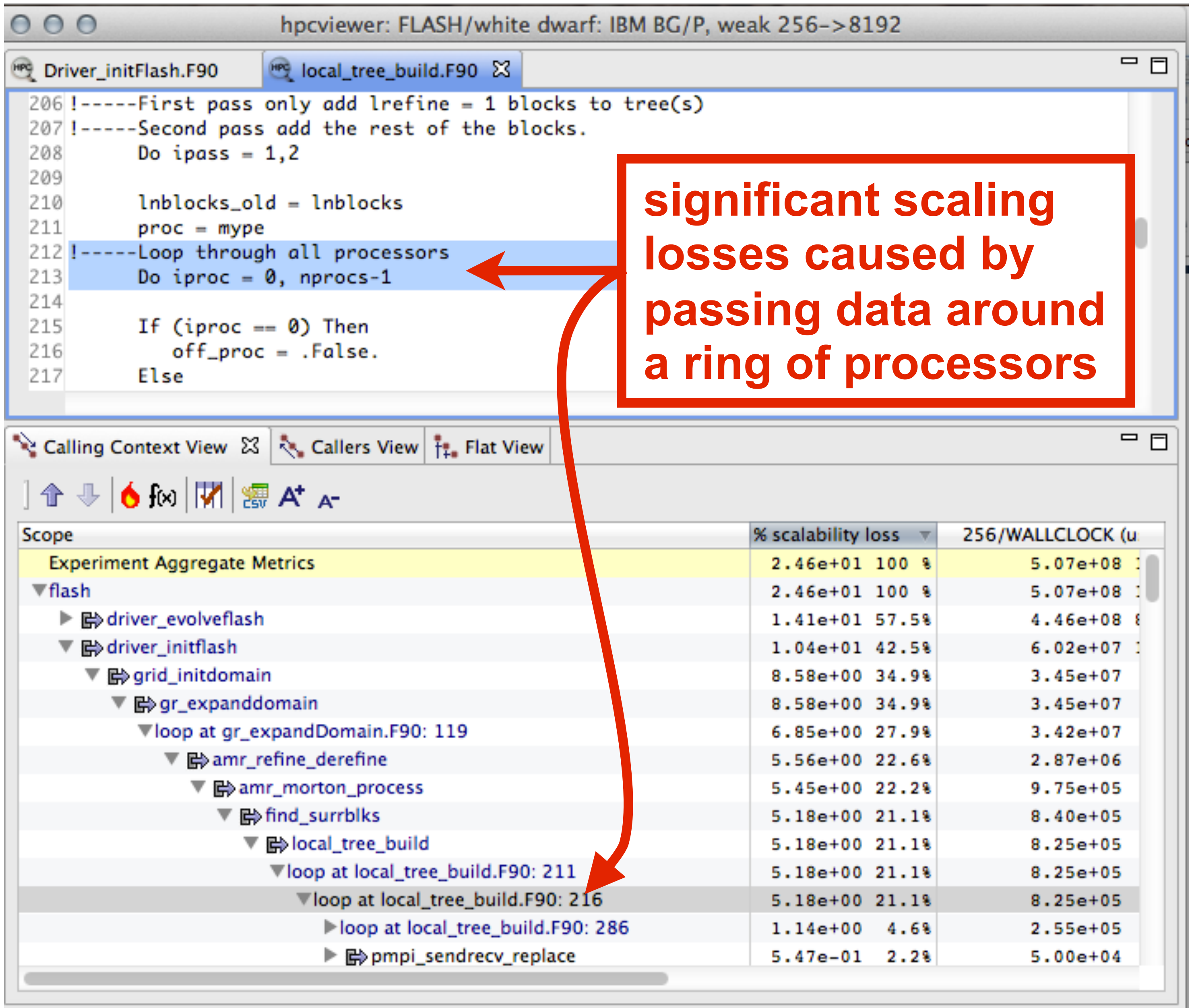
Figures courtesy of FLASH Team, University of Chicago

Scalability Analysis of Flash (Demo)

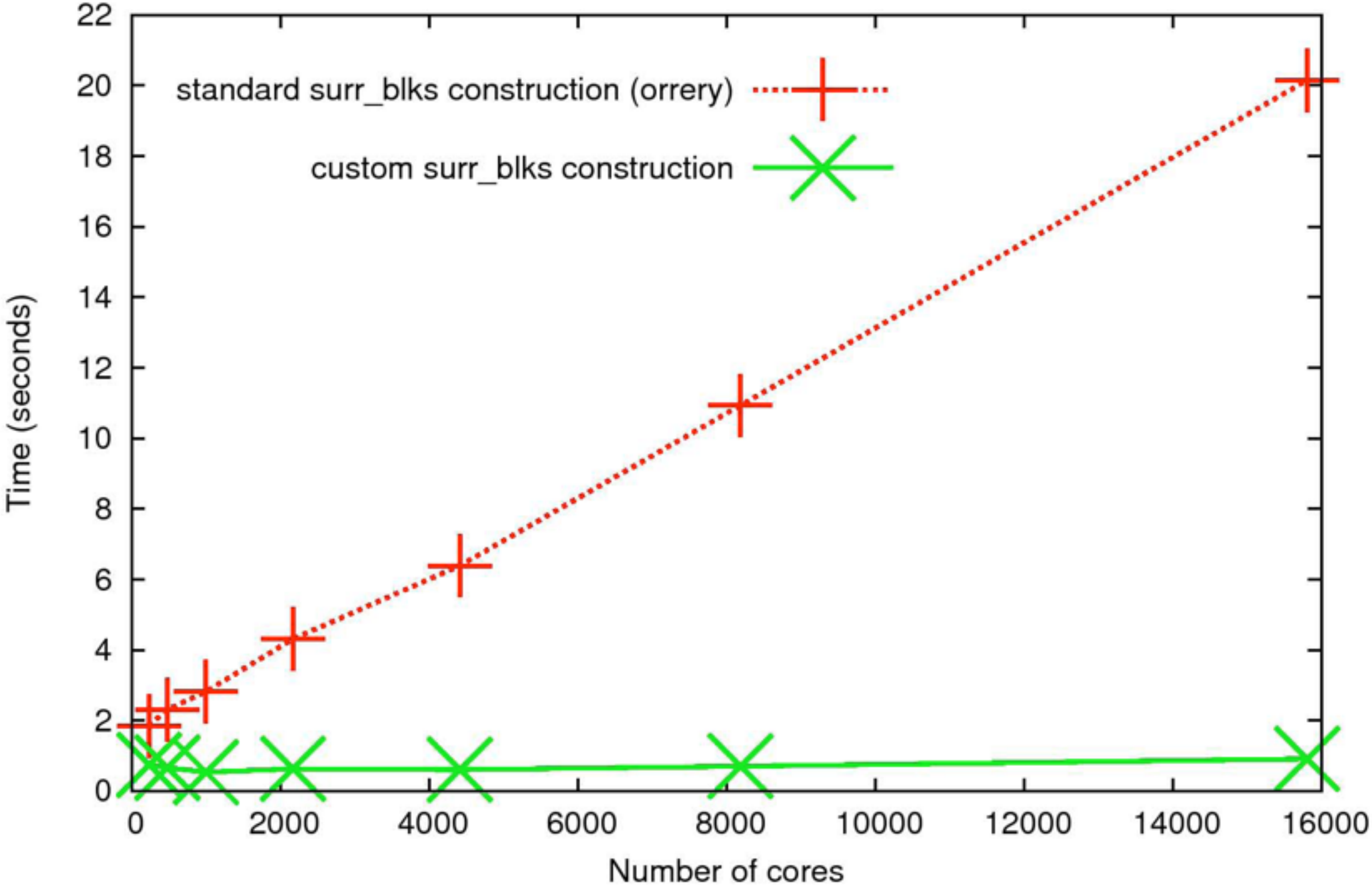


Scalability Analysis

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



Improved Flash Scaling of AMR Setup

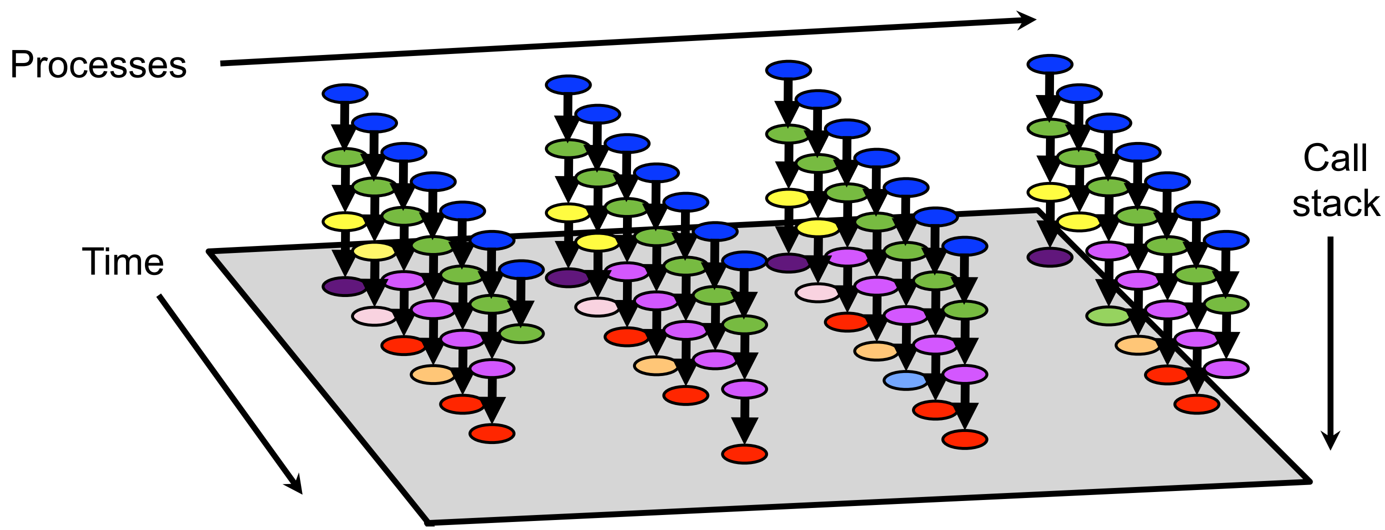


Graph courtesy of Anshu Dubey, U Chicago

Understanding Temporal Behavior

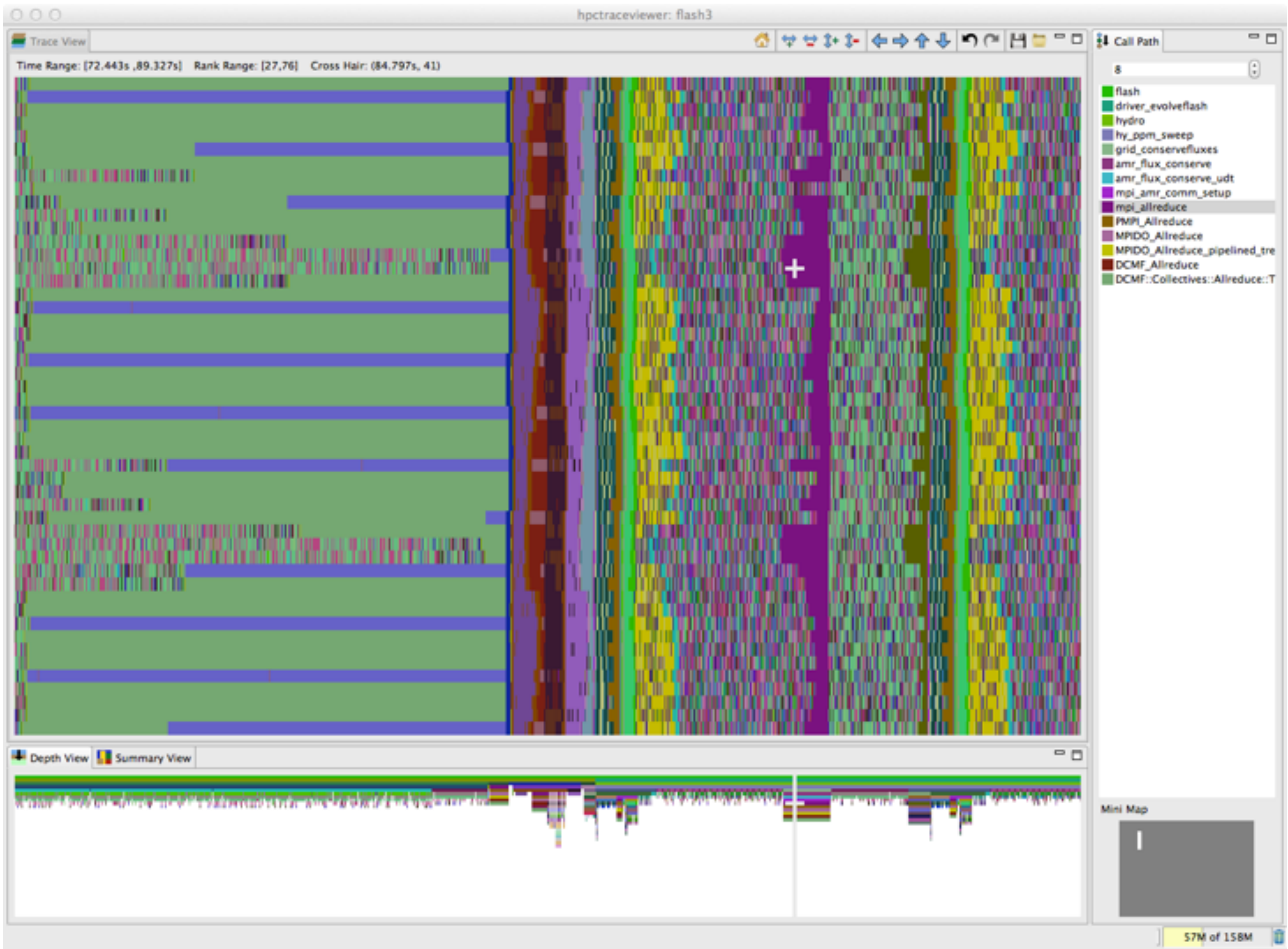
- **Profiling compresses out the temporal dimension**
  - **—temporal patterns, e.g. serialization, are invisible in profiles**
- **What can we do? Trace call path samples**
  - **—sketch:**
    - **N times per second, take a call path sample of each thread**
    - **organize the samples for each thread 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



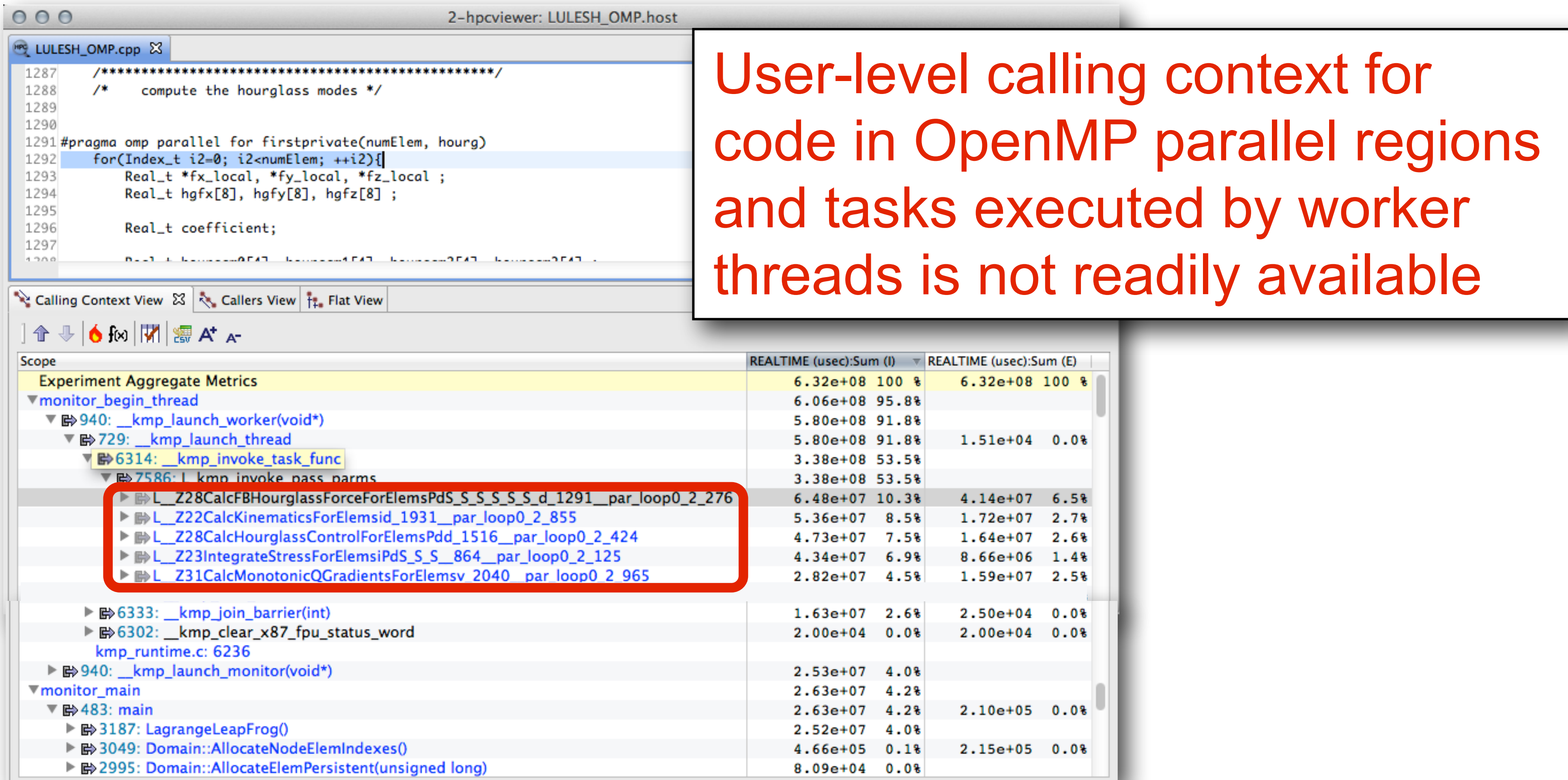
hpctraceviewer: detail of FLASH@256PE

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 between threaded programming models and their implementations**



- **Runtime support is necessary for tools to bridge the gap**

Challenges for OpenMP Node Programs

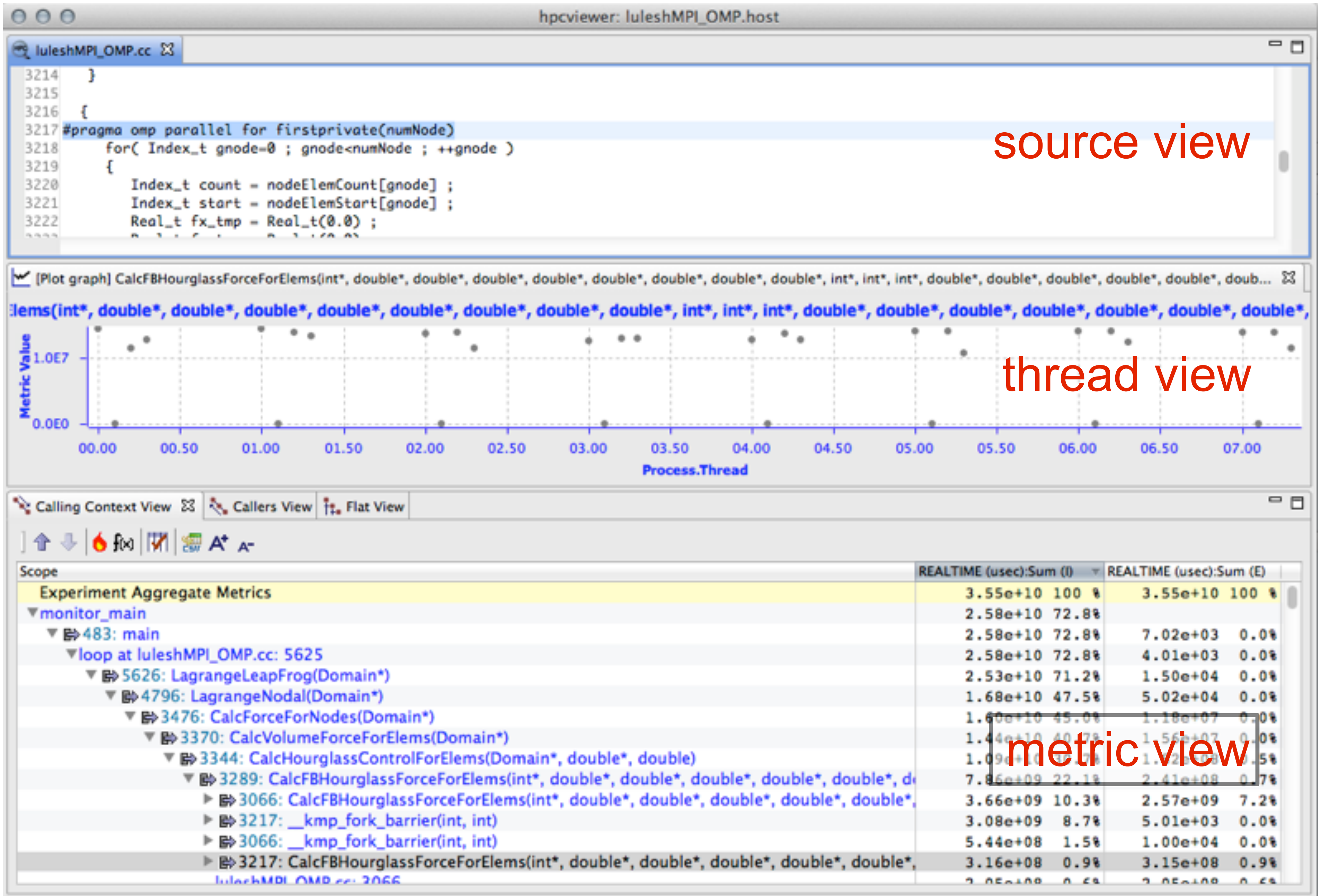
- Tools provide implementation-level view of OpenMP threads
  - asymmetric threads
    - master thread
    - worker thread
  - run-time frames are interspersed with user code
- Hard to understand causes of idleness
  - long serial sections
  - load imbalance in parallel regions
  - waiting for critical 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

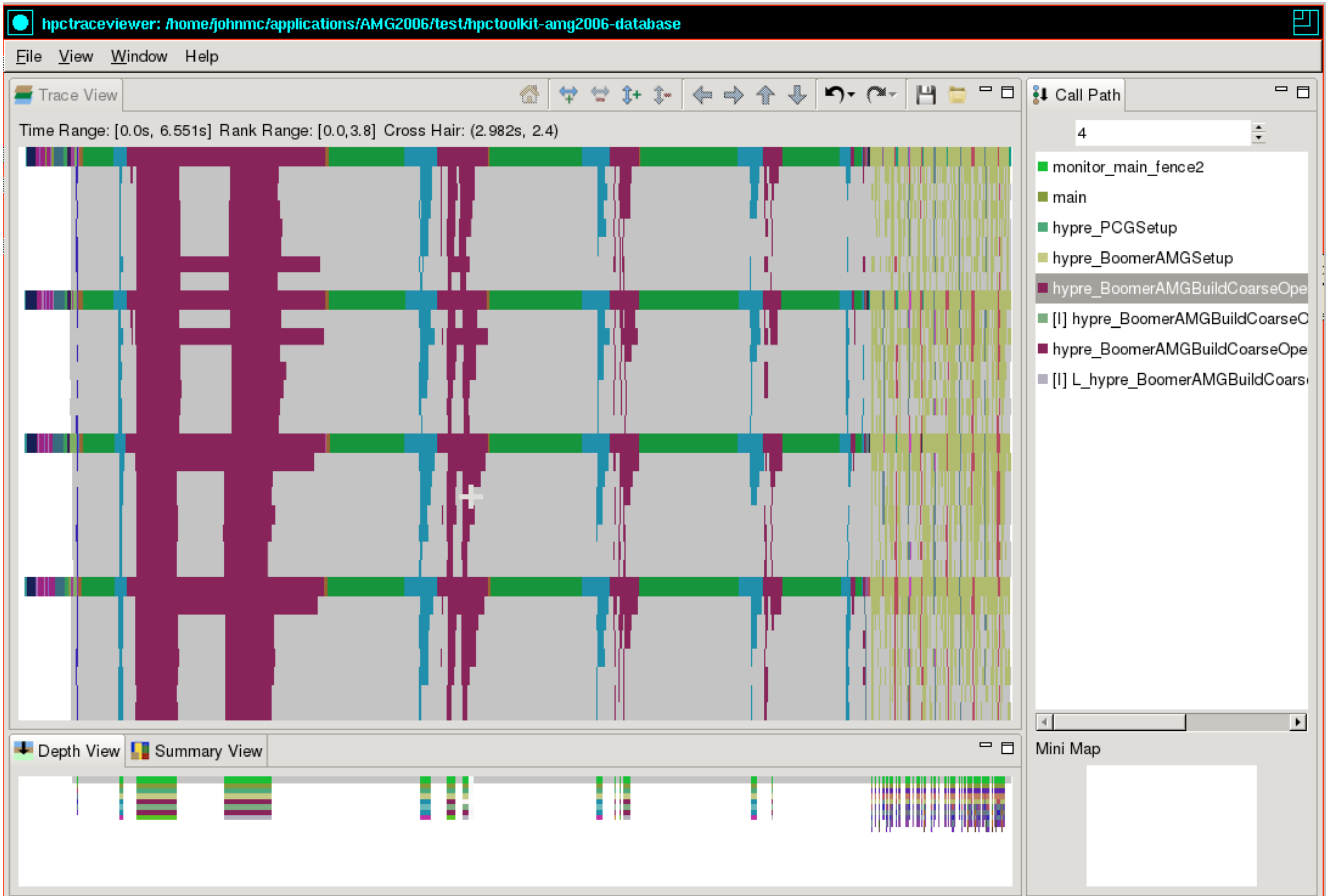
Integrated View of MPI+OpenMP with OMPT

LLNL's luleshMPI_OMP (8 MPI x 3 OMP), 30, REALTIME@1000



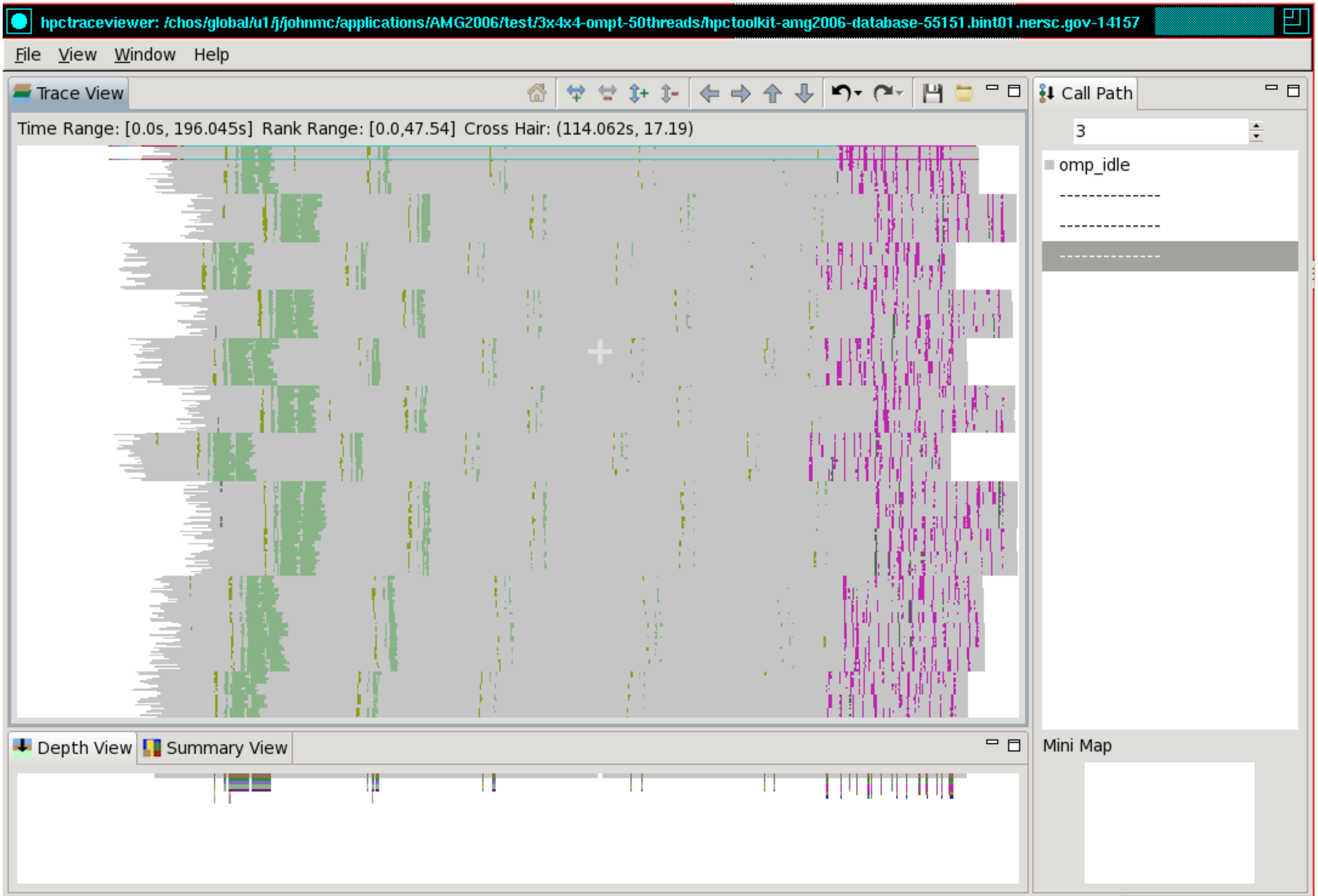
2 18-core Haswell
4 MPI ranks
6+3 threads per rank

Case Study: AMG2006



12 nodes on Babbage@NERSC
24 Xeon Phi
48 MPI ranks
50+5 threads per rank

Case Study: AMG2006



12 nodes on Babbage@NERSC
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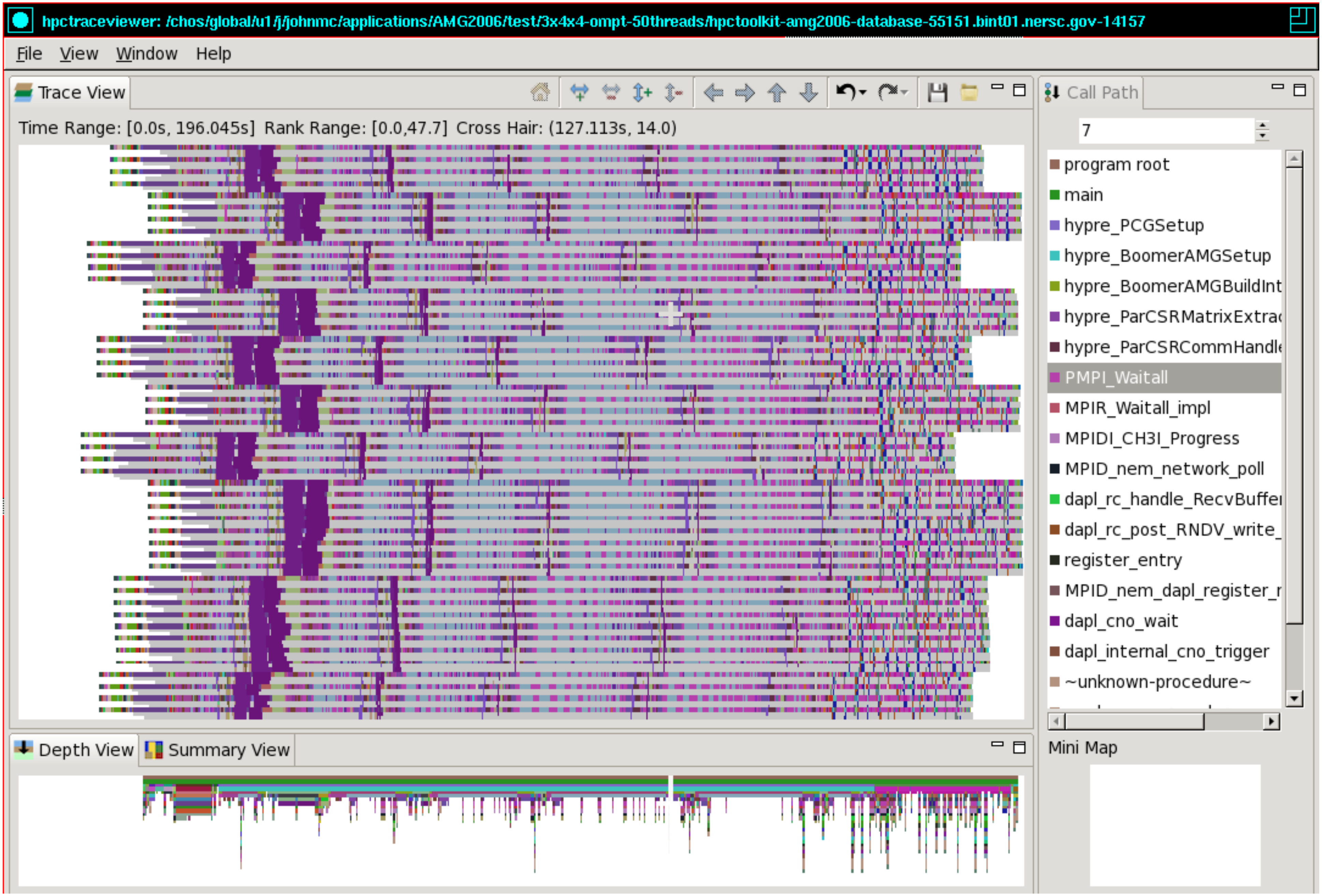
Case Study: AMG2006

<u>Slice</u>
Thread 0 from each MPI rank
First two OpenMP workers



Blame-shifting: Analyze Thread Performance

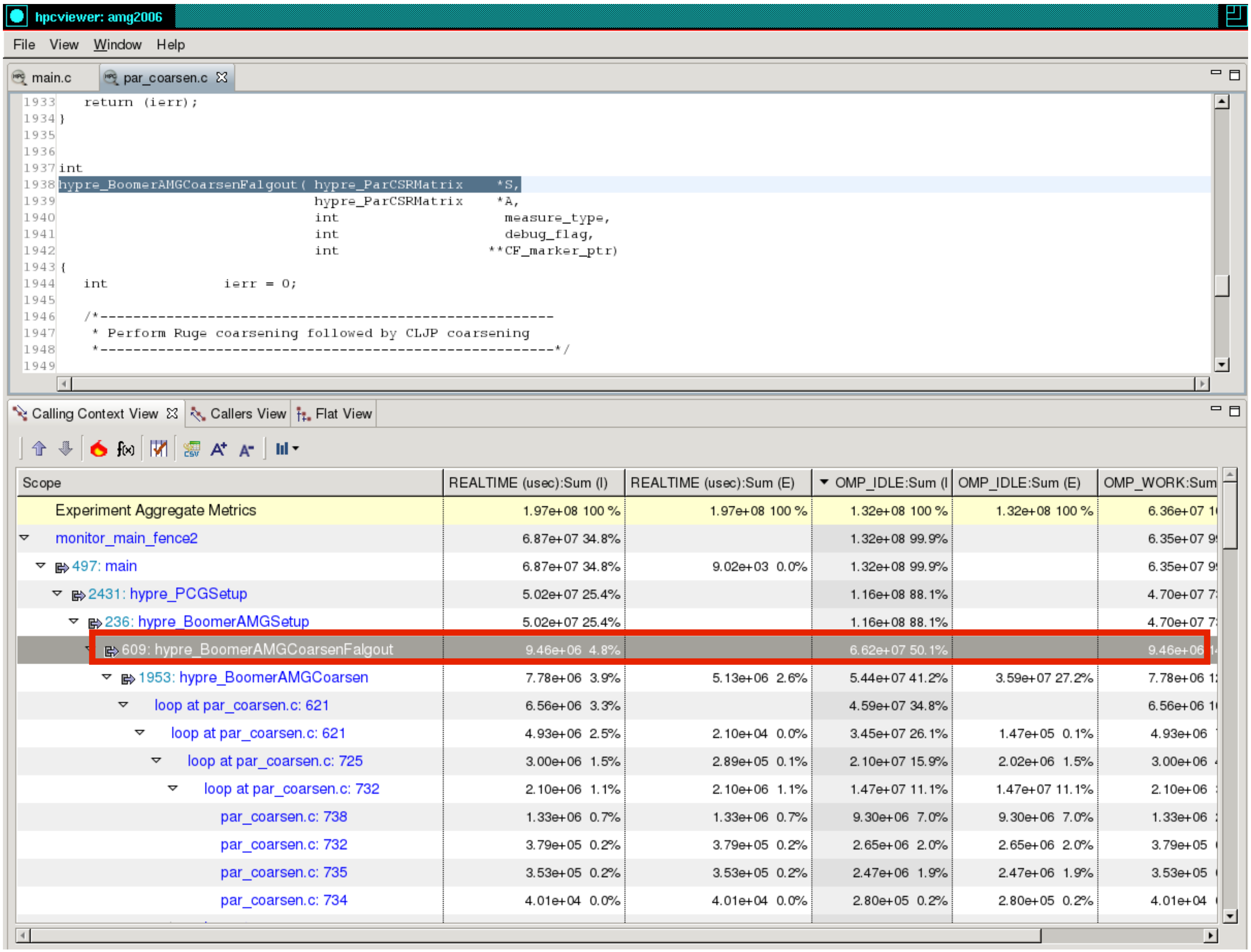
	Problem	Approach
Undirected Blame Shifting[1,3]	A thread is idle waiting for work	Apportion blame among working threads for not shedding enough parallelism to keep all threads busy
Directed Blame Shifting[2,3]	A thread is idle waiting for a mutex	Blame the thread holding the mutex for idleness of threads waiting for the mutex

[1]Tallent & Mellor-Crummey: PPoPP 2009

[2]Tallent, Mellor-Crummey, Porterfield: PPoPP 2010

[3]Liu, Mellor-Crummey, Fagan: ICS 2013

Blame Shifting: Idleness in AMG2006



OpenMP Tool API Status

- Currently HPCToolkit supports OMPT interface based on OpenMP TR2 (April 2014)
- Migrating to emerging OpenMP 5.0 (preview, Nov 2016)
- OMPT prototype implementations
  - —LLVM (current: OpenMP TR2; soon: OpenMP 5)
    - – interoperable with GNU, Intel compilers
  - —IBM LOMP (currently targets OpenMP 5)
- Ongoing work
  - —refining OpenMP 5.0 definition of OMPT
  - —refining OpenMP 5.0 OMPT support in LLVM
  - —refining HPCToolkit OMPT to match emerging standard

Ongoing Work and Future Plans

- **Ongoing work**
  - measurement and analysis using Linux perf_events
    - call stacks for kernel activity in addition to application work
    - measurement and attribution of kernel blocking
  - compliance with emerging OpenMP 5.0 standard
    - updates to HPCToolkit, LLVM OpenMP, vendor OpenMP implementations
    - support for measurement and attribution of GPU accelerated code
  - support for 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:**
  http://hpctoolkit.org/manual/HPCToolkit-users-manual.pdf
  - 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 <u>full</u> 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 \
    -I /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 GUIs 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 GUIs 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.

Blue Gene/Q Notes

Measurement & Analysis of L2 Activity on BG/Q

- **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