# Using HPCToolkit to Measure and Analyze the Performance of GPU-Accelerated Applications

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Download GPU application examples to run and measure:
git clone https://github.com/HPCToolkit/hpctoolkit-tutorial-examples

# Acknowledgments


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  - Industry: AMD
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    - Lead: Prof. Barton Miller

# Performance Analysis Challenges for GPU-accelerated Supercomputers

- **Myriad performance concerns**
  - Computation performance
    - Principal concern: keep GPUs busy and computing productively
      - need extreme-scale data parallelism!
  - Data movement costs within and between memory spaces
  - Internode communication
  - I/O
- **Many ways to hurt performance**
  - insufficient parallelism, load imbalance, serialization, replicated work, parallel overheads …
- **Hardware and execution model complexity**
  - Multiple compute engines with vastly different characteristics, capabilities, and concerns
  - Multiple memory spaces with different performance characteristics
    - CPU and GPU have different complex memory hierarchies
  - Asynchronous execution

# Measurement Challenges for GPU-accelerated Supercomputers

- **Extreme-scale parallelism**
  - Serialization within tools will disrupt parallel performance
- **Multiple measurement modalities and interfaces**
  - Sampling on the CPU
  - Callbacks when GPU operations are launched
  - GPU event stream
- **Frequent GPU kernel launches require a low-overhead measurement substrate**
- **Importance of third-party measurement interfaces**
  - Tools can only measure what GPU hardware can monitor
    - support for fine-grain measurement will be essential to diagnose GPU inefficiencies
  - Linux perf_events for kernel measurement
  - GPU monitoring libraries from vendors

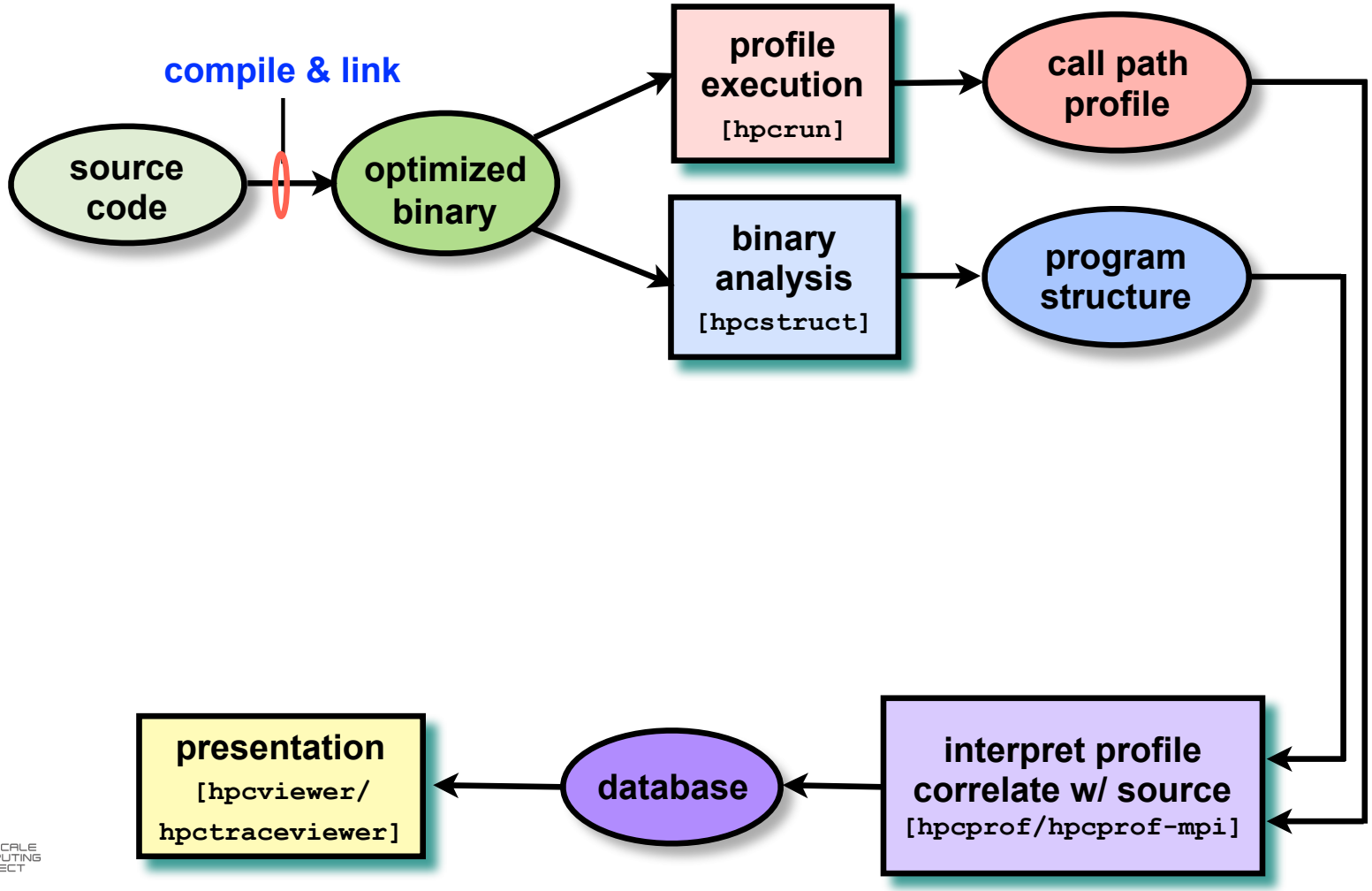
# Outline

- **Performance measurement and analysis challenges for GPU-accelerated supercomputers**
- **Introduction to HPCToolkit performance tools**
  - Overview of HPCToolkit components and their workflow
  - HPCToolkit's graphical user interfaces and using them effectively
- **Analyzing the performance of GPU-accelerated supercomputers with HPCToolkit**
  - Overview of HPCToolkit's GPU performance measurement capabilities
  - Collecting measurements
  - Analysis and attribution
  - Exploring measurements and analysis results
- **Experiences with analysis and tuning of GPU-accelerated codes**
  - Computation, memory hierarchy, and data movement issues
- **Obtaining HPCToolkit**

# Rice University's HPCToolkit Performance Tools

- **Employs binary-level measurement and analysis**
  - Observes executions of fully optimized, dynamically-linked applications
  - Supports multi-lingual codes with external binary-only libraries
- **Collects sampling-based measurements on CPU**
  - Controllable overhead
  - Minimize systematic error and avoid blind spots
  - Enable data collection for large-scale parallelism
- **GPU performance using measurement APIs provided by vendors**
  - Callbacks to monitor launch of GPU operations
  - Activity API to monitor and present information about asynchronous operations on GPU devices
  - PC sampling for fine-grain measurement
- **Associates metrics with both static and dynamic context**
  - Loop nests, procedures, inlined code, calling context on both CPU and GPU
- **Enables one to specify and compute derived CPU and GPU performance metrics of your choosing**
  - Diagnosis often requires more than one species of metric
- **Supports top-down performance analysis**
  - Identify costs of interest and drill down to causes: up and down call chains, over time

# HPCToolkit Workflow



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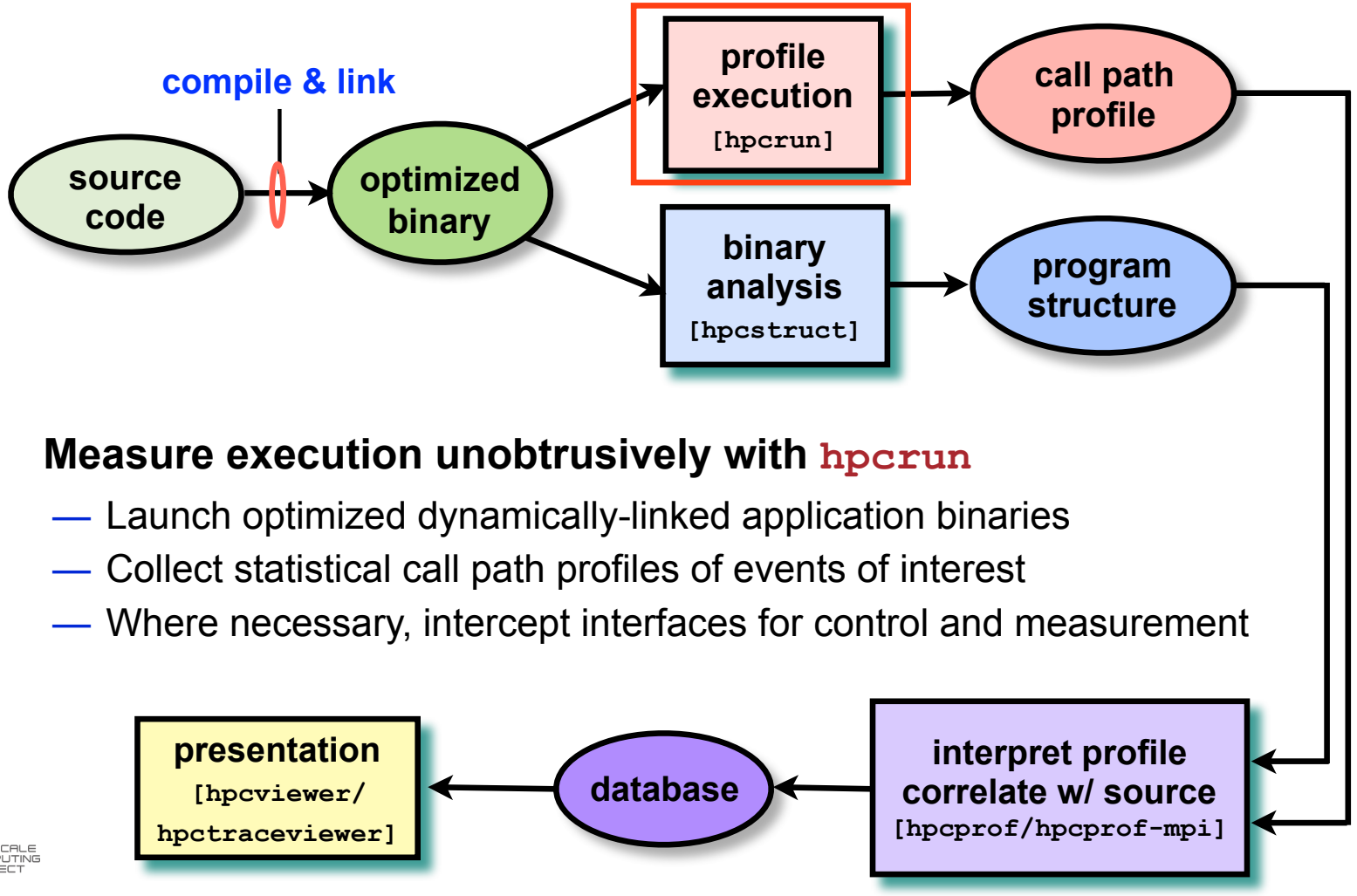


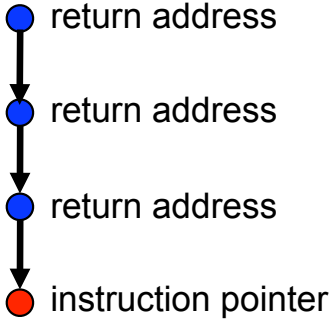

**Measure execution unobtrusively with `hpcrun`**

- Launch optimized dynamically-linked application binaries
- Collect statistical call path profiles of events of interest
- Where necessary, intercept interfaces for control and measurement

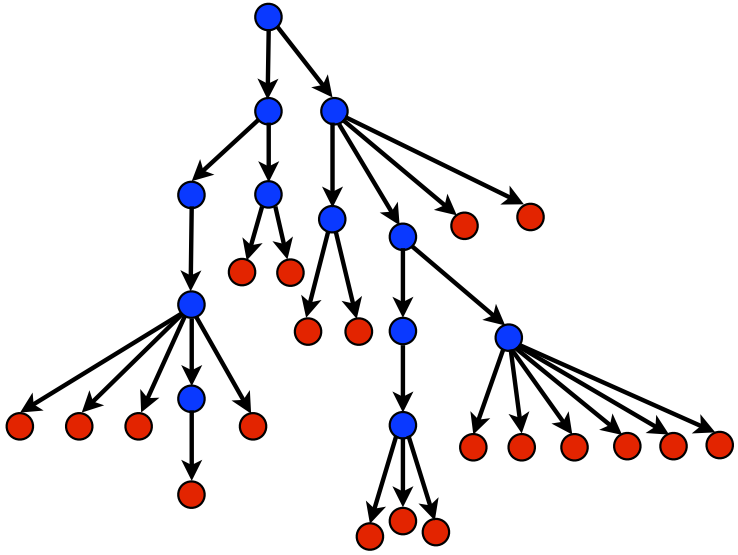
# Call Path Profiling

- **Measure and attribute costs in context**
  - Sample timer or hardware counter overflows
  - Gather CPU calling context using stack unwinding

Call path sample

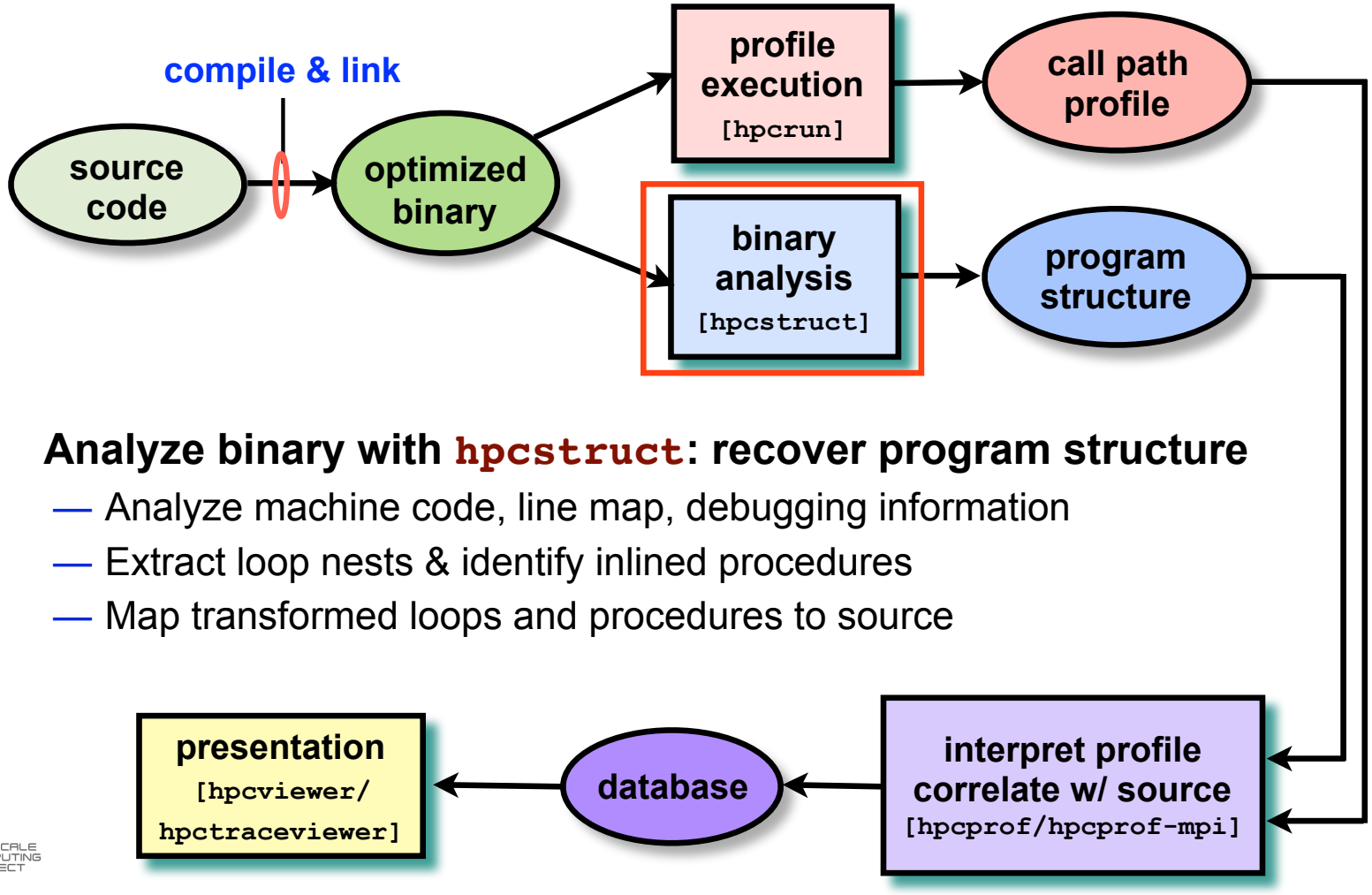



Calling context tree



**Overhead proportional to sampling frequency, not call frequency**

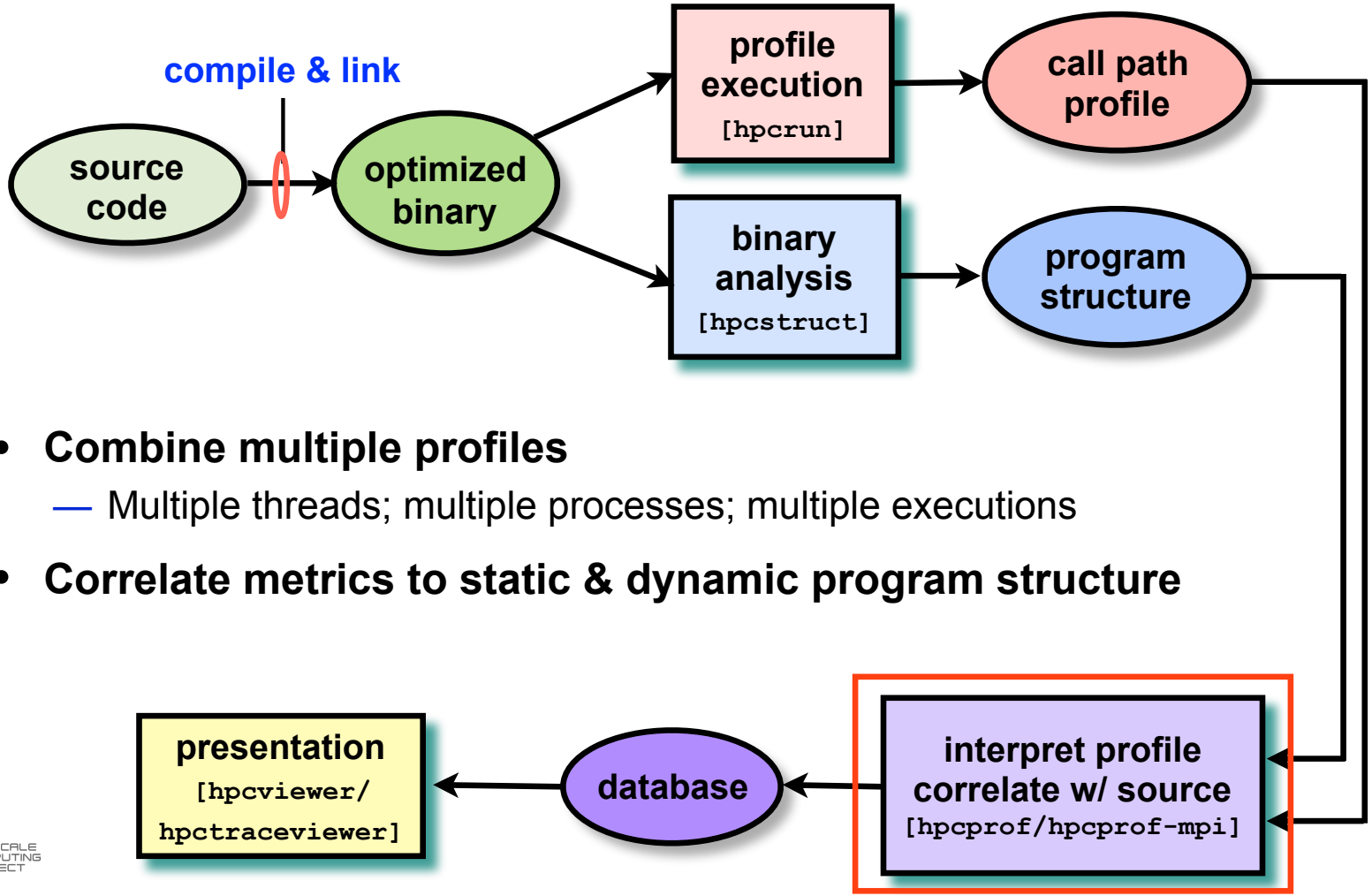
# HPCToolkit Workflow




**Analyze binary with `hpcstruct`: recover program structure**

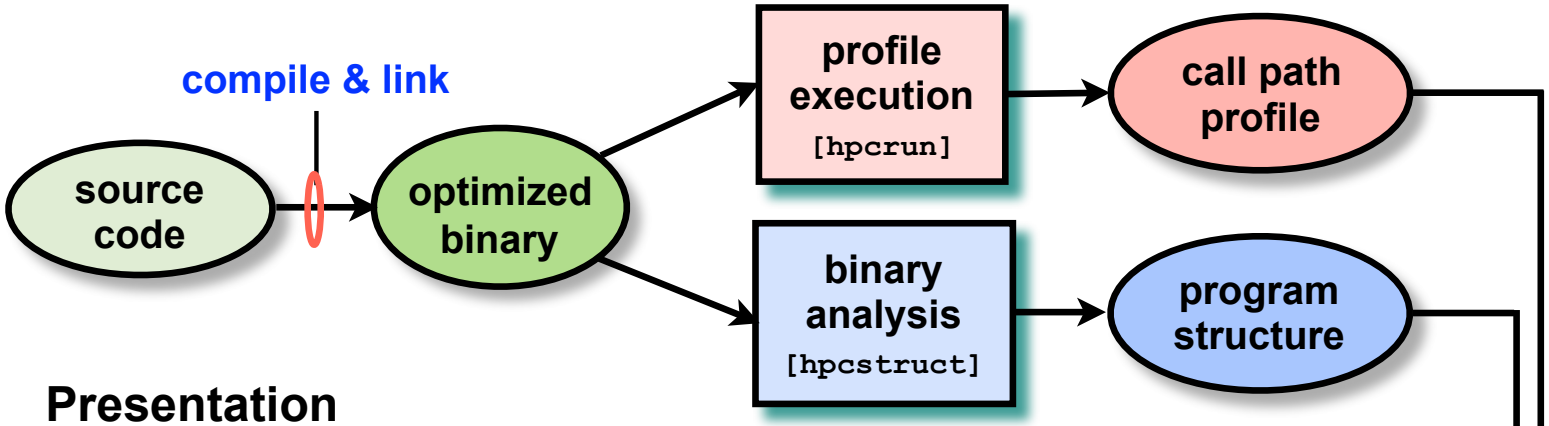
- Analyze machine code, line map, debugging information
- Extract loop nests & identify inlined procedures
- Map transformed loops and procedures to source

# HPCToolkit Workflow



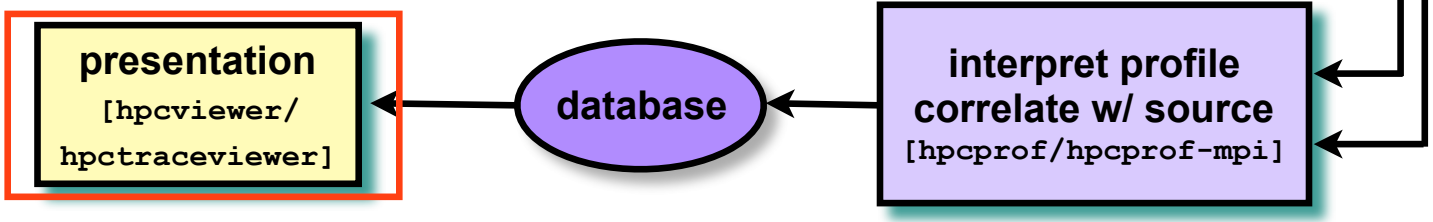

- **Combine multiple profiles**
  - Multiple threads; multiple processes; multiple executions
- **Correlate metrics to static & dynamic program structure**

# HPCToolkit Workflow

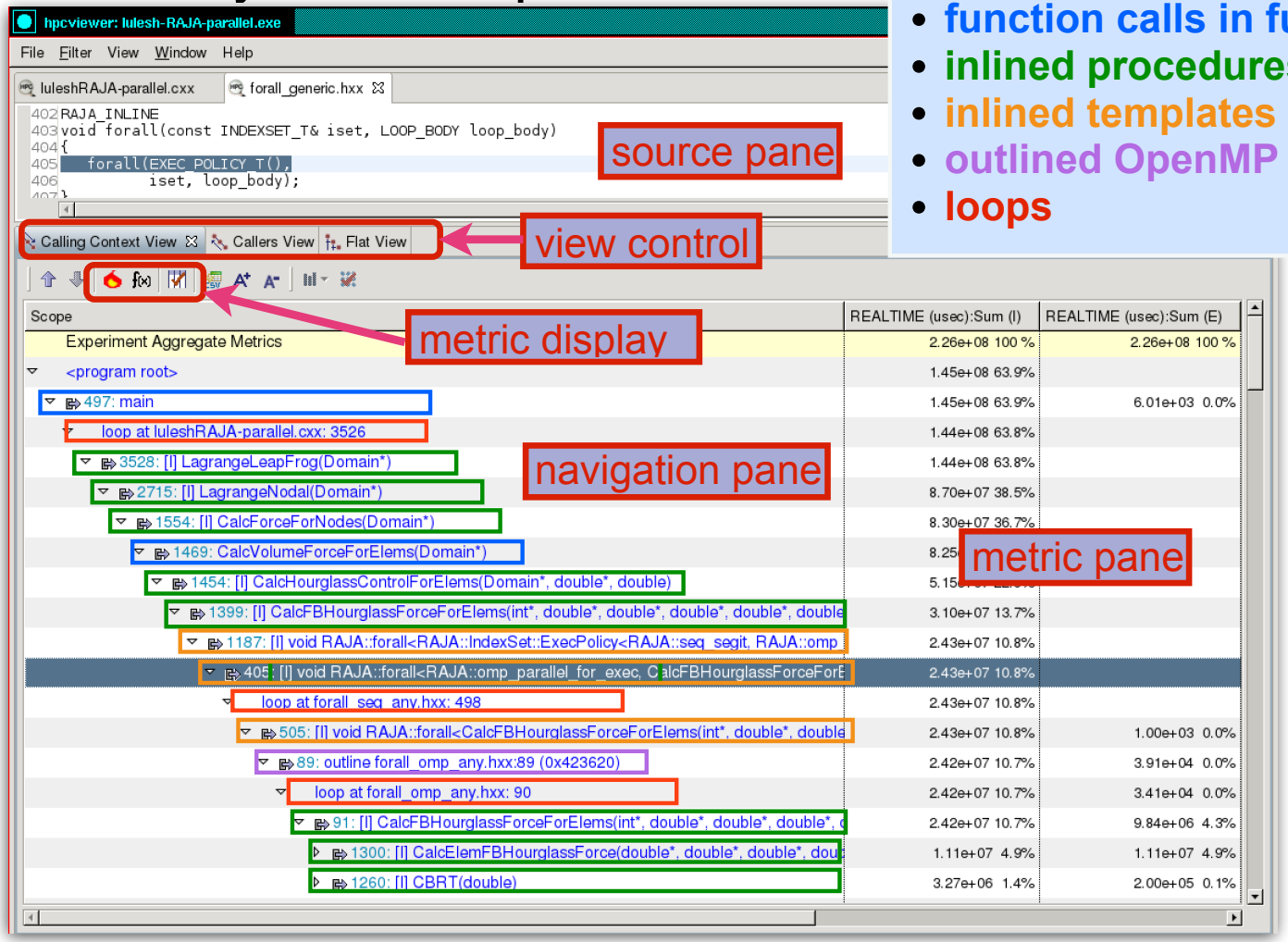



## Presentation

- Explore performance data from multiple perspectives
  - Rank order by metrics to focus on what's important
    e.g., cycles, instructions, GPU instructions, GPU stalls
  - Compute derived metrics to help gain insight
    e.g. scalability losses
- Explore evolution of behavior over time



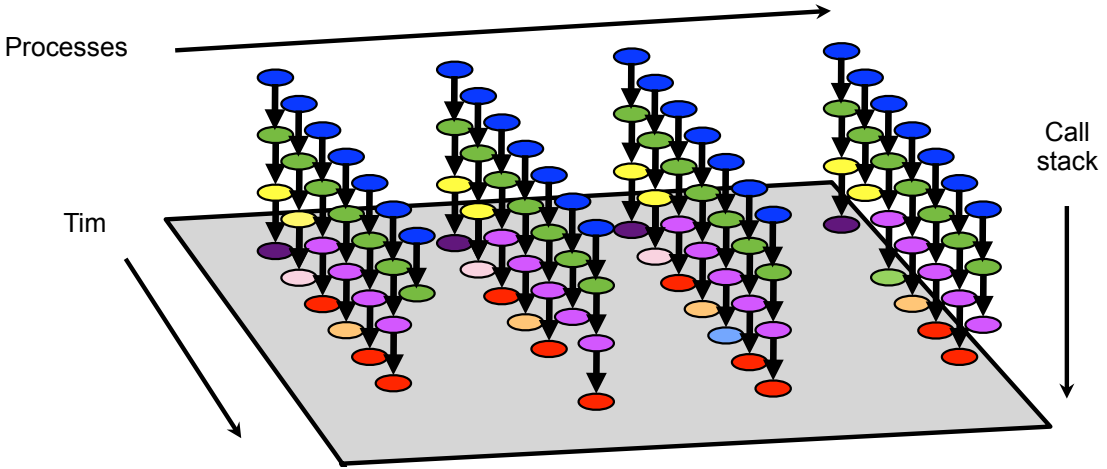
# Code-centric Analysis with hpcviewer




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

# Understanding Temporal Behavior

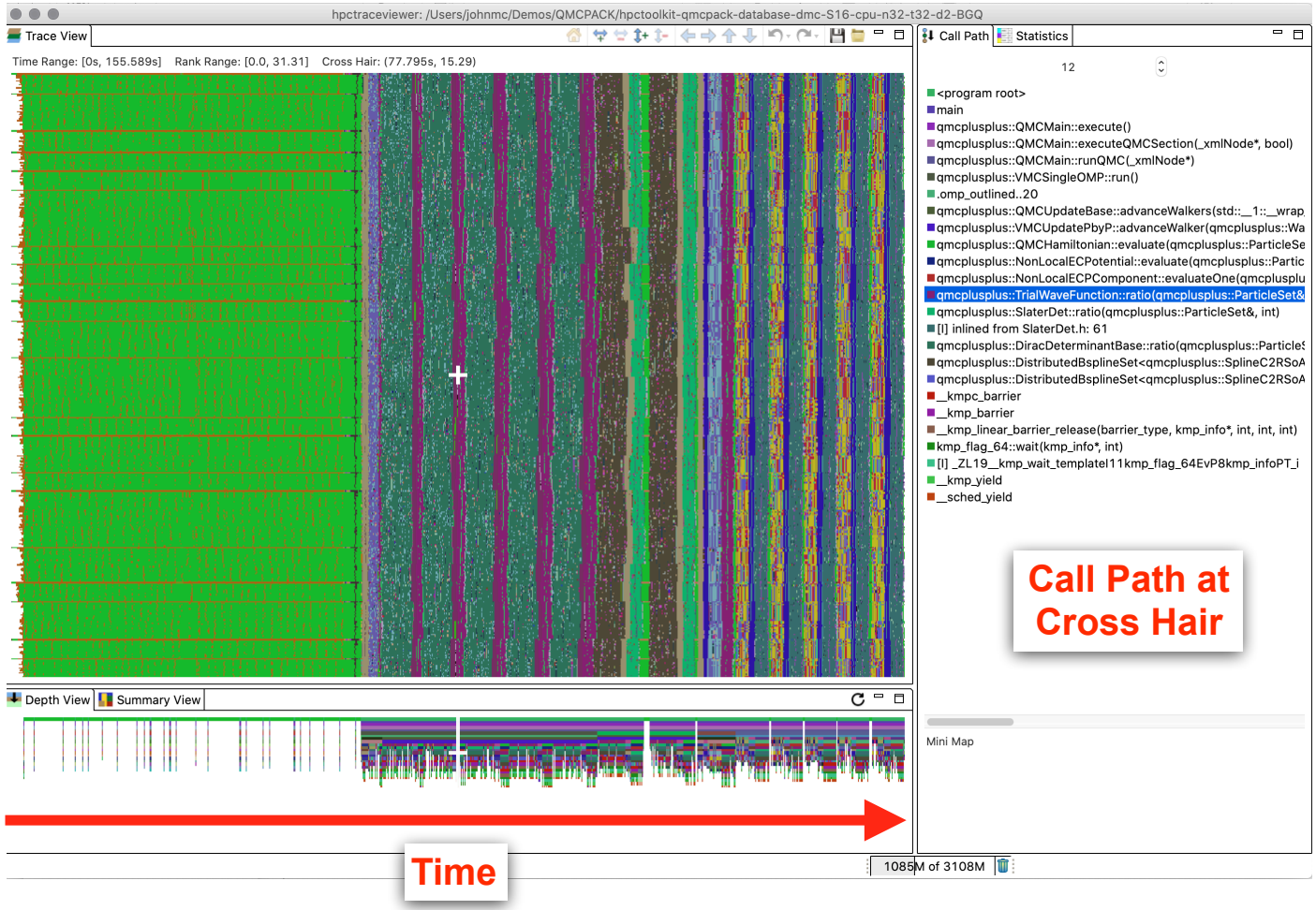
- **Profiling compresses out the temporal dimension**
  - Temporal patterns, e.g. serial sections and dynamic load imbalance are invisible in profiles
- **What can we do? Trace call path samples**
  - N times per second, take a call path sample of each thread
  - Organize the samples for each thread 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



# Time-centric Analysis with hpctraceviewer

**Experimental version of QMCPack on Blue Gene Q**

- 32 ranks
- 32 threads each



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# hpctraceviewer Panes and their Purposes

- **Trace View pane**
  - Displays a sequence of samples for each trace line rendered
  - Title bar shows time interval rendered, rank interval rendered, cross hair location
- **Call Path pane**
  - Show the call path of the selected thread at the cross hair
- **Depth View pane**
  - Show the call stack over time for the thread marked by the cross hair
  - Unusual changes or clustering of deep call stacks can indicate behaviors of potential interest
- **Summary View pane**
  - At each point in time, a histogram of colors above in a vertical column of the Trace View

# Rendering Traces with hpctraceviewer

- **hpctraceviewer renders traces by sampling the [rank x time] rectangle in the viewport**
  - Don’t try to summarize activity in a time interval represented by a pixel
  - Just pick the last activity before the sample point in time
- **Cost of rendering a large execution is [H x T lg N] for traces of length N**
  - The number of trace lines that can be rendered is limited by the number of vertical pixels H
  - Binary search along rendered trace lines to extract values for pixels
- **It can be used to analyze large data: thousands of ranks and threads**
  - Data is kept on disk, memory mapped, and read only as needed

# Understanding How hpctraceviewer Paints Traces

- **CPU trace lines**
  - Given: (procedure f, t) (procedure g, t') (procedure h, t'')
    - Default painting algorithm
      - paint color "f" in [t,t'); paint color "g" in [t', t'')
    - Midpoint painting algorithm
      - paint color "f" in [t, (t+t')/2); paint color "g" in [(t+t')/2, (t'+t'')/2)
- **GPU trace lines**
  - Given GPU operations "f" in interval [t, t') and and "g" in interval [t'', t''')
    - paint color "f" in [t, t'); paint color white in [t', t''); paint color "g" in [t'', t''')

# Analysis Strategies with Time-centric hpctraceviewer

- **Use top-down analysis to understand the broad characteristics of the parallel execution**
- **Click on a point of interest in the Trace View to see the call path there**
- **Zoom in on individual phases of the execution or more generally subsets of [rank, time]**
  - The mini-map tracks what subset of the execution you are viewing
- **Home, undo, redo buttons allow you to move back and forth in a sequence of zooms**
- **Drill down the call path to see what is going on at the call path leaves**
  - Hold your mouse over the call path depth selector. a tool tip will tell you the maximum depth
  - Type the maximum call stack depth number into the depth selector
- **Use the summary view to see a histogram about what fraction of threads or ranks is doing at each time**
- **The summary view can facilitate analysis of how behavior changes over time**
- **The statistics view can show you the fraction of [rank x time] spent in each procedure at the selected depth level**

# Understanding the Navigation Pane in Code-centric hpcviewer

- **<program root>: the top of the call chain for the executable**
- **<thread root>: the top of the call chain for any pthreads**
- **<partial call paths>**
  - The presence of partial call paths indicates that hpcrun was unable to fully unwind the call stack
  - Even if a large fraction of call paths are “partial” unwinds, bottom-up and flat views can be very informative
- **Sometimes functions appear in the navigation pane and appear to be a root**
  - This means that hpcrun believed that the unwind was complete and successful
  - Ideally, this would have been placed under <partial call paths>

# Understanding the Navigation Pane in Code-centric hpcviewer

- **Treat inlined functions as if regular functions**
- **Calling an inlined function**


**[I] is a tag used to indicate that the called function is inlined**

**callsite is a hyperlink to the file and source line where the inlined function is called**

**callee is a hyperlink to the definition of the inlined function**

- **If no source file is available, the caller line number and the callee will be in black**

# Analysis Strategies with Code-centric hpcviewer

- **Use top-down analysis to understand the broad characteristics of the execution**
  - Are there specific unique subtrees in the computation that use or waste a lot of resources?
  - Select a costly node and drill down the “hottest path” rooted there with the flame button
  - One can select a node other than the root and use the flame button to look in its subtree
  - Hold your mouse over a long name in the navigation pane to see the full name in a tool tip
- **Use bottom-up analysis to identify costly procedures and their callers**
  - Pick a metric of interest, e.g. cycles
  - Sort by cycles in descending order
  - Pick the top routine and use the flame button to look up the call stack to its callers
  - Repeat for a few routines of particular interest, e.g. network wait, lock wait, memory alloc, …
- **Use the flat view to explore the full costs associated with code at various granularities**
  - Sort by a cost of interest; use the flame button to explore an interesting load module
  - Use the “flatten” button to melt away load modules, files, and functions to identify the most costly loop

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# Measurement and Analysis of GPU-accelerated Computations

- **What HPCToolkit GUIs present for GPU-accelerated applications**
  - Profile views displaying call paths that integrate CPU and GPU call paths
  - Trace views that attribute CPU threads and GPU streams to full heterogeneous call paths
- **What HPCToolkit collects**
  - Heterogeneous call path profiles and call path traces
- **How HPCToolkit collects information**
  - CPU
    - Sampling-based measurement of application thread activity in user space and in the kernel
    - Measurement of blocking time using Linux perf_events context switch notifications
  - GPU
    - Coarse-grain measurement of GPU operations (memory copies, kernel launches, …)
    - Fine-grain measurement of GPU kernels using PC Sampling (NVIDIA only)

# GPU Monitoring Capabilities of HPCToolkit

| Measurement Capability | NVIDIA CUPTI | AMD ROC-tracer |
|---|---|---|
| kernel launches, explicit memory copies, synchronization | callbacks + activity API | callbacks + Activity API |
| instruction-level measurement and analysis | PC sampling, analysis of GPU binaries | no |
| kernel characteristics | Activity API | (available statically, but not yet used by HPCToolkit) |

Intel oneAPI Level 0 runtime: specification (December 2019); implementation (not yet available)
https://spec.oneapi.com/versions/latest/oneL0/index.html

# Preparing a GPU-accelerated Program for HPCToolkit

- **HPCToolkit doesn't need any modifications to your Makefiles**
  - it can measure fully-optimized code without special preparation
- **To get the most from your measurement and analysis**
  - Compile your program with line numbers
    - CPU (all compilers)
      - add "-g" to your compiler optimization flags
    - NVIDIA GPUs
      - compiling with nvcc
        - add "-lineinfo" to your optimization flags for GPU line numbers
        - adding -G provides full information about inlining and GPU code structure but disables optimization
      - compiling with xlc
        - line information is unavailable for optimized code (last confirmed May 2019)
    - AMD GPUs, no special preparation needed
      - current AMD GPUs and ROCM software stack lack capabilities for fine-grain measurement and attribution
    - Intel GPUs
      - HPCToolkit is currently oblivious to their presence

# Using HPCToolkit to Measure an Execution

- **Sequential program**
  - `hpcrun [measurement options] program [program args]`
- **Parallel program**
  - `mpirun -n <nodes> [mpi options] hpcrun [measurement options] \ program [program args]`
  - Similar launches with job managers
    - LSF: jsrun
    - SLURM: srun

# CPU Time-based Sample Sources - Linux thread-centric timers

- **CPUTIME (DEFAULT if no sample source is specified)**
  - CPU time used by the thread in microseconds
  - Does not include time blocked in the kernel
    - **disadvantage: completely overlooks time a thread is blocked**
    - **advantage: a blocked thread is never unblocked by sampling**
- **REALTIME**
  - Real time used by the thread in microseconds
  - Includes time blocked in the kernel
    - **advantage: shows where a thread spends its time, even when blocked**
    - **disadvantages**
      - **activates a blocked thread to take a sample**
      - **a blocked thread appears active even when blocked**

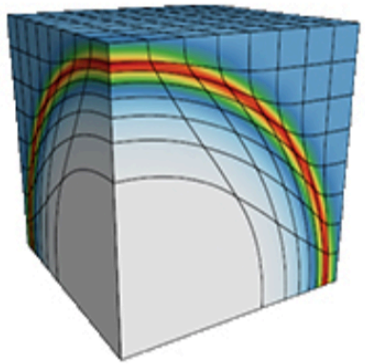
**Note: Only use one Linux timer to measure an execution**

# CPU Sample Sources - Linux perf_event monitoring subsystem

- **Kernel subsystem for performance monitoring**
- **Access and manipulate**
  - Hardware counters: cycles, instructions, …
  - Software counters: context switches, page faults, …
- **Available in Linux kernels 2.6.31+**
- **Capabilities**
  - Can monitor ‘cycles’ to observe activity in user space and in the kernel
    - including costs in GPU drivers
  - Can monitor time threads spend blocked by tracking context switches
    - HPCToolkit’s ‘BLOCKTIME’ metric

# Case Study: Measurement and Analysis of GPU-accelerated Laghos

Laghos (LAGrangian High-Order Solver) is a LLNL ASC co-design mini-app that was developed as part of the CEED software suite, a collection of software benchmarks, miniapps, libraries and APIs for efficient exascale discretization based on high-order finite element and spectral element methods.



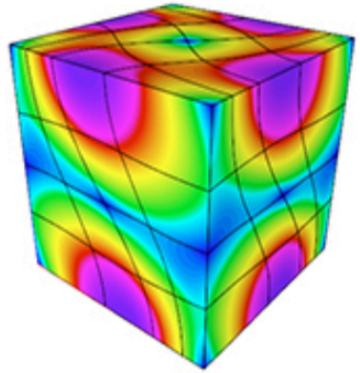



Figure credit: https://computing.llnl.gov/projects/co-design/laghos

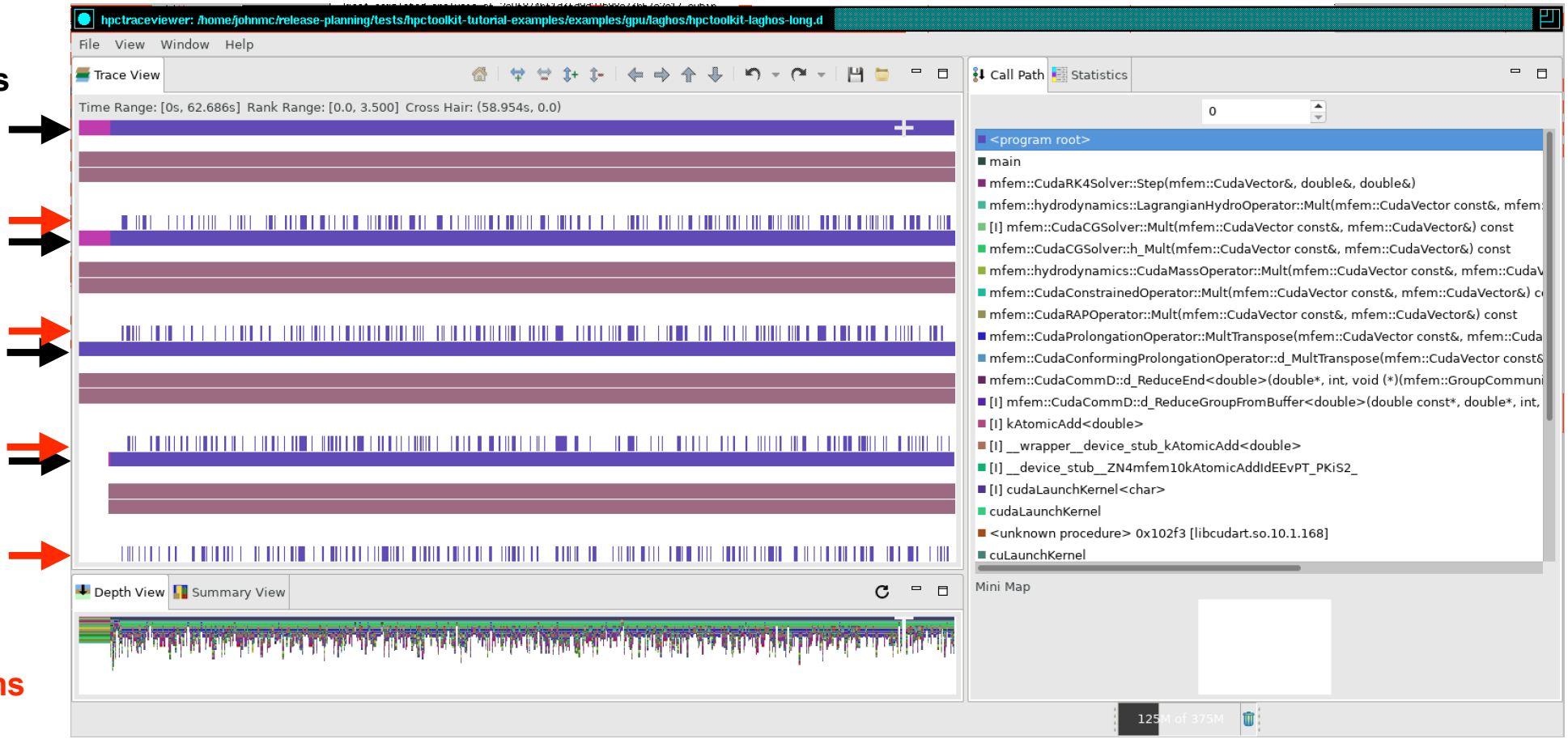
# Applying the GPU Operation Measurement Workflow to Laghos

```
# measure an execution of laghos
time mpirun -np 4 hpcrun -o $OUT -e cycles -e gpu=nvidia -t \
   ${LAGHOS_DIR}/laghos -p 0 -m ${LAGHOS_DIR}/../data/square01_quad.mesh \
   -rs 3 -tf 0.75 -pa

# compute program structure information for the laghos binary
hpcstruct -j 16 laghos

# compute program structure information for the laghos cubins
hpcstruct -j 16 $OUT

# combine the measurements with the program structure information
mpirun -n 4  hpcprof-mpi -S laghos.hpcstruct $OUT
```

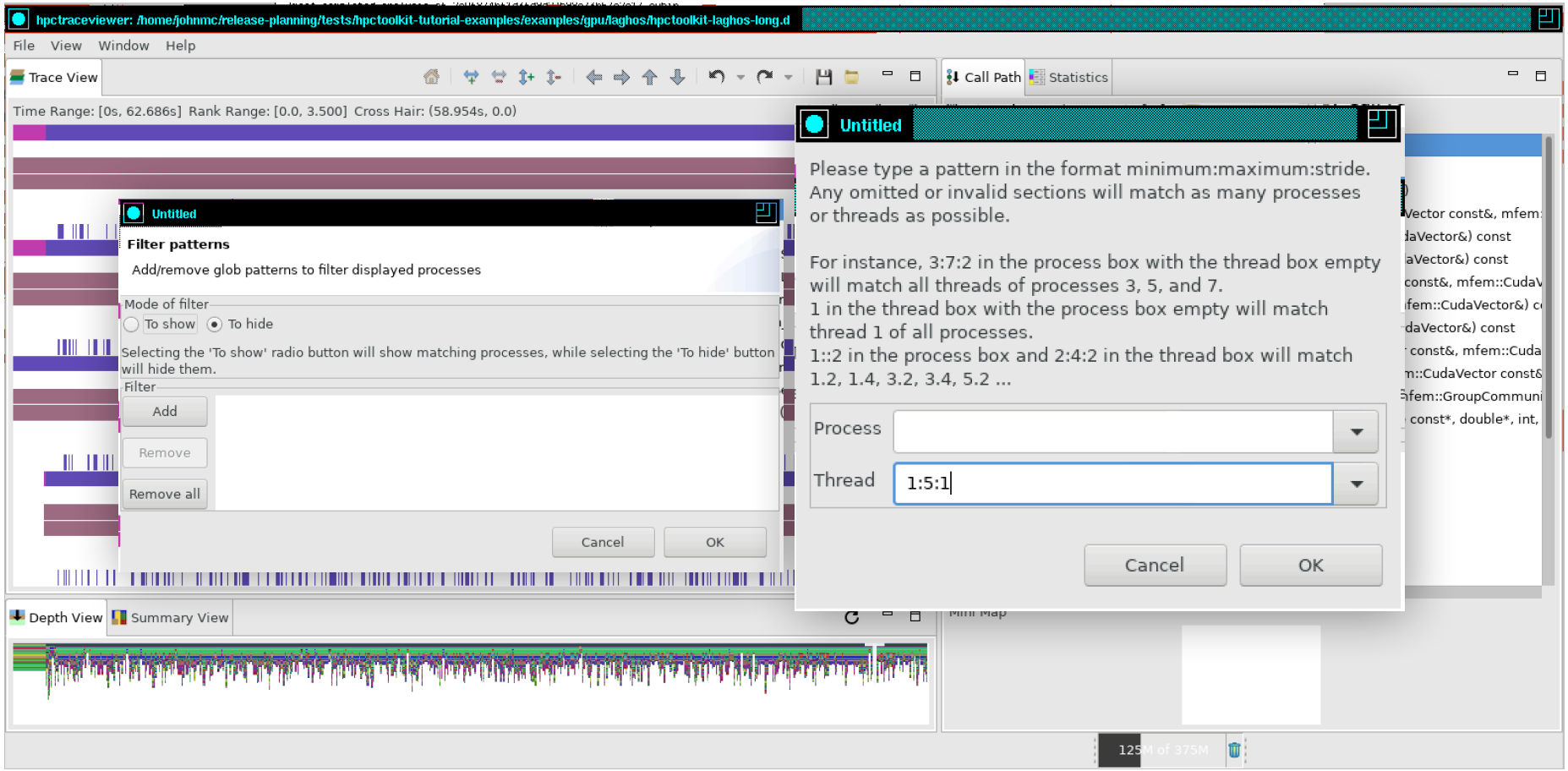
# Computing Program Structure Information for NVIDIA cubins

- **When a GPU-accelerated application runs, HPCToolkit collects unique GPU binaries**
  - Currently, NVIDIA does not provide an API that provides a URI for cubins it launches
  - CUPTI presents cubins to tools as an interval in the heap (starting address, length)
  - HPCToolkit computes an MD5 hash for each cubin and saves one copy
    - stores save cubins in hpcrun's measurement directory: <measurement directory>/cubins
- **Analyze the cubins collected during an execution**
  - **`hpcstruct -j 16 <measurement directory>`**
    - lightweight analysis based only on cubin symbols and line map
  - **`hpcstruct -j 16 –gpucfg yes <measurement directory>`**
    - heavyweight analysis based only on cubin symbols, line map, control flow graph
      - uses nvdisasm to compute control flow graph
    - fine-grain analysis only needed to interpret PC sampling experiments
  - **`hpcstruct`** analyzes a collection of cubins in parallel using thread count specified with -j

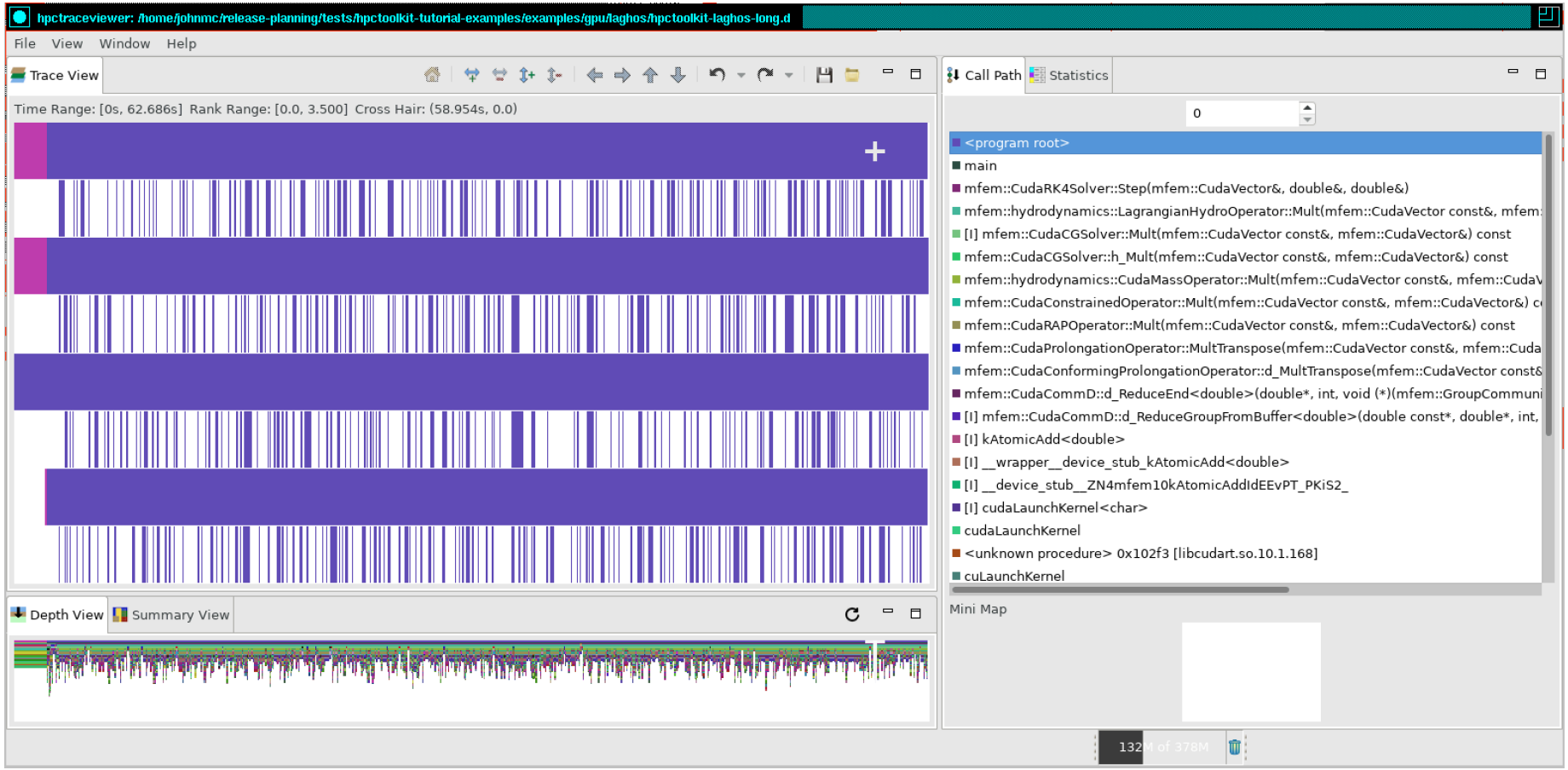
# Initial hpctraceviewer view of Laghos (long) Execution



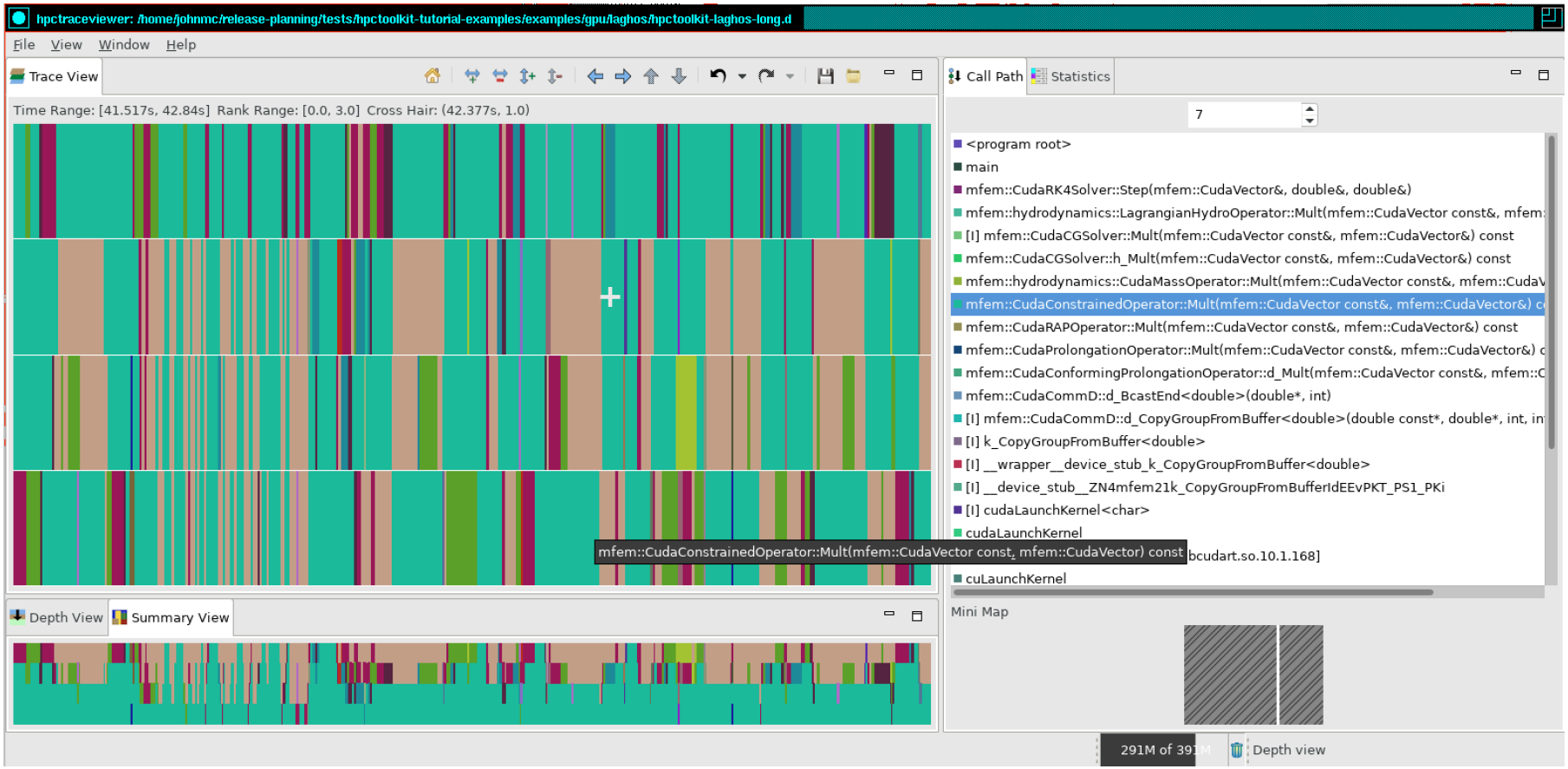
# Hiding the Empty MPI Helper Threads



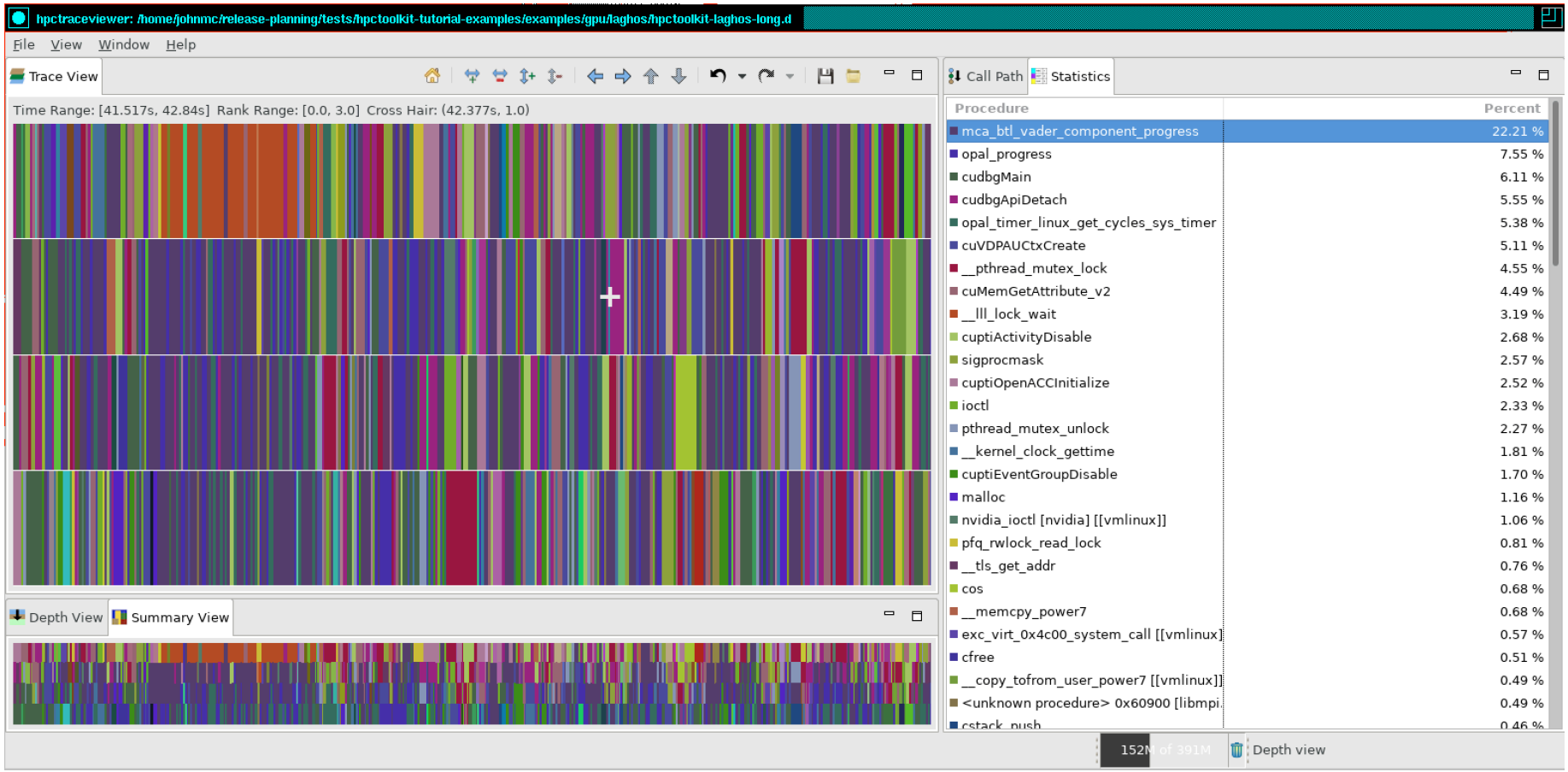
# After Hiding the Empty MPI Helper Threads



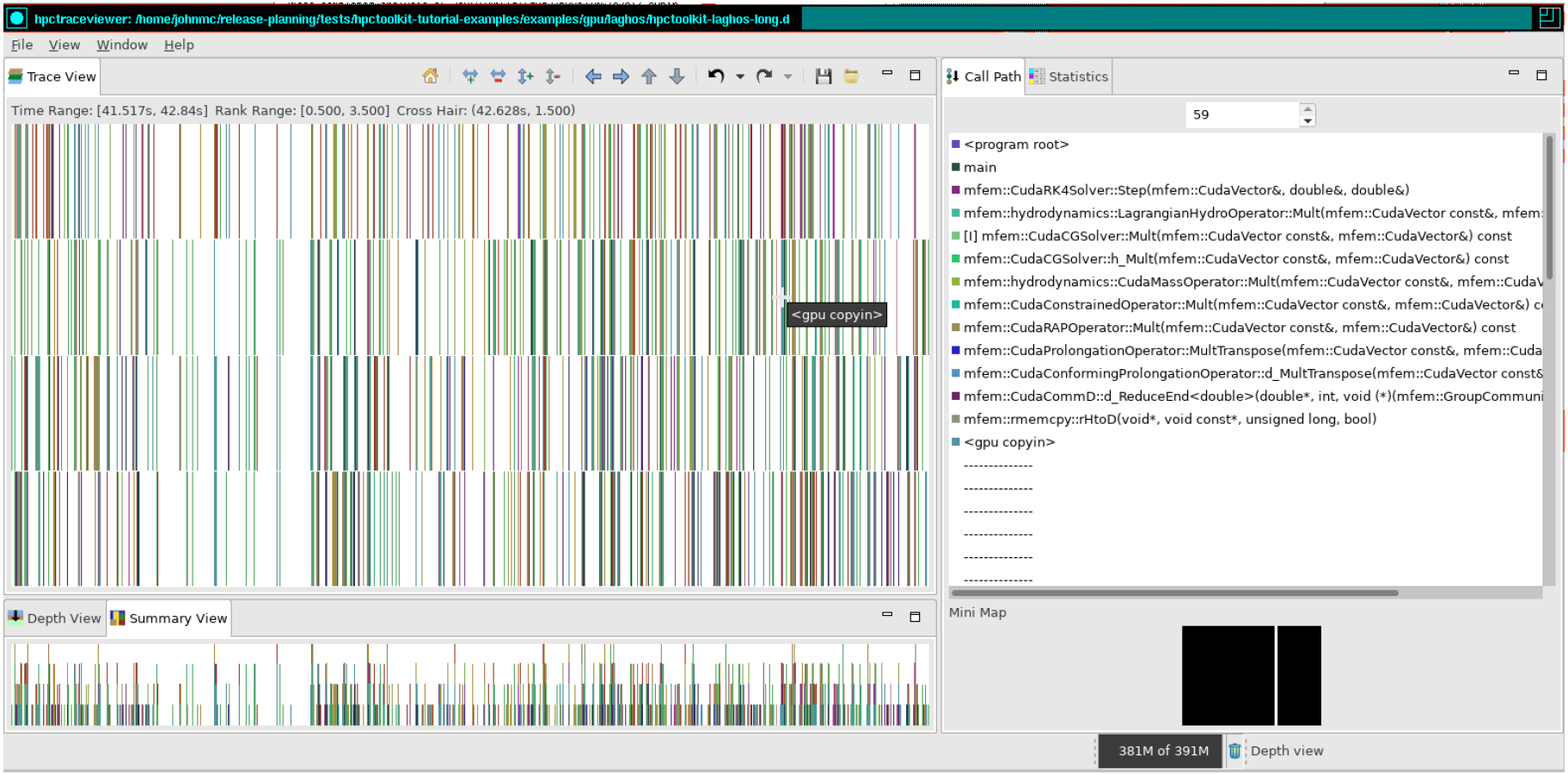
# A Detail of Only the MPI Threads



# Only the MPI Threads - Analysis using the Statistics Panel



# Only the GPU Threads - Inspecting the Callpath for a Kernel



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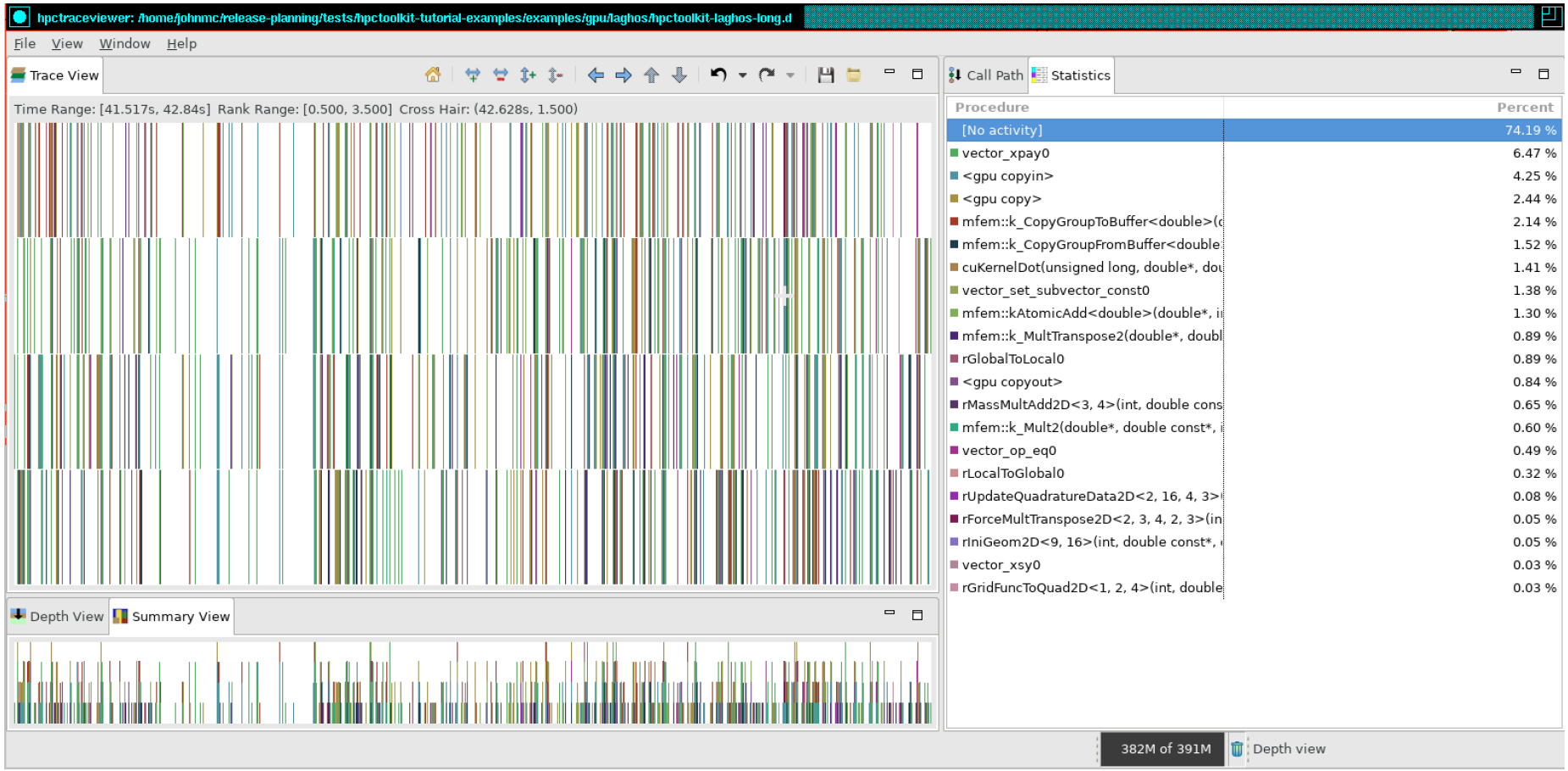
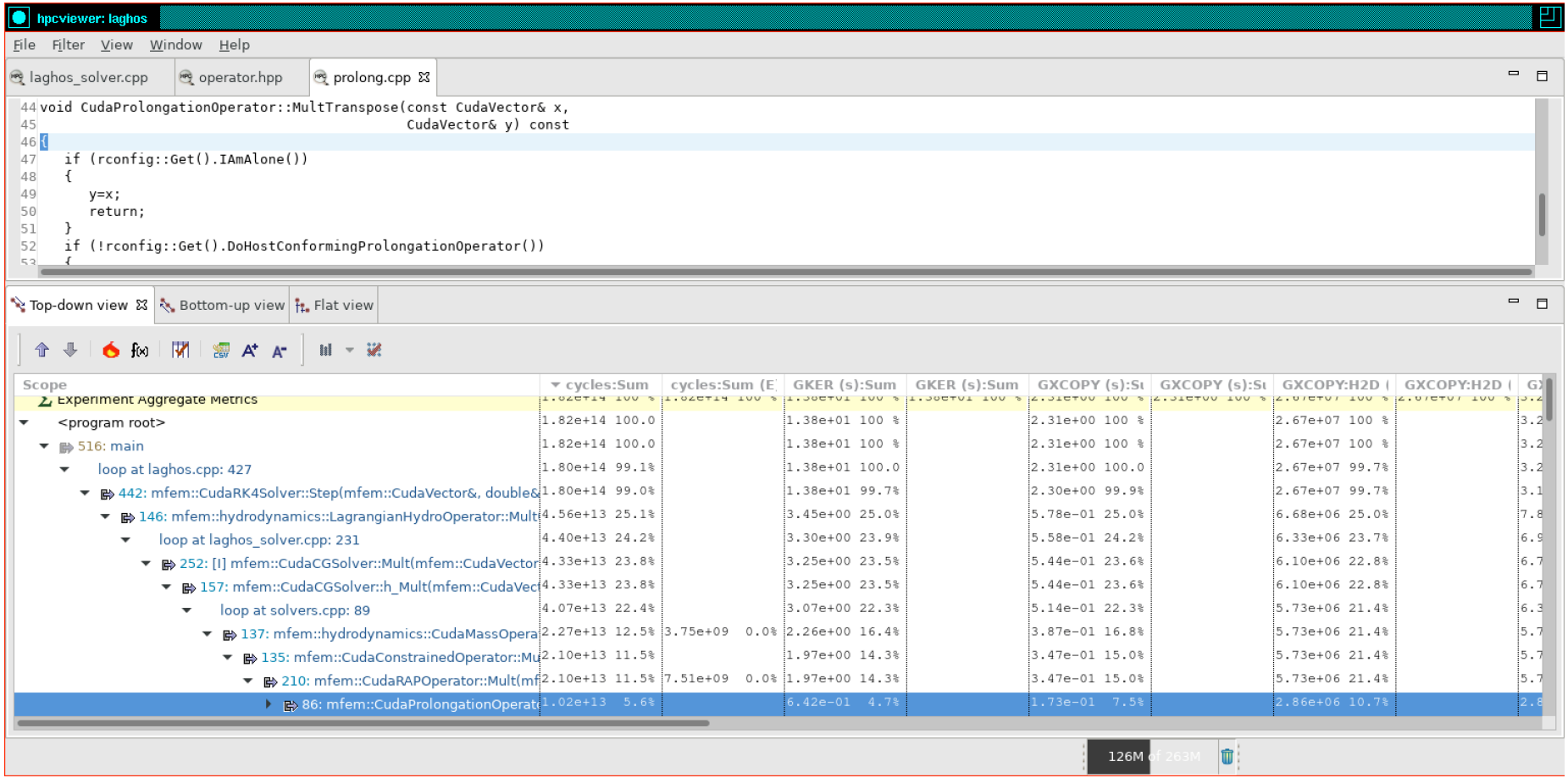


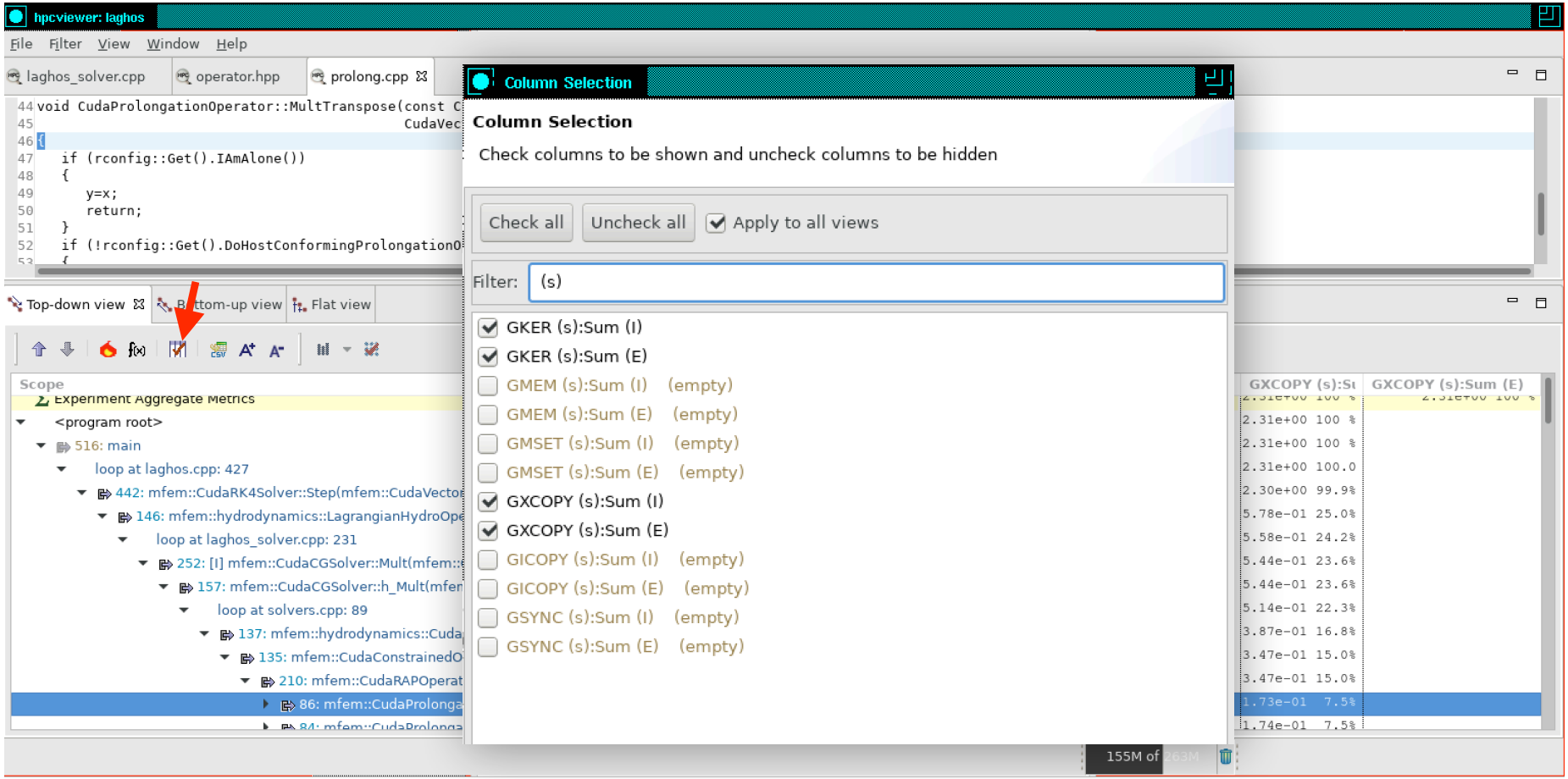
# Some Cautions When Analyzing GPU Traces

- **There are overheads introduced by NVIDIA's monitoring API that we can't avoid**
- **When analyzing traces from your program and compare GPU activity to [no activity]**
  - Time your program without any tools
  - Time your program when tracing with HPCToolkit or nvprof
  - Re-weight [no activity] by the ratio of unmonitored time to monitored time
- **While this is a concern for traces, this should be less a concern for profiles**
  - On the CPU, HPCToolkit compensates for monitoring overhead in profiles by not measuring it

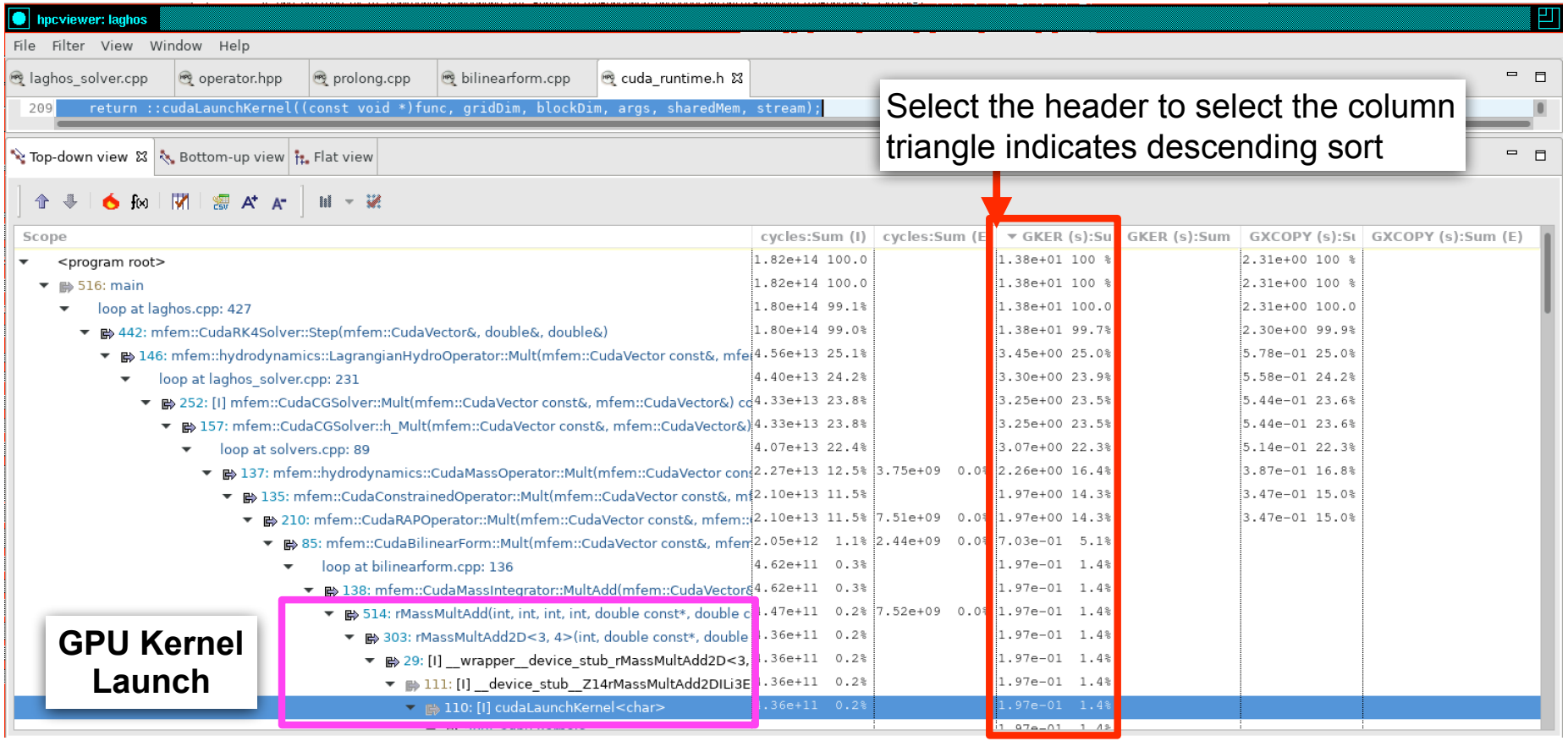
# Using hpcviewer to See the Source-centric View



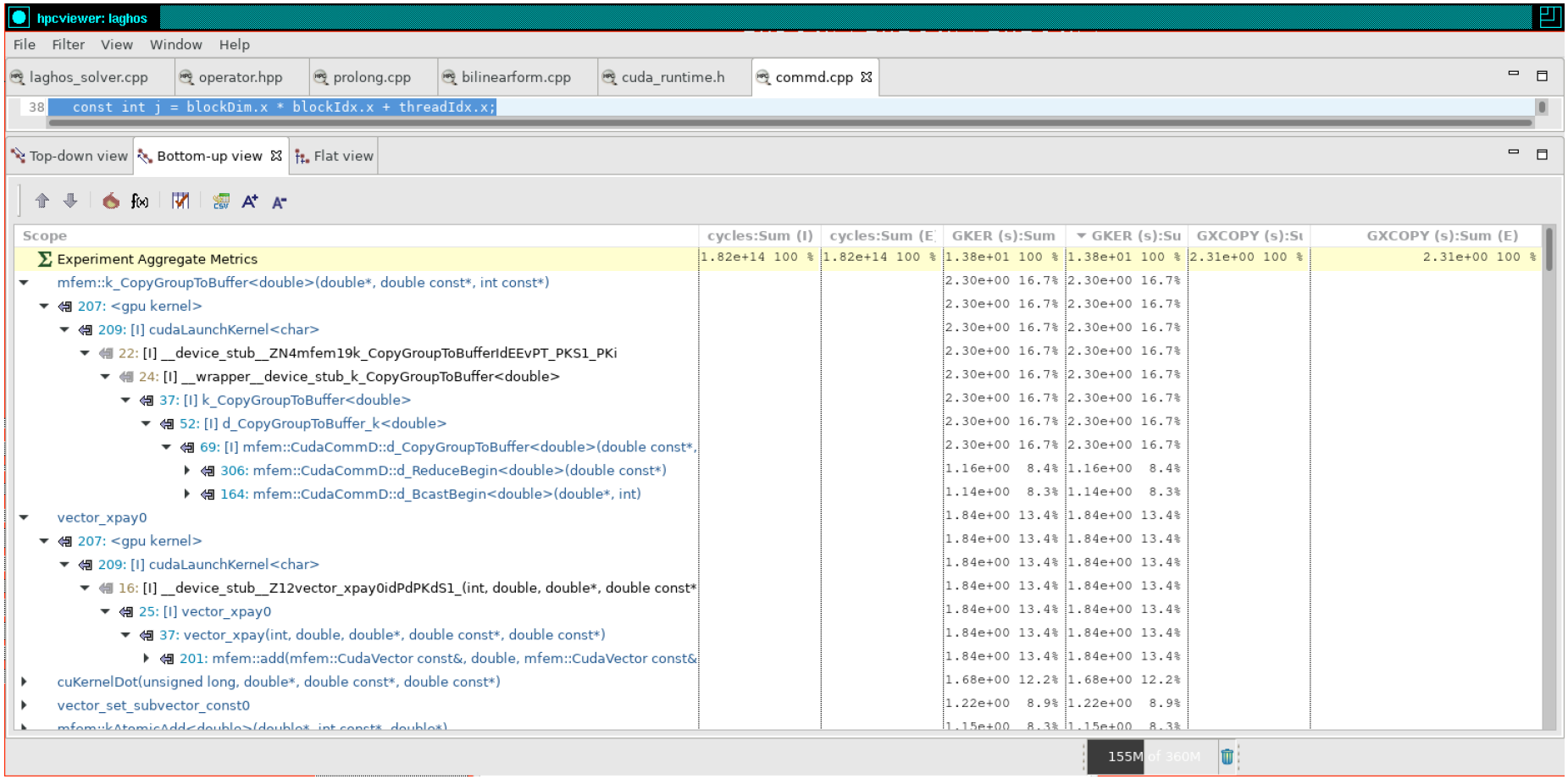
# Selecting Metrics to Display Using the Column Selector



# Using GPU Kernel Time to Guide Top-down Exploration



# Using GPU Kernel Time to Guide Bottom-up Exploration



# Applying the GPU PC Sampling Measurement Workflow to Laghos

```
# measure an execution of laghos using pc sampling
time mpirun -np 4 hpcrun -o $OUT -e cycles -e gpu=nvidia,pc -t \
   ${LAGHOS_DIR}/laghos -p 0 -m ${LAGHOS_DIR}/../data/square01_quad.mesh \
   -rs 1 -tf 0.05 -pa

# compute program structure information for the laghos binary
hpcstruct -j 16 laghos

# compute program structure information for the laghos cubins with CFG
hpcstruct --gpucfg yes -j 16 $OUT

# combine the measurements with the program structure information
mpirun -n 4  hpcprof-mpi -S laghos.hpcstruct $OUT
```

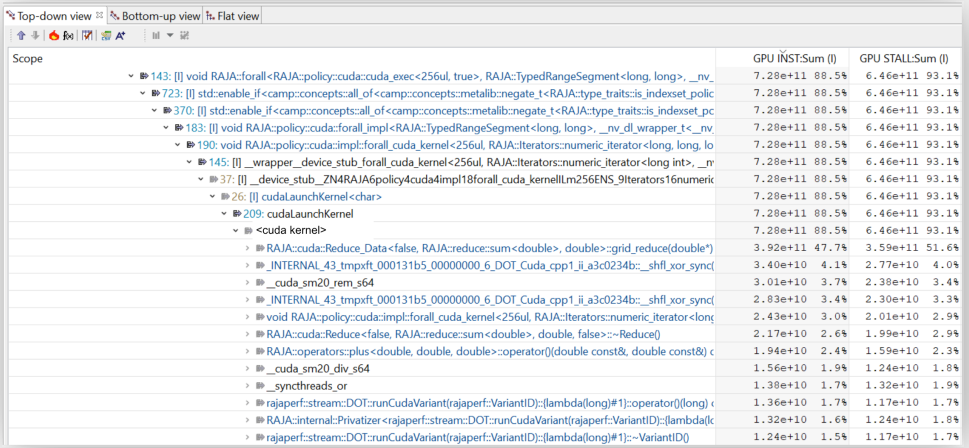
# HPCToolkit's GPU Instruction Sampling Metrics (NVIDIA Only)

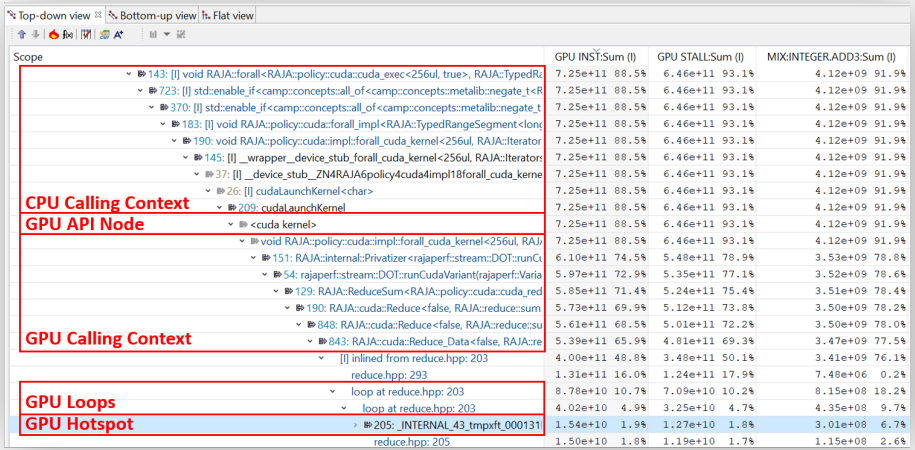
| Metric | Definition |
|---|---|
| **GINST:STL_ANY** | GPU instruction stalls: any (sum of all **STALL** metrics other than **NONE**) |
| **GINST:STL_NONE** | GPU instruction stalls: no stall |
| **GINST:STL_IFET** | GPU instruction stalls: await availability of next instruction (fetch or branch delay) |
| **GINST:STL_IDEP** | GPU instruction stalls: await satisfaction of instruction input dependence |
| **GINST:STL_GMEM** | GPU instruction stalls: await completion of global memory access |
| **GINST:STL_TMEM** | GPU instruction stalls: texture memory request queue full |
| **GINST:STL_SYNC** | GPU instruction stalls: await completion of thread or memory synchronization |
| **GINST:STL_CMEM** | GPU instruction stalls: await completion of constant or immediate memory access |
| **GINST:STL_PIPE** | GPU instruction stalls: await completion of required compute resources |
| **GINST:STL_MTHR** | GPU instruction stalls: global memory request queue full |
| **GINST:STL_NSEL** | GPU instruction stalls: not selected for issue but ready |
| **GINST:STL_OTHR** | GPU instruction stalls: other |
| **GINST:STL_SLP** | GPU instruction stalls: sleep |

# Approximation of GPU Calling Contexts to Understand Performance

- GPU code from C++ template-based programming models is complex
- NVIDIA GPUs collect flat PC samples
- Flat profiles for instantiations of complex C++ templates are inscrutable

- HPCToolkit reconstructs approximate GPU calling contexts
  - Reconstruct call graph from machine code
  - Infer calls at call sites
    - PC samples of call instructions indicate calls
      - Use call counts to apportion costs to call sites
    - PC samples in a routine



# Approximation of GPU Calling Contexts to Understand Performance

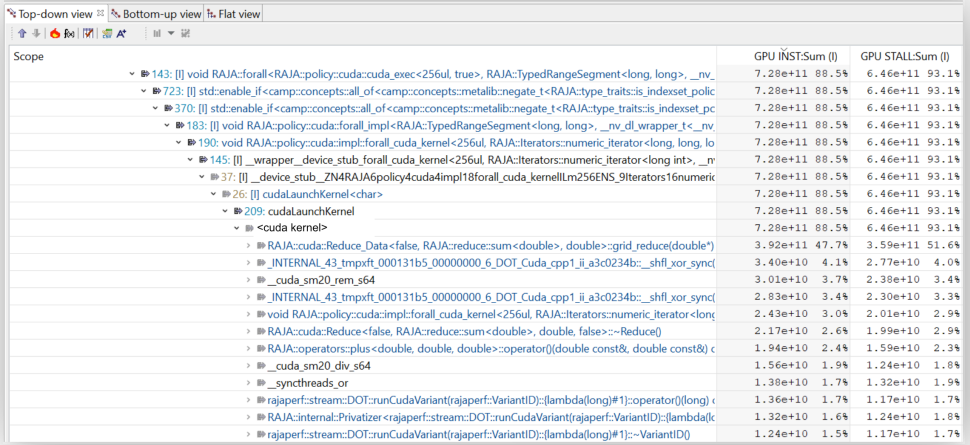
Top-down view | Bottom-up view | Flat view

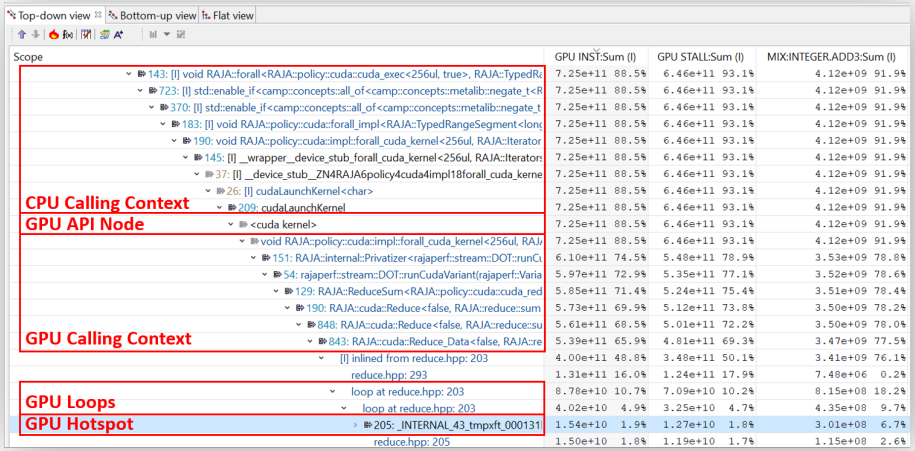
| Scope | GPU INST:Sum (I) | | GPU STALL:Sum (I) | |
|---|---|---|---|---|
| 143: [I] void RAJA::forall<RAJA::policy::cuda::cuda_exec<256ul, true>, RAJA::TypedRangeSegment<long, long>, __nv_ | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 723: [I] std::enable_if<camp::concepts::all_of<camp::concepts::metalib::negate_t<RAJA::type_traits::is_indexset_polic | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 370: [I] std::enable_if<camp::concepts::all_of<camp::concepts::metalib::negate_t<RAJA::type_traits::is_indexset_pc | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 183: [I] void RAJA::policy::cuda::forall_impl<RAJA::TypedRangeSegment<long, long>, __nv_dl_wrapper_t<__nv_ | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 190: void RAJA::policy::cuda::impl::forall_cuda_kernel<256ul, RAJA::Iterators::numeric_iterator<long, long, lo | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 145: [I] __wrapper__device_stub_forall_cuda_kernel<256ul, RAJA::Iterators::numeric_iterator<long int>, __n | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 37: [I] __device_stub__ZN4RAJA6policy4cuda4impl18forall_cuda_kernelILm256ENS_9Iterators16numeric | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 26: [I] cudaLaunchKernel<char> | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| 209: cudaLaunchKernel | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| <cuda kernel> | 7.28e+11 | 88.5% | 6.46e+11 | 93.1% |
| RAJA::cuda::Reduce_Data<false, RAJA::reduce::sum<double>, double>::grid_reduce(double*) | 3.92e+11 | 47.7% | 3.59e+11 | 51.6% |
| _INTERNAL_43_tmpxft_000131b5_00000000_6_DOT_Cuda_cpp1_ii_a3c0234b::__shfl_xor_sync( | 3.40e+10 | 4.1% | 2.77e+10 | 4.0% |
| __cuda_sm20_rem_s64 | 3.01e+10 | 3.7% | 2.38e+10 | 3.4% |
| _INTERNAL_43_tmpxft_000131b5_00000000_6_DOT_Cuda_cpp1_ii_a3c0234b::__shfl_xor_sync( | 2.83e+10 | 3.4% | 2.30e+10 | 3.3% |
| void RAJA::policy::cuda::impl::forall_cuda_kernel<256ul, RAJA::Iterators::numeric_iterator<long | 2.43e+10 | 3.0% | 2.01e+10 | 2.9% |
| RAJA::cuda::Reduce<false, RAJA::reduce::sum<double>, double, false>::~Reduce() | 2.17e+10 | 2.6% | 1.99e+10 | 2.9% |
| RAJA::operators::plus<double, double, double>::operator()(double const&, double const&) c | 1.94e+10 | 2.4% | 1.59e+10 | 2.3% |
| __cuda_sm20_div_s64 | 1.56e+10 | 1.9% | 1.24e+10 | 1.8% |
| __syncthreads_or | 1.38e+10 | 1.7% | 1.32e+10 | 1.9% |
| rajaperf::stream::DOT::runCudaVariant(rajaperf::VariantID)::{lambda(long)#1}::operator()(long) c | 1.36e+10 | 1.7% | 1.17e+10 | 1.7% |
| RAJA::internal::Privatizer<rajaperf::stream::DOT::runCudaVariant(rajaperf::VariantID)::{lambda(lc | 1.32e+10 | 1.6% | 1.24e+10 | 1.8% |
| rajaperf::stream::DOT::runCudaVariant(rajaperf::VariantID)::{lambda(long)#1}::~VariantID() | 1.24e+10 | 1.5% | 1.17e+10 | 1.7% |

# Approximation of GPU Calling Contexts to Understand Performance

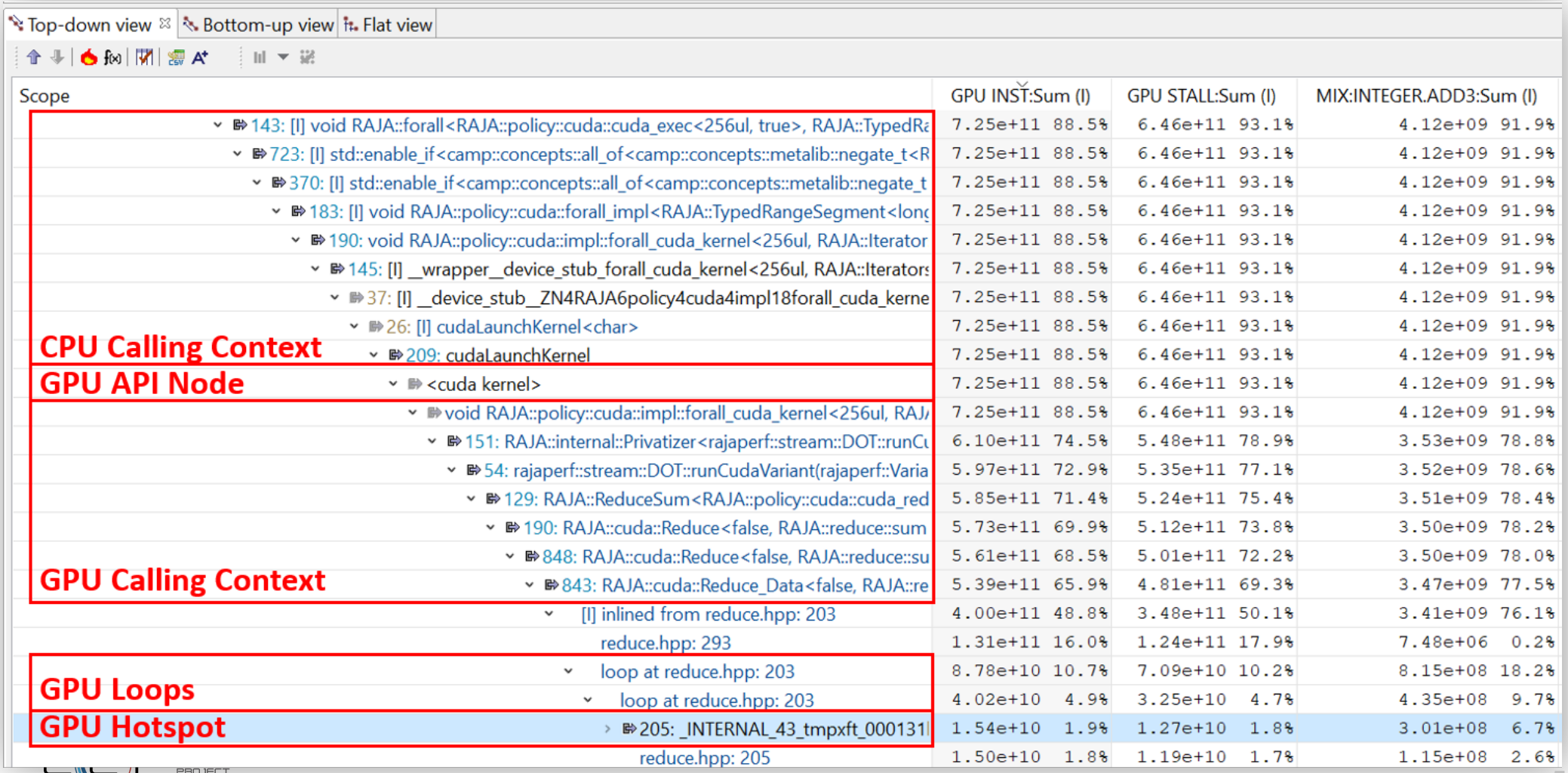
- GPU code from C++ template-based programming models is complex
- NVIDIA GPUs collect flat PC samples
- Flat profiles for instantiations of complex C++ templates are inscrutable

- HPCToolkit reconstructs approximate GPU calling contexts
  - PC samples of call instructions indicate calls
    - Use counts to split costs
  - PC samples in a routine
    - Infer caller or distribute costs equally to potential callers



# Approximation of GPU Calling Contexts to Understand Performance



# Accuracy of GPU Calling Context Recovery: Case Studies

- **Compute approximate call counts as the basis for partitioning the cost of function invocations across call sites**
  - Use call samples at call sites, data flow analysis to propagate call approximation upward
    - if samples were collected in some function f, if no calls to f were sampled, equally attribute f to each of its call sites
  - How accurate is our approximation?
- **Evaluation methodology**
  - Use NVIDIA's nvbit to
    - instrument call and return for GPU functions
    - instrument basic blocks to collect block histogram

# Accuracy of GPU Calling Context Recovery: Case Studies

- **Error partitioning a function's cost among call sites**

$$Error = \sqrt{\sum_{i=0}^{n-1} \frac{\left(\sqrt{\sum_{j=0}^{i_c-1} \frac{(f_N(i,j)-f_H(i,j))^2}{i_c}}\right)^2}{n}}$$

geometric mean across GPU functions of (root mean square error of call attribution across all of a function's call sites comparing our approximation vs. attribution using exact nvbit measurements)

- **Experimental study**

| Test Case | Unique Call Paths | Error |
|---|---|---|
| Basic_INIT_VIEW1D_OFFSET | 9 | 0 |
| Basic_REDUCE3_INT | 113 | 0.03 |
| Stream_DOT | 60 | 0.006 |
| Stream_TRIAD | 5 | 0 |
| Apps_PRESSURE | 6 | 0 |
| Apps_FIR | 5 | 0 |
| Apps_DEL_DOT_VEC_2D | 3 | 0 |
| Apps_VOL3D | 4 | 0 |

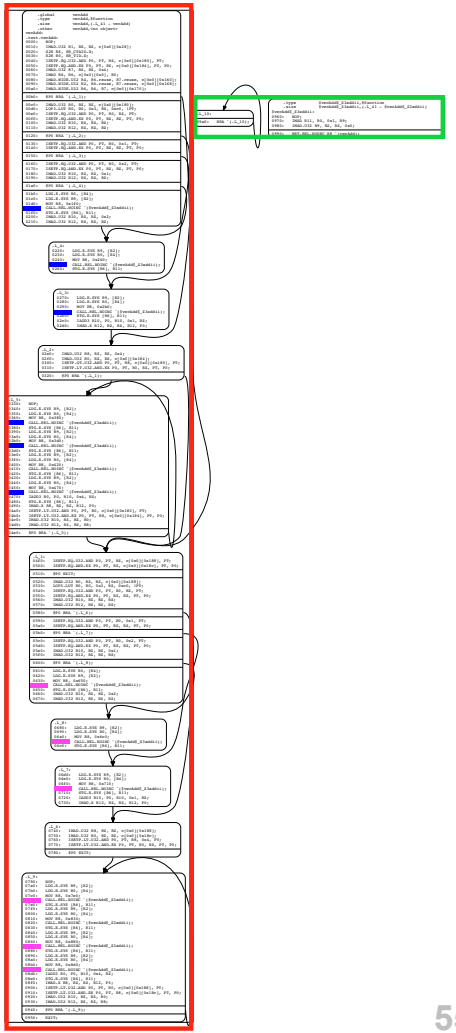
# Costs of GPU Functions Distributed Among Their Call Sites

- **Use call site frequency approximation**
- **Use Gprof assumption: all calls to a function incur exactly the same cost**
  - known to not be true in all cases, but a useful assumption nevertheless

# GPU call site attribution example

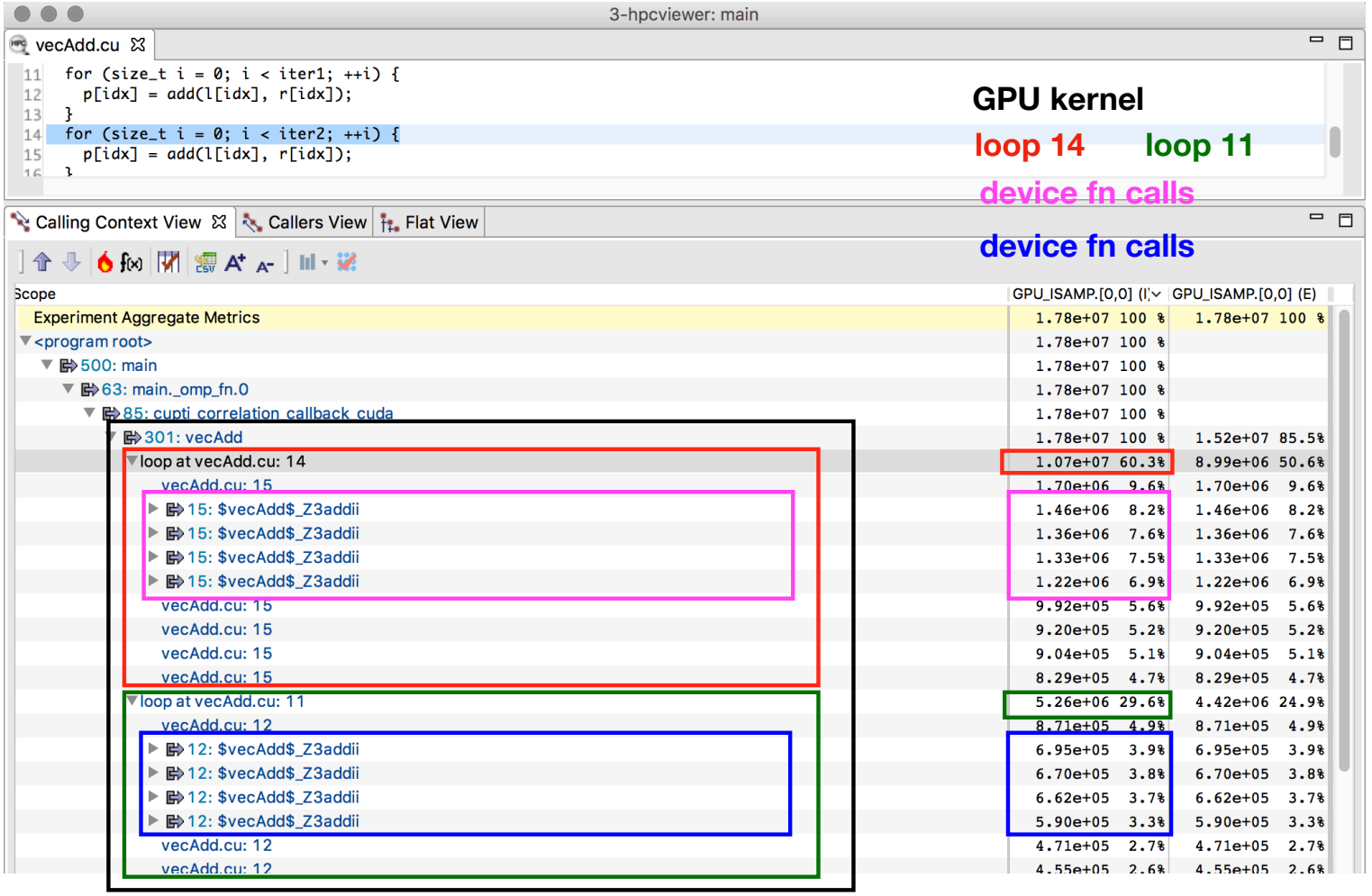
- **Case study: call function GPU “vectorAdd”***
  - iter1 = N
  - iter2 = 2N

```
1  __device__
2  int __attribute__ ((noinline)) add(int a, int b) {
3    return a + b;
4  }
5
6
7  extern "C"
8  __global__
9  void vecAdd(int *l, int *r, int *p, size_t N, size_t iter1,
       size_t iter2) {
10   size_t idx = blockDim.x * blockIdx.x + threadIdx.x;
11   for (size_t i = 0; i < iter1; ++i) {
12     p[idx] = add(l[idx], r[idx]);
13   }
14   for (size_t i = 0; i < iter2; ++i) {
15     p[idx] = add(l[idx], r[idx]);
16   }
17 }
18
```



Note: the computation by the function is synthetic and is not a vector addition. The name came from code that was hacked to perform an unrelated computation.

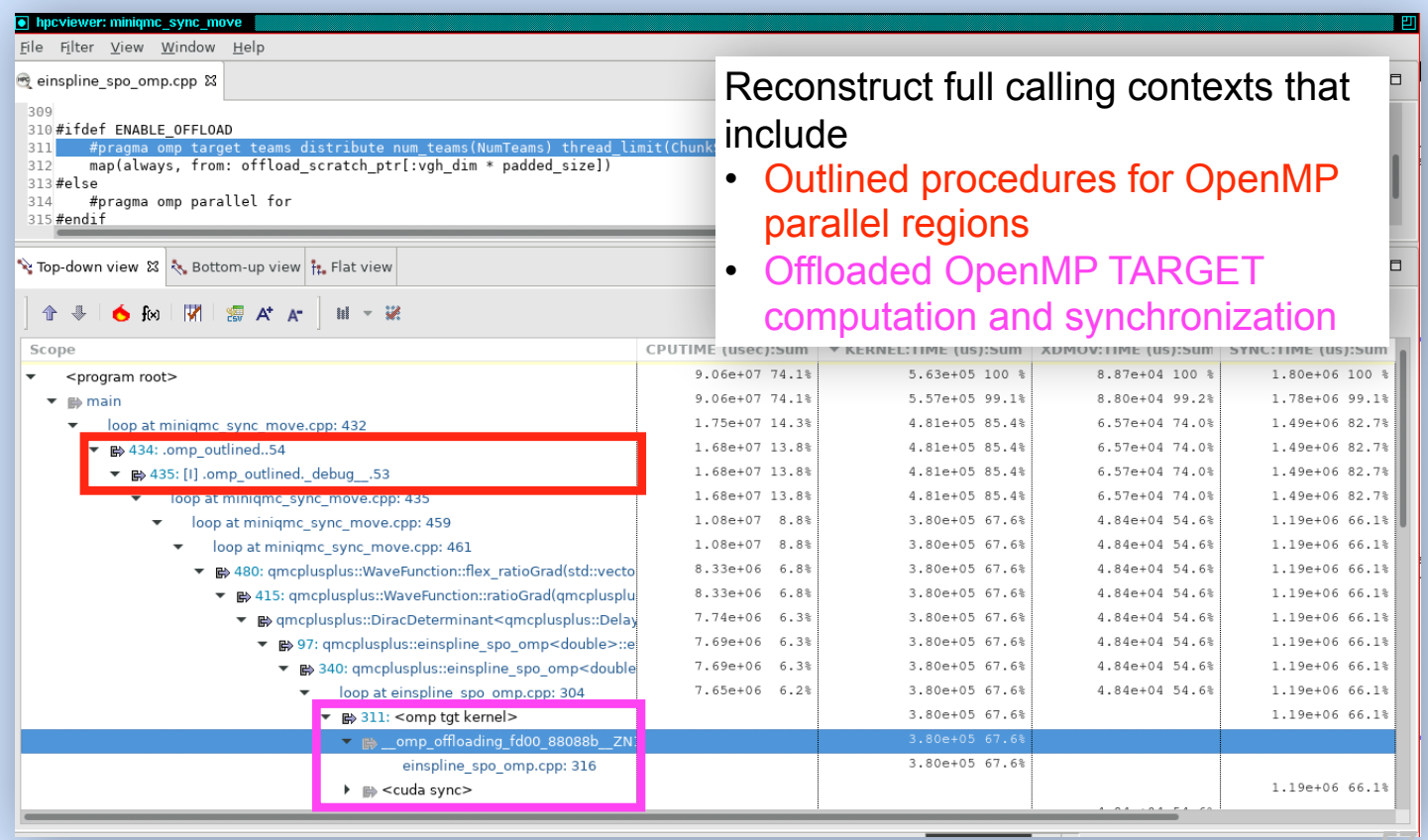
# Profiling Result for GPU-accelerated Example



# Support for OpenMP TARGET

- HPCToolkit implementation of OMPT OpenMP API
  - host monitoring
    - leverages callbacks for regions, threads, tasks
    - employs OMPT API for call stack introspection
  - GPU monitoring
    - leverages callbacks for device initialization, kernel launch, data operations
  - reconstruction of user-level calling contexts
- Leverages implementation of OMPT in LLVM OpenMP and libomptarget

ECP QMCPACK Project: miniqmc using OpenMP TARGET (Power9 + NVIDIA V100)



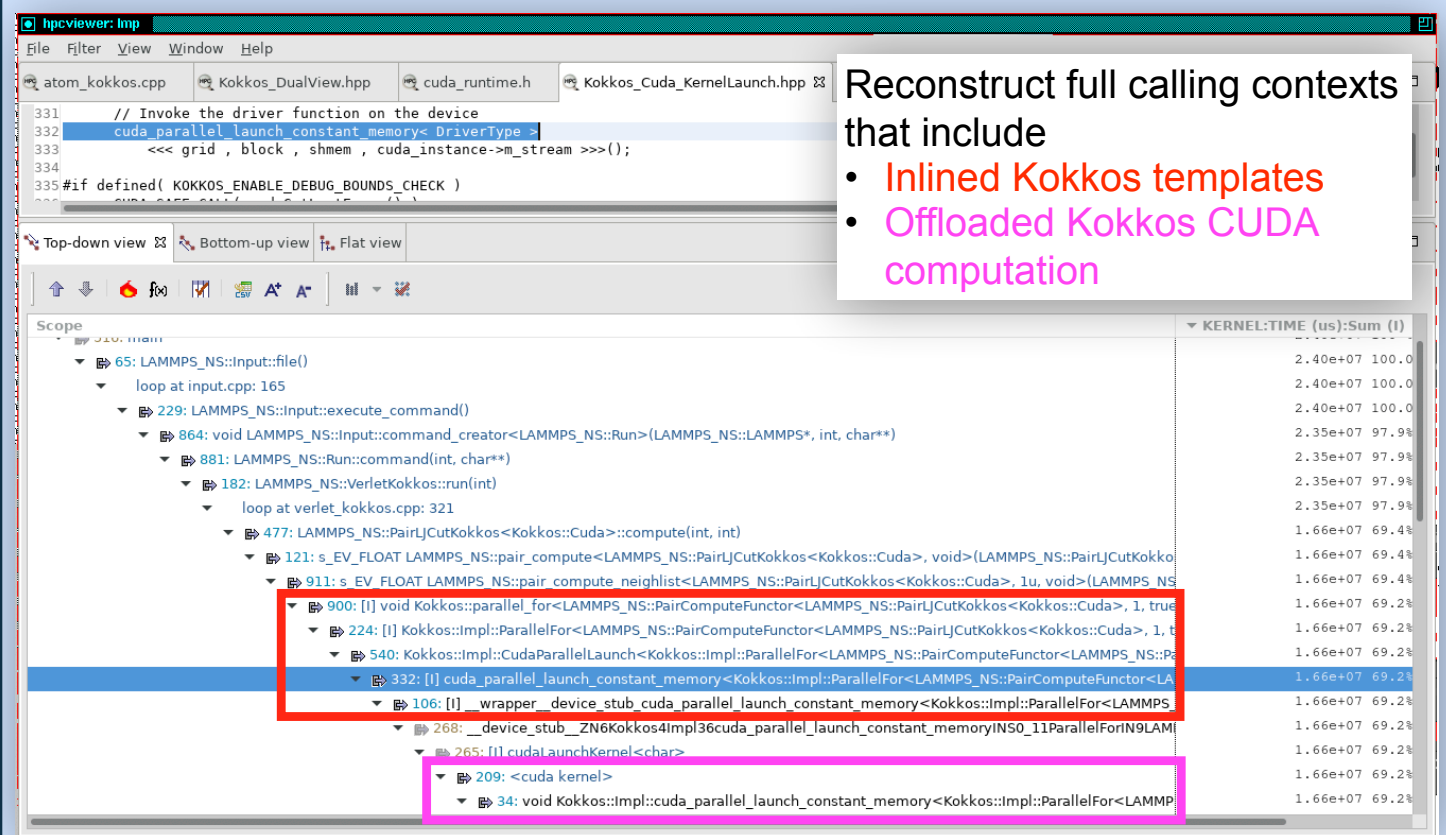

Reconstruct full calling contexts that include

- Outlined procedures for OpenMP parallel regions
- Offloaded OpenMP TARGET computation and synchronization

# Support for RAJA and and Kokkos C++ Template-based Models

- RAJA and Kokkos provide portability layers atop C++ template-based programming abstractions
- HPCToolkit employs binary analysis to recover information about procedures, inlined functions and templates, and loops
  - Enables both developers and users to understand complex template instantiation present with these models

ECP EXAALT Project: lammps using Kokkos over CUDA (Power9 + NVIDIA V100)



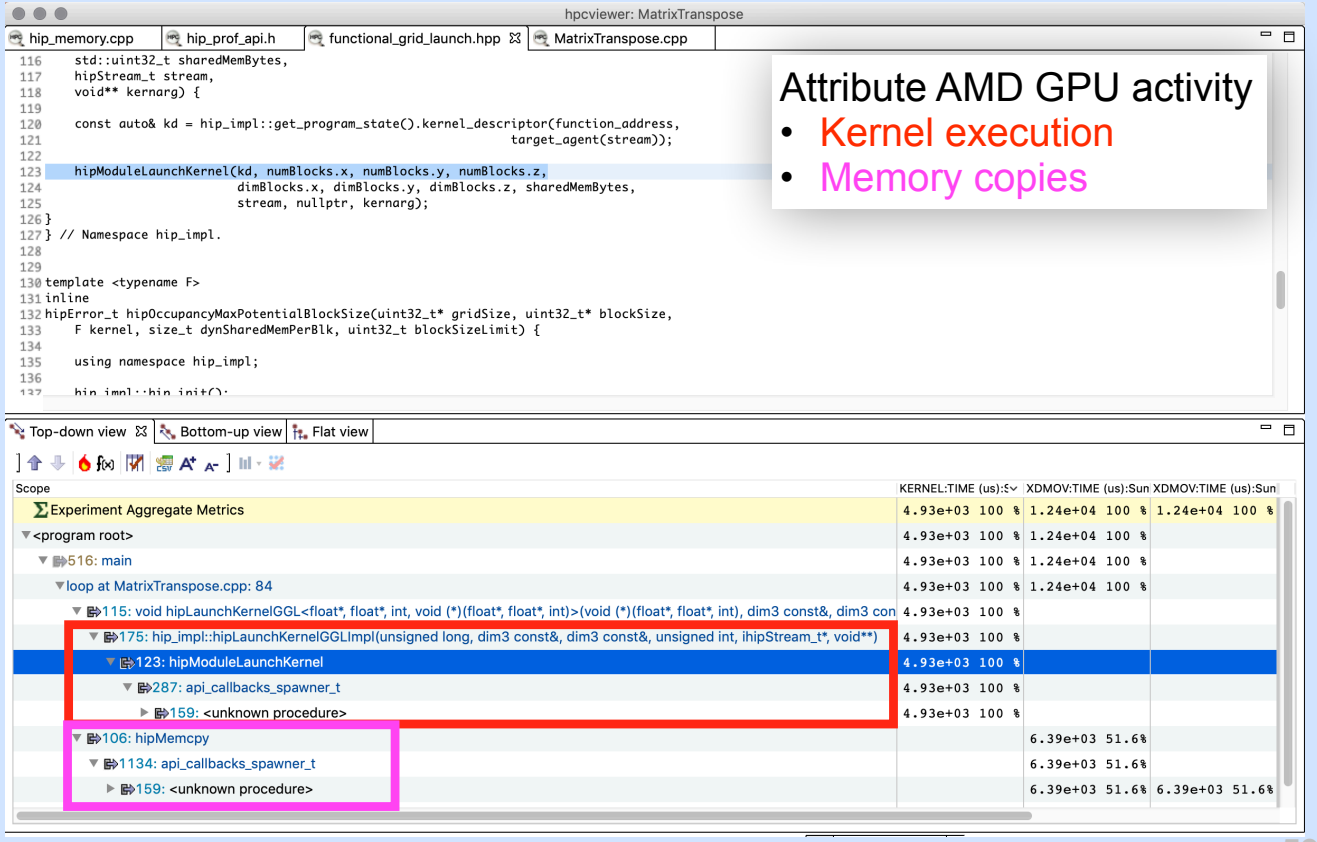

Reconstruct full calling contexts that include

- Inlined Kokkos templates
- Offloaded Kokkos CUDA computation

# Prototype Integration with AMD's Roctracer GPU Monitoring Framework

- Use AMD Roctracer activity API to trace GPU activity
  - kernel launches
  - explicit memory copies
- Current prototype supports AMD's HIP programming model

## AMD MatrixTranspose Testcase for Roctracer (AMD Ryzen + AMD 580 GPU)



# HPCToolkit Challenges and Limitations

- **Fine-grain measurement and attribution of GPU performance**
  - PC sampling overhead on NIVIDIA GPUs is currently very high: a function of NVIDIA's CUPTI implementation
  - Currently, no hardware support for fine-grain measurement on Intel and AMD GPUs
- **GPU tracing in HPCToolkit**
  - Creates one tool thread per GPU stream when tracing
  - OK for a small number of streams but many streams can be problematic
- **Cost of call path sampling**
  - Call path unwinding of GPU kernel invocations is costly (~2x execution dilation for Laghos)
  - Best solution is to avoid some of it, e.g. sample GPU kernel invocations
- **Currently, hpcprof and hpcprof-mpi compute dense vectors of metrics**
  - Designed for few CPU metrics, not O(100) GPU metrics: space and time problem for analysis

# Outline

- **Performance measurement and analysis challenges for GPU-accelerated supercomputers**
- **Introduction to HPCToolkit performance tools**
  - Overview of HPCToolkit components and their workflow
  - HPCToolkit's graphical user interfaces and using them effectively
- **Analyzing the performance of GPU-accelerated supercomputers with HPCToolkit**
  - Overview of HPCToolkit's GPU performance measurement capabilities
  - Collecting measurements
  - Analysis and attribution
  - Exploring measurements and analysis results
- **Experiences with analysis and tuning of GPU-accelerated codes**
  - Computation, memory hierarchy, and data movement issues
- **Obtaining HPCToolkit**

# Analysis and Optimization Case Studies

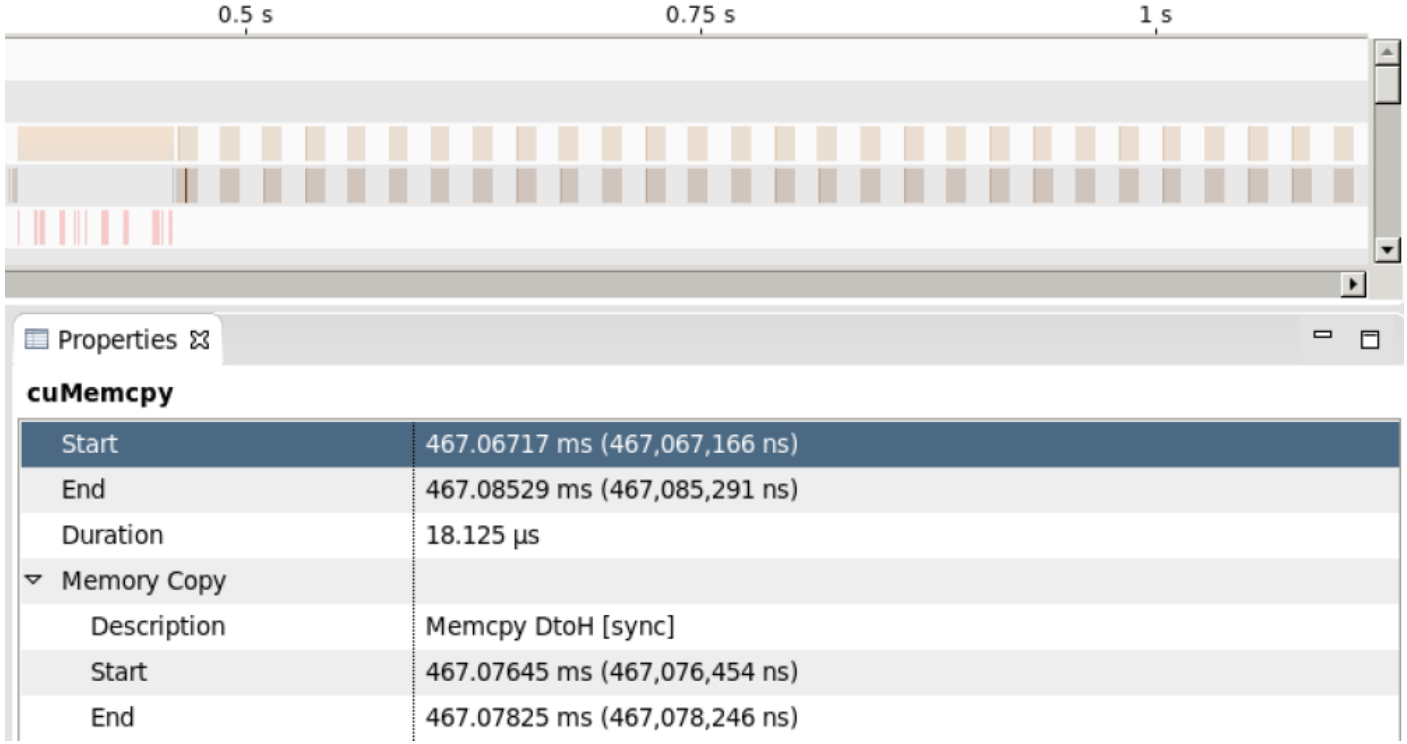
- **Environments**
  - Summit
    - cuda/10.1.168
    - gcc/6.4.0
  - Local
    - cuda/10.1.168
    - gcc/7.3.0

# Case 1: Locating Expensive GPU APIs with Profile View

- **Laghos**
  - 1 MPI process
  - 1 GPU stream per process

# nvprof: Doesn’t Report CPU Calling Context

- **Goal: Associate every GPU API with its CPU calling context**



# HPCToolkit: Metrics in Context Guide Analysis and Optimization

| Scope | XDMOV_IMPORTANCE |
|---|---|
| <cuda copy> | 13.23 % |
| 72: mfem::rmemcpy::rDtoD(void*, void const*, unsigned long, bool) | 6.83 % |
| 34: [I] mfem::CudaVector::SetSize(unsigned long, void const*) | 6.83 % |
| 109: mfem::CudaVector::operator=(mfem::CudaVector const&) | 6.83 % |
| 49: mfem::CudaProlongationOperator::MultTranspose(mfem::CudaVector const&, mfen | 2.20 % |
| 86: mfem::CudaRAPOperator::Mult(mfem::CudaVector const&, mfem::CudaVector&) | 2.14 % |
| 245: mfem::hydrodynamics::LagrangianHydroOperator::Mult(mfem::CudaVector con: | 0.06 % |
| 29: mfem::CudaProlongationOperator::Mult(mfem::CudaVector const&, mfem::CudaVec | 2.20 % |
| 84: mfem::CudaRAPOperator::Mult(mfem::CudaVector const&, mfem::CudaVector&) | 2.14 % |
| 256: mfem::hydrodynamics::LagrangianHydroOperator::Mult(mfem::CudaVector con: | 0.06 % |
| 130: mfem::hydrodynamics::CudaMassOperator::Mult(mfem::CudaVector const&, mfem | 2.14 % |
| 212: mfem::hydrodynamics::LagrangianHydroOperator::Mult(mfem::CudaVector const& | 0.15 % |
| 39: mfem::CudaCGSolver::h_Mult(mfem::CudaVector const&, mfem::CudaVector&) cons | 0.12 % |
| 436: main | 0.01 % |
| 61: cuVectorDot(unsigned long, double const*, double const*) | 6.16 % |

Case 1

Case 2

Case 3

# Laghos Insight: Frequent, Small Data Transfers

- **A small amount of memory is transferred from device to host, repeated 197000 times**

| Scope | GXCOPY (s):Sum (I) | GXCOPY:COUNT:Sum (I) | GXCOPY:D2H (B):Sum (I) |
|---|---|---|---|
| 61: cuVectorDot(unsigned long, double const*, double const*) | 3.67e-01 46.3% | 1.97e+05 37.9% | 7.81e+06 20.4% |

- **Avoid the cost of the transfer between pageable and pinned host arrays by directly allocating a host array in pinned memory**
  - Use pinned memory when data movement frequency is high but size is small

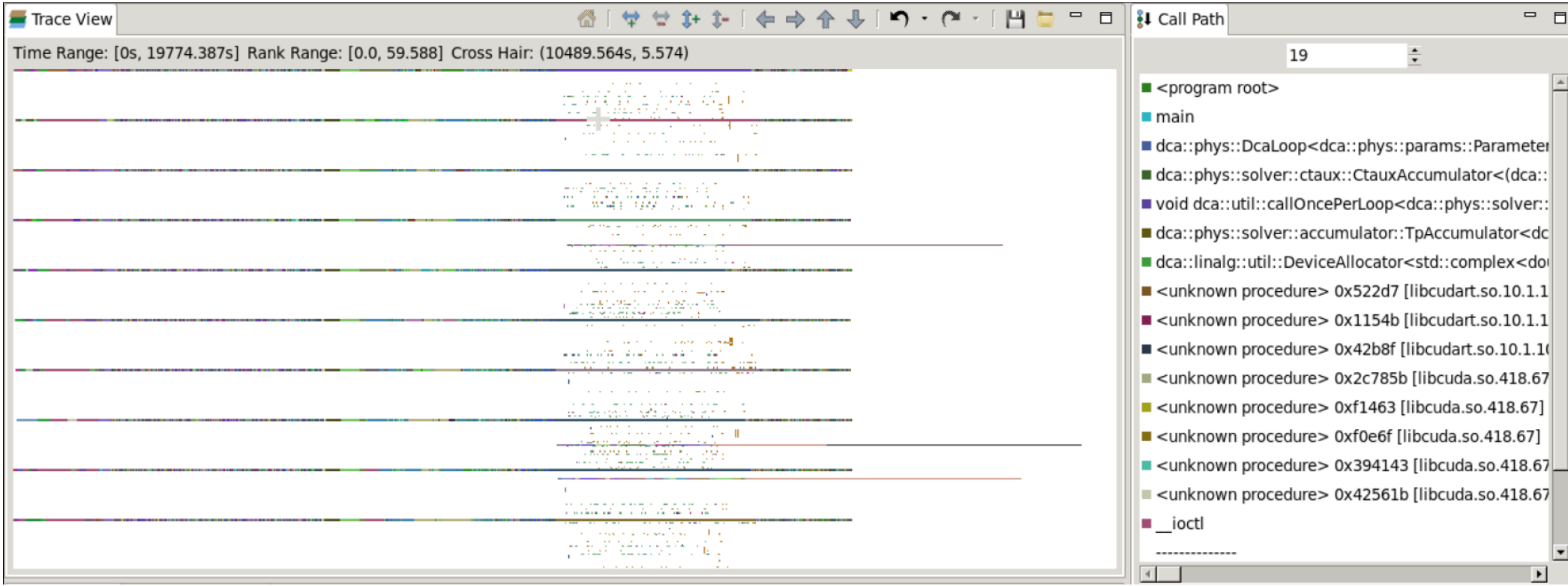
# Case 2: Trace Multi-process Applications

- **DCA++**
  - 60 MPI processes
  - 128 GPU streams per process
- **Nyx**
  - 6 MPI processes
  - 16 GPU stream per process

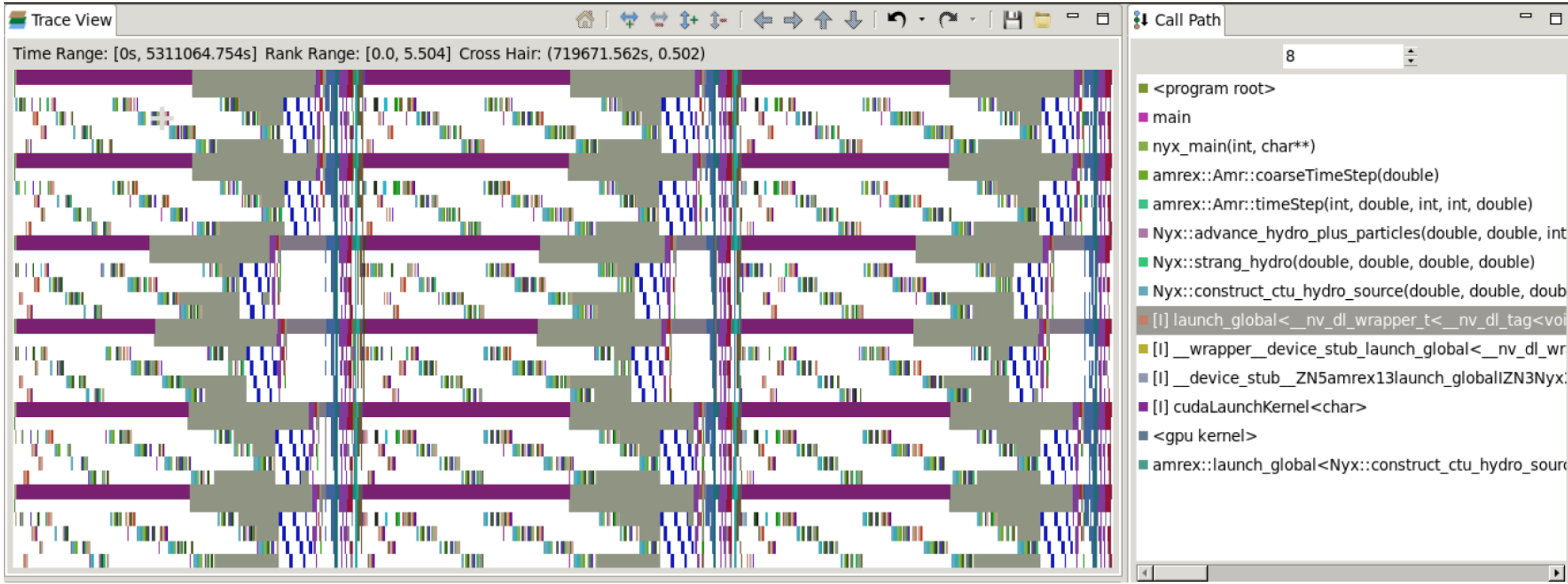
# nvprof: Non-scalable Tracing of DCA++

- **nvprof**
  - With CPU profiling enabled, hangs on Summit
  - Without CPU profiling
    - Collects 1.1 GB data
- **HPCToolkit**
  - CPU+GPU hybrid profiling with full calling context
    - Collects 0.13 GB data
    - Data can be further reduced by sampling GPU events

# DCA++ Trace View: 60 MPI Ranks / 128 Streams Each

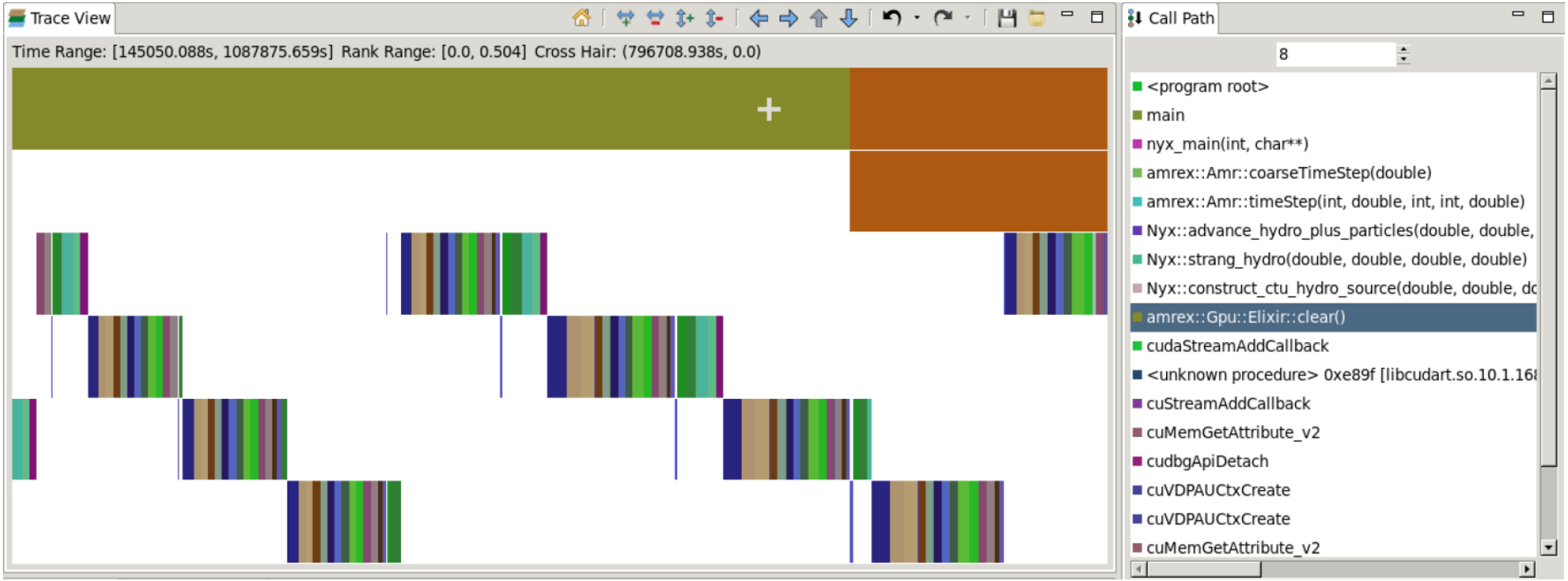


# Nyx Trace View: 5 MPI Ranks / 4 GPU Streams Each



# Nyx Insight: Insufficient GPU Stream Parallelism

- **On GPU, streams are not working concurrently**



# Nyx cudaCallBack Issue

- **On CPU, amrex::Gpu::Elixir::clear() invokes stream callbacks**

```
33 void
34 Elixir::clear () noexcept
35 {
36 #ifdef AMREX_USE_GPU
37     if (Gpu::inLaunchRegion())
38     {
39         if (m_p != nullptr) {
40             void** p = static_cast<void**>(std::malloc(2*sizeof(void*)));
41             p[0] = m_p;
42             p[1] = (void*)m_arena;
43             AMREX_HIP_OR_CUDA(
44                 AMREX_HIP_SAFE_CALL ( hipStreamAddCallback(Gpu::gpuStream(),
45                                                            amrex_elixir_delete, p, 0));,
46                 AMREX_CUDA_SAFE_CALL(cudaStreamAddCallback(Gpu::gpuStream(),
47                                                            amrex_elixir_delete, p, 0)););
48             Gpu::callbackAdded();
49         }
50     }
51     else
52 #endif
```

# Nyx Performance Insight

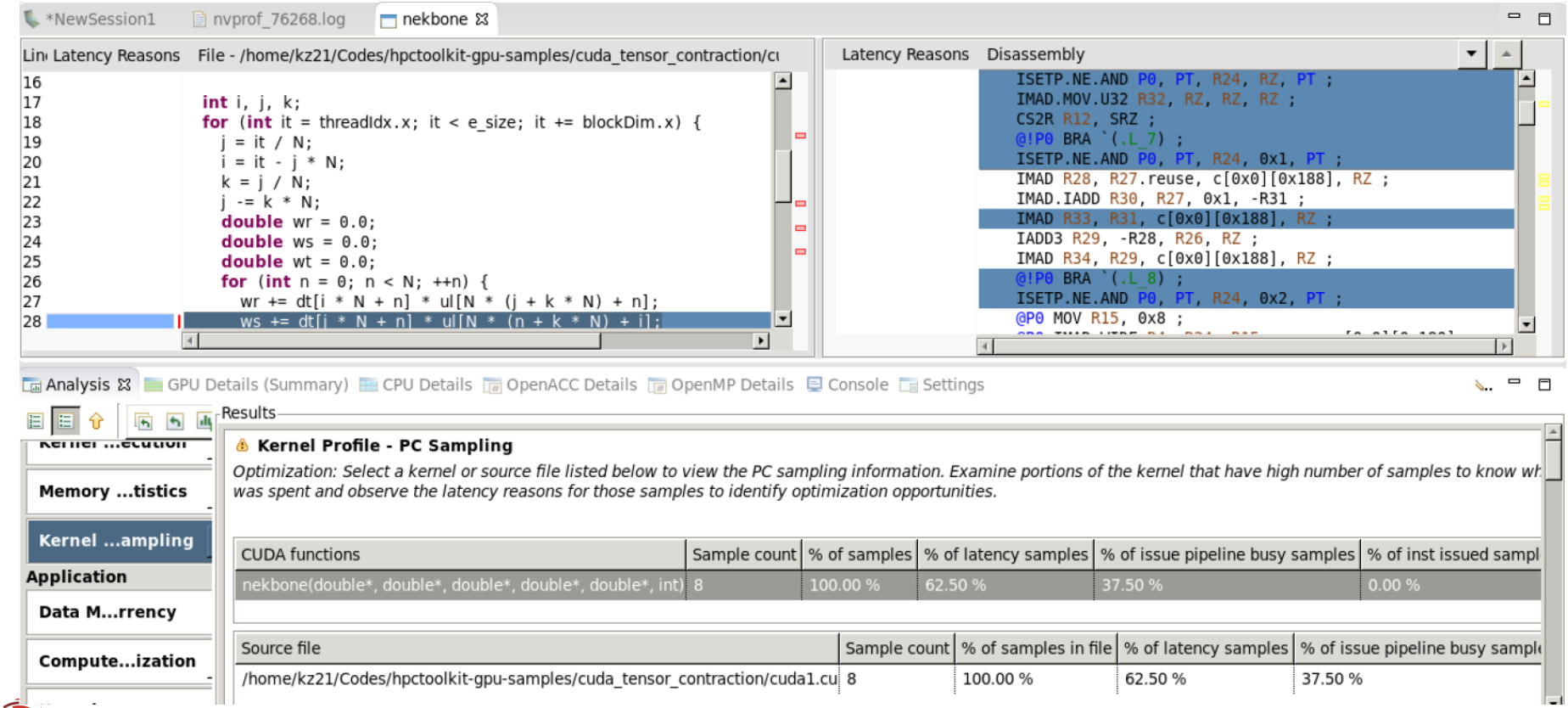
- **A bug present in the current version of CUDA (10.1). If a callBack is called in a place where multiple streams are used, the device kernels artificially synchronize and have no overlap.**
- **Fixed in CUDA-10.2?**
- **Workaround**
  - The Elixir object holds a copy of the data pointer to prevent it from being destroyed before the related device kernels are completed
  - Allocate new objects outside the compute loop and delete them after work completes

# Case 3: Fine-grained GPU Kernel Tuning

- **Nekbone: A lightweight subset of Nek5000 that mimics the essential computational complexity of Nek5000**

# nvprof: Limited source level performance metrics

- **No loop structure, No GPU calling context, No instruction mix**



# Nekbone Profile View

cuda1.cu | gpu-op-placeholders.c

```
16
17  int i, j, k;
18  for (int it = threadIdx.x; it < e_size; it += blockDim.x) {
19    j = it / N;
20    i = it - j * N;
21    k = j / N;
22    j -= k * N;
23    double wr = 0.0;
```

Top-down view | Bottom-up view | Flat view

| Scope | GINS:Sum (I) | GINS:Sum (E) |
|---|---|---|
| 516: main | 6.59e+08 100 % | |
| 150: [I] nekbone | 6.59e+08 100 % | |
| 2: __device_stub__Z7nekbonePdS_S_S_S_i(double*, double*, double*, double*, double*, int) | 6.59e+08 100 % | |
| 13: [I] cudaLaunchKernel<char> | 6.59e+08 100 % | |
| 209: <gpu kernel> | 6.59e+08 100 % | |
| 174: nekbone(double*, double*, double*, double*, double*, int) | 6.59e+08 100 % | 6.59e+08 100 % |
| loop at cuda1.cu: 18 | 3.17e+08 48.1% | 3.17e+08 48.1% |
| loop at cuda1.cu: 39 | 2.21e+08 33.6% | 2.21e+08 33.6% |
| loop at cuda1.cu: 11 | 6.47e+07 9.8% | 6.47e+07 9.8% |
| cuda1.cu: 39 | 3.30e+07 5.0% | 3.30e+07 5.0% |
| cuda1.cu: 11 | 1.31e+07 2.0% | 1.31e+07 2.0% |
| cuda1.cu: 15 | 2.76e+06 0.4% | 2.76e+06 0.4% |

# Performance Insight 1: Execution Dependency

- **The hotspot statement is waiting for *j* and *k***

cuda1.cu

```
14
15  __syncthreads();
16
17  int i, j, k;
18  for (int it = threadIdx.x; it < e_size; it += blockDim.x) {
19    j = it / N;
20    i = it - j * N;
21    k = j / N;
22    j -= k * N;
23    double wr = 0.0;
24    double ws = 0.0;
25    double wt = 0.0;
26    for (int n = 0; n < N; ++n) {
27      wr += dt[i * N + n] * ul[N * (j + k * N) + n];
28      ws += dt[j * N + n] * ul[N * (n + k * N) + i];
29      wt += dt[k * N + n] * ul[N * (j + n * N) + i];
30    }
```

Top-down view | Bottom-up view | Flat view

| Scope | GINS:Sum (I) | GINS:Sum (E) | GINS:STL_ANY:Sl | GINS:STL_ANY:Sl | GI |
|---|---|---|---|---|---|
| 209: <gpu kernel> | 6.59e+08 100 % | | 3.70e+08 100 % | | 3.0 |
| 174: nekbone(double*, double*, double*, double*, double*, int) | 6.59e+08 100 % | 6.59e+08 100 % | 3.70e+08 100 % | 3.70e+08 100 % | 3.0 |
| loop at cuda1.cu: 18 | 3.17e+08 48.1% | 3.17e+08 48.1% | 1.79e+08 48.3% | 1.79e+08 48.3% | 6.1 |
| cuda1.cu: 27 | 8.80e+07 13.4% | 8.80e+07 13.4% | 4.92e+07 13.3% | 4.92e+07 13.3% | 1.1 |
| cuda1.cu: 32 | 7.72e+07 11.7% | 7.72e+07 11.7% | 5.36e+07 14.5% | 5.36e+07 14.5% | |
| cuda1.cu: 28 | 5.95e+07 9.0% | 5.95e+07 9.0% | 3.25e+07 8.8% | 3.25e+07 8.8% | |
| cuda1.cu: 29 | 5.19e+07 7.9% | 5.19e+07 7.9% | 2.95e+07 8.0% | 2.95e+07 8.0% | |

# Strength Reduction

- **MISC.CONVERT: I2F, F2I, MUFU instructions**
  - NVIDIA GPUs convert integer to float for division
  - Division is a latency and low throughput instruction
- **Replace *j = it / N* by *j = it x (1/N)* and precompute *1/N***

```
18  for (int it = threadIdx.x; it < e_size; it += blockDim.x) {
19    j = it / N;
20    i = it - j * N;
21    k = j / N;
22    j -= k * N;
23    double wr = 0.0;
24    double ws = 0.0;
25    double wt = 0.0;
26    for (int n = 0; n < N; ++n) {
27      wr += dt[i * N + n] * ul[N * (j + k * N) + n];
```

Top-down view | Bottom-up view | Flat view

| Scope | MISC.CONVERT:Sum (I) | MISC.CONVERT:Sum (E) |
|---|---|---|
| 174: nekbone(double*, double*, d | 2.01e+05 100 % | 2.01e+05 100 % |
| loop at cuda1.cu: 18 | 1.02e+05 51.0% | 1.02e+05 51.0% |
| cuda1.cu: 27 | | |
| cuda1.cu: 32 | | |
| cuda1.cu: 28 | | |
| cuda1.cu: 29 | | |
| cuda1.cu: 19 | 1.02e+05 51.0% | 1.02e+05 51.0% |

# Coming Attraction: Instruction-level Analysis

**Separate GPU instructions into classes**

- **Memory operations**
  - instruction (load, store)
  - size
  - memory kind (global memory, texture memory, constant memory)
- **Floating point**
  - instruction (add, mul, mad)
  - size
  - compute unit (tensor unit, floating point unit)
- **Integer operations**
- **Control operations**
  - branches, calls

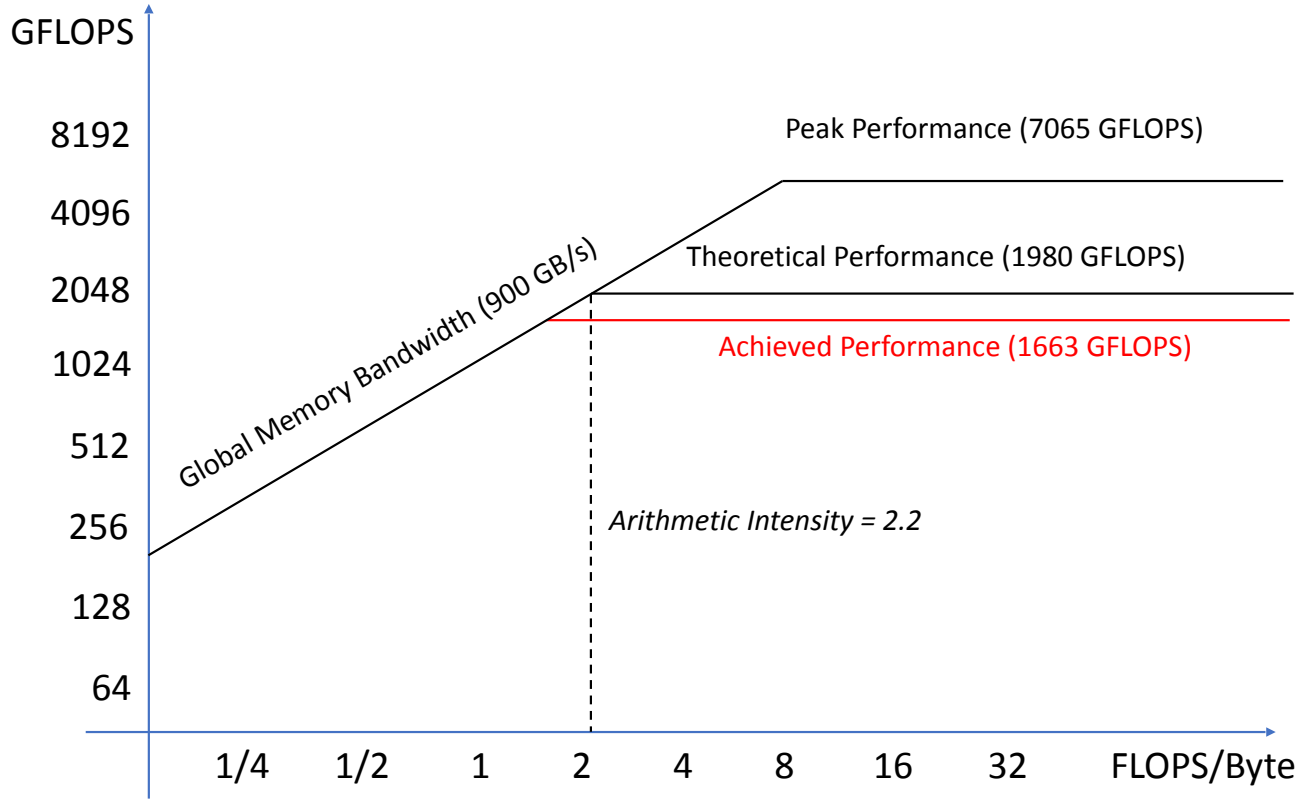
# Performance Insight 2: Instruction Throughput

- **Estimate instruction throughput based on pc samples**
- $THROUGHPUT = \frac{INS}{TIME}$
- $GFLOPS = THROUGHPUT_{DP}$
- $Arithmetic\ Intensity = \frac{THROUGHPUT_{GMEM}}{THROUGHPUT_{DP}}$

| Scope | MEMORY.LOAD.GLOBAL.64 | MEMORY.STORE.GLOBAL.64 | FLOAT.MAD.64:Sum | FLOAT.MUL.64:Sum | FLOAT.ADD.64:Sum |
|---|---|---|---|---|---|
| <program root> | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 516: main | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| [I] inlined from cuda4.cu: 2 | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 2: __device_stub__Z7nekboneP | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| [I] inlined from cuda_runtime.h | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 209: <gpu kernel> | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 174: nekbone(double*, | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |

# Roofline Analysis

- **83.9% of peak performance**



# Performance Insight 3: Unfused DMUL and DADD

- **DMUL:** $6.51 \times 10^5$
- **DADD:** $4.55 \times 10^5$
- **If all paired DMUL and DADD instructions are fused to MAD instructions**
  - $$\frac{\left(4.55 \times 10^5 + 3.08 \times 10^6\right)}{3.08 \times 10^6} = 14.7\%$$
  - 1663 GFLOPS × 114.7% = 1908 GFLOPS (99% of peak)

| Scope | MEMORY.LOAD.GLOBAL.64 | MEMORY.STORE.GLOBAL.64 | FLOAT.MAD.64:Sum | FLOAT.MUL.64:Sum | FLOAT.ADD.64:Sum |
|---|---|---|---|---|---|
| <program root> | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 516: main | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| [I] inlined from cuda4.cu: 2 | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 2: __device_stub__Z7nekboneP | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| [I] inlined from cuda_runtime.h | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 209: <gpu kernel> | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |
| 174: nekbone(double*, | 3.36e+05 100 % | 5.32e+04 100 % | 3.08e+06 100 % | 6.51e+05 100 % | 4.55e+05 100 % |

# Case Study Acknowledgements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# Outline

- **Performance measurement and analysis challenges for GPU-accelerated supercomputers**
- **Introduction to HPCToolkit performance tools**
  - Overview of HPCToolkit components and their workflow
  - HPCToolkit's graphical user interfaces and using them effectively
- **Analyzing the performance of GPU-accelerated supercomputers with HPCToolkit**
  - Overview of HPCToolkit's GPU performance measurement capabilities
  - Collecting measurements
  - Analysis and attribution
  - Exploring measurements and analysis results
- **Experiences with analysis and tuning of GPU-accelerated codes**
  - Computation, memory hierarchy, and data movement issues
- **Obtaining HPCToolkit**

# Installing HPCToolkit for Analysis of GPU-accelerated Codes

- **Complete instructions: http://hpctoolkit.org/software-instructions.html**
- **Sketch**
  - Clone spack
    - command: **`git clone https://github.com/spack/spack`**
  - Configure a packages.yaml file
    - specify your platform's installation of CUDA or ROCM
    - specify your platform's installation of MPI
    - use an appropriate GCC compiler
      - ensure that a GCC version >= 5 is on your path. typically, we use GCC 7.3
      - **`spack compiler find`**
  - Install software for your platform using spack
    - NVIDIA GPUs: **`spack install hpctoolkit +cuda +mpi`**
    - AMD GPUs: **`spack install hpctoolkit +rocm +mpi`**