ARGONNE
ATPESC 10
EXTREME-SCALE COMPUTING

HPCToolkit Performance Tools

Performance analysis of CPU and GPU-accelerated applications

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ECP Argonne NATIONAL LABORATORY

HPCToolkit Funding Acknowledgments

- Government
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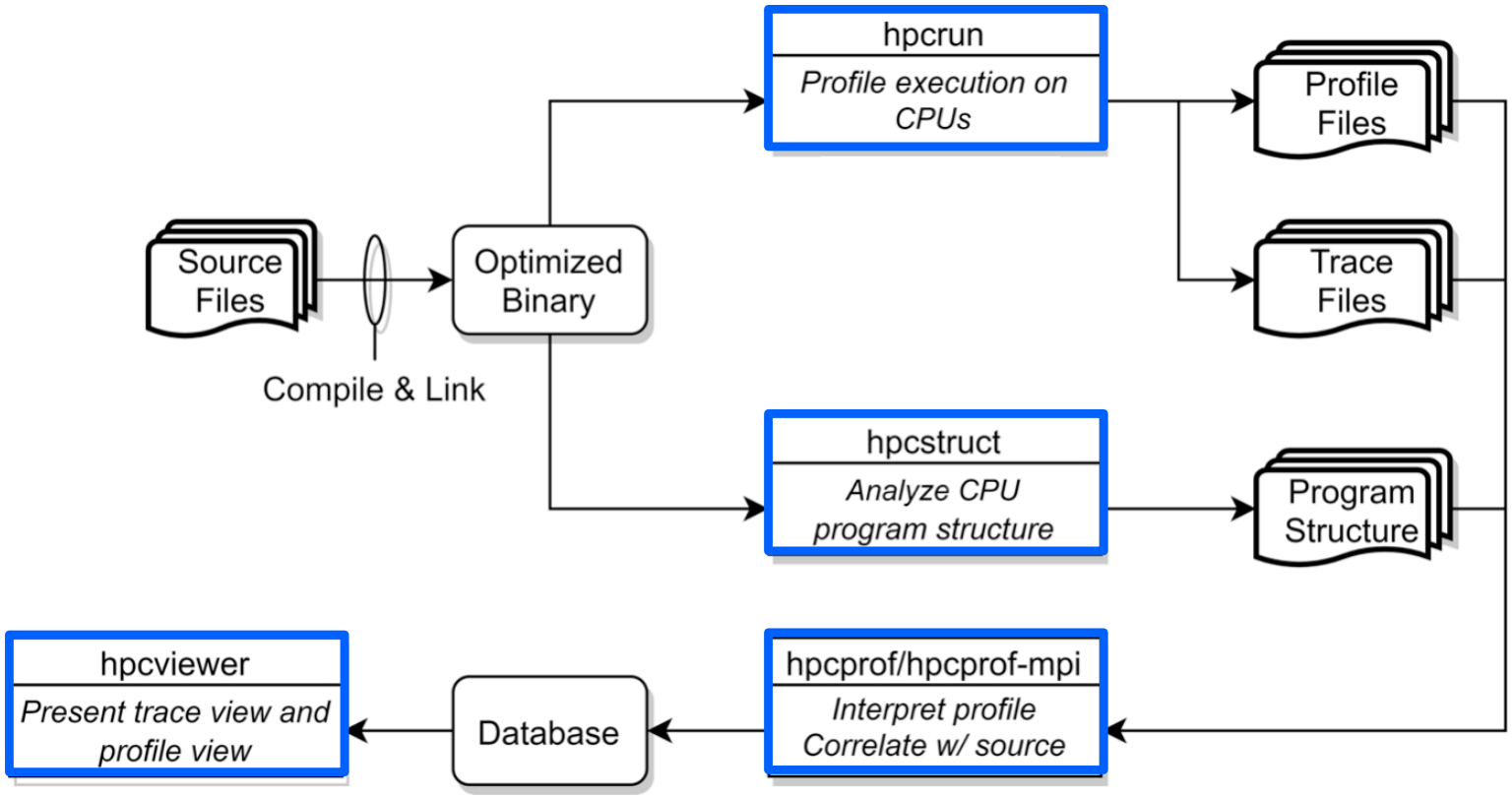
  - —Advanced Micro Devices
  - —Intel Corporation
  - —TotalEnergies EP Research & Technology USA, LLC.

Rice University's HPCToolkit Performance Tools

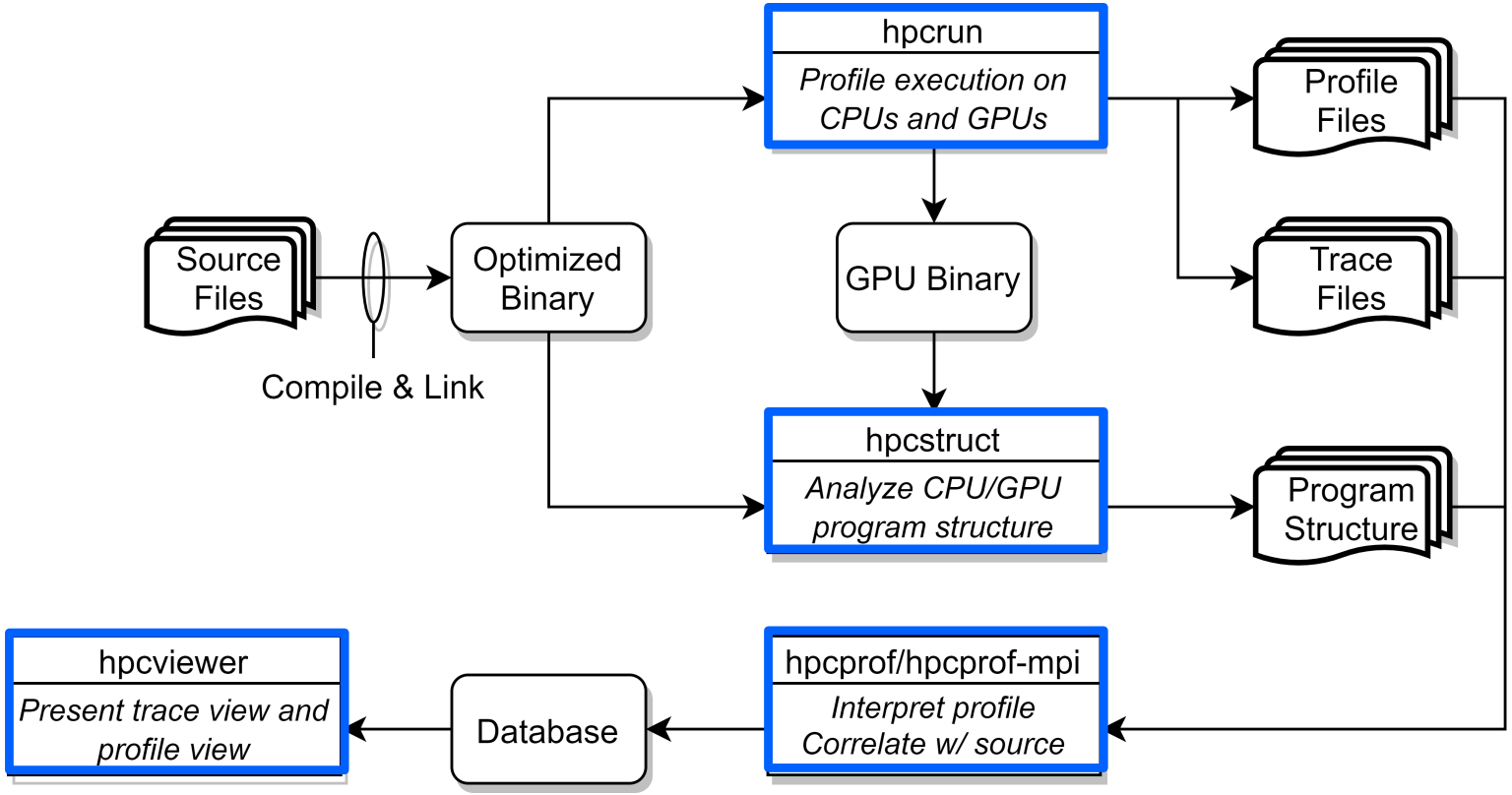
Measure and analyze performance of CPU and GPU-accelerated applications

- Easy: profile unmodified application binaries
- Fast: low-overhead measurement
- Informative: understand where an application spends its time and why
  - —call path profiles associate metrics with application source code contexts
  - —optional hierarchical traces to understand execution dynamics
- Broad audience
  - —application developers
  - —framework developers
  - —runtime and tool developers

HPCToolkit's Workflow for CPU Applications



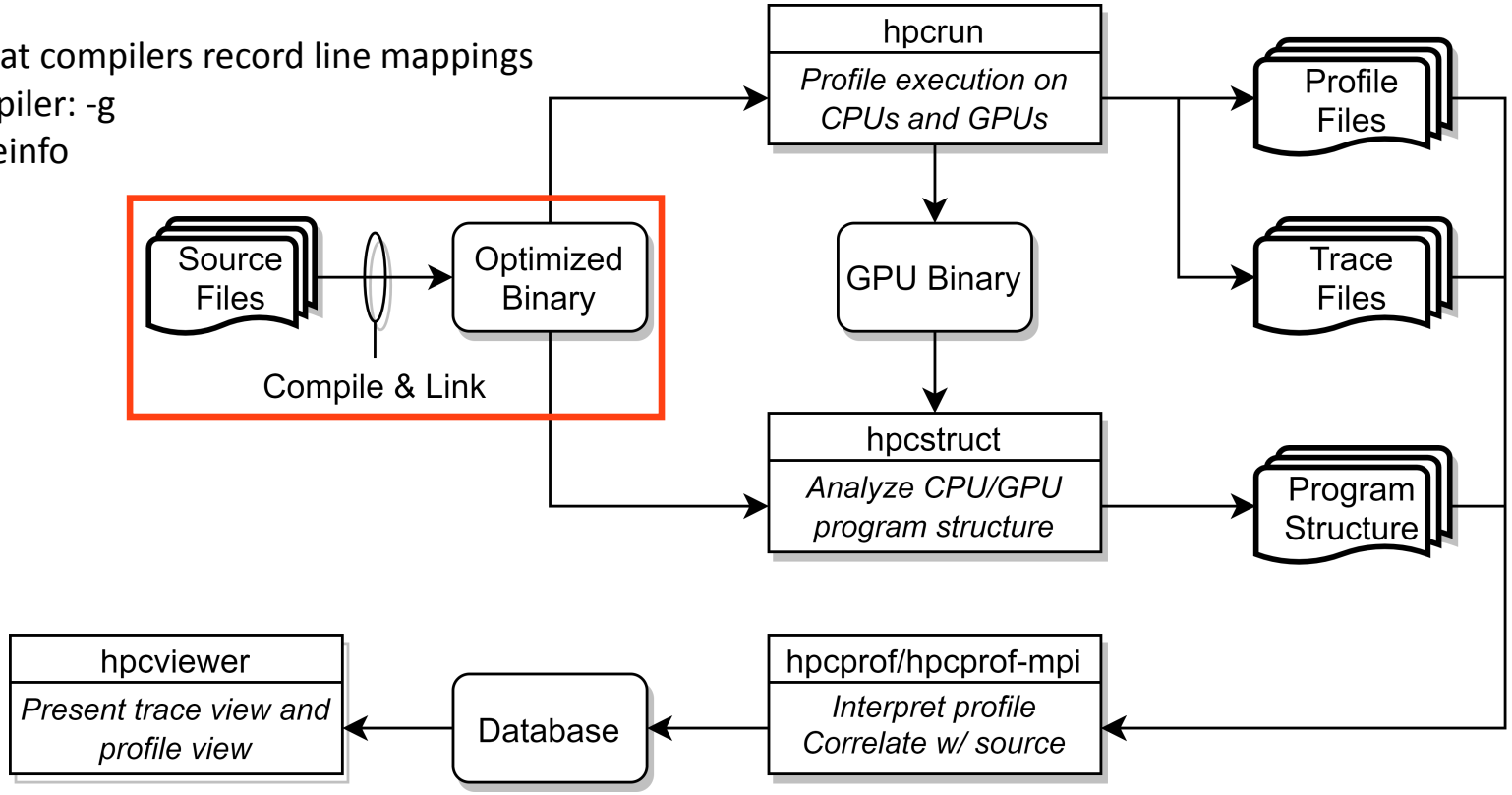
HPCToolkit's Workflow for GPU-accelerated Applications



HPCToolkit's Workflow for GPU-accelerated Applications

Step 1:

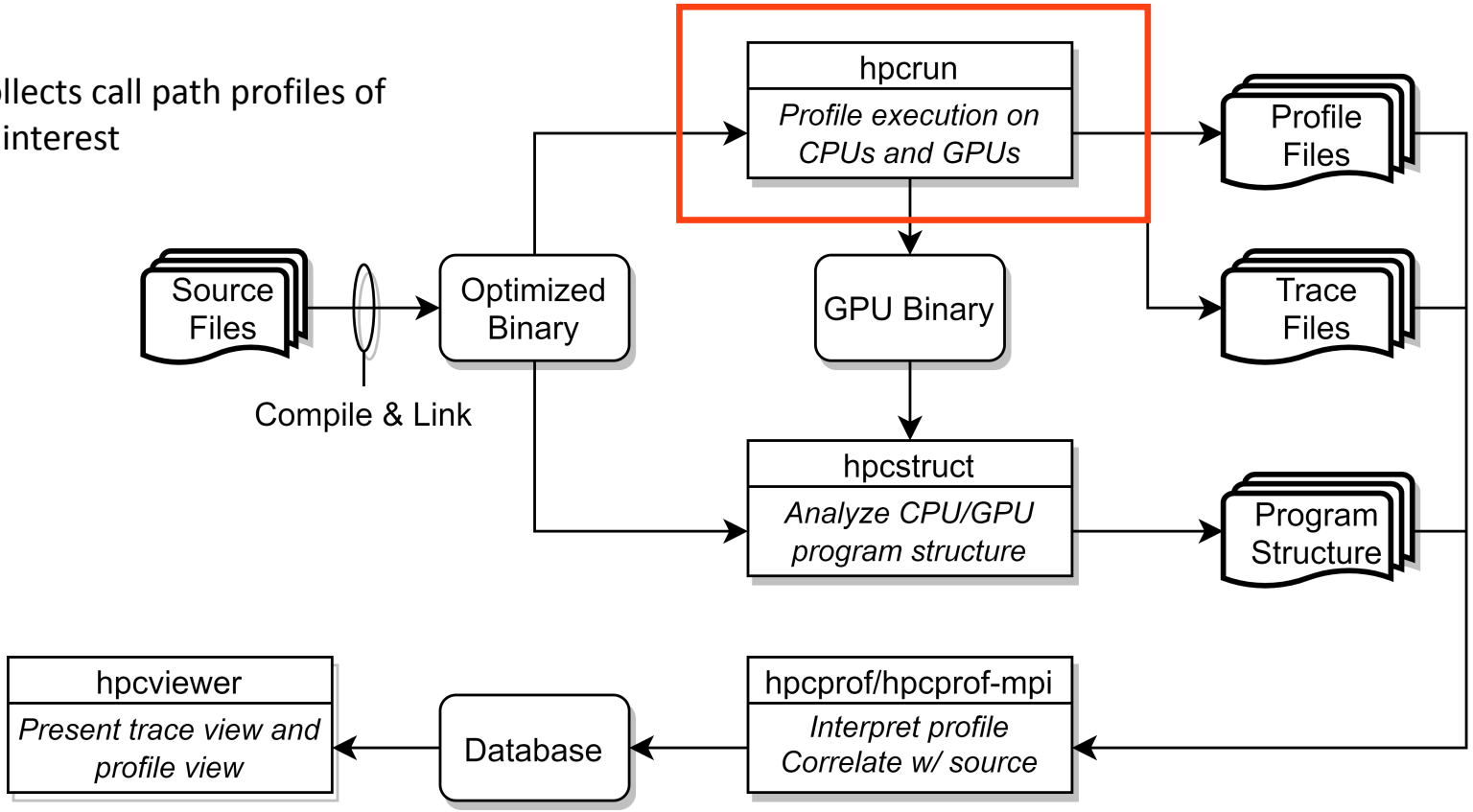
- Ensure that compilers record line mappings
- host compiler: -g
- nvcc: -lineinfo



HPCToolkit's Workflow for GPU-accelerated Applications

Step 2:

- *hpcrun* collects call path profiles of events of interest



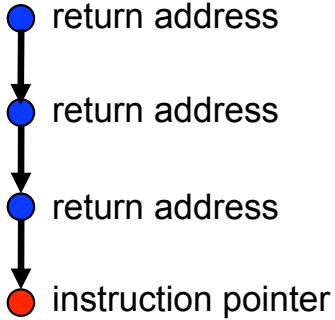
Measurement of CPU and GPU-accelerated Applications

- Sampling using timers and hardware counter overflow on the CPU
- Callbacks when GPU operations are launched and (sometimes) completed
- GPU event stream for GPU operations; PC Samples (NVIDIA)

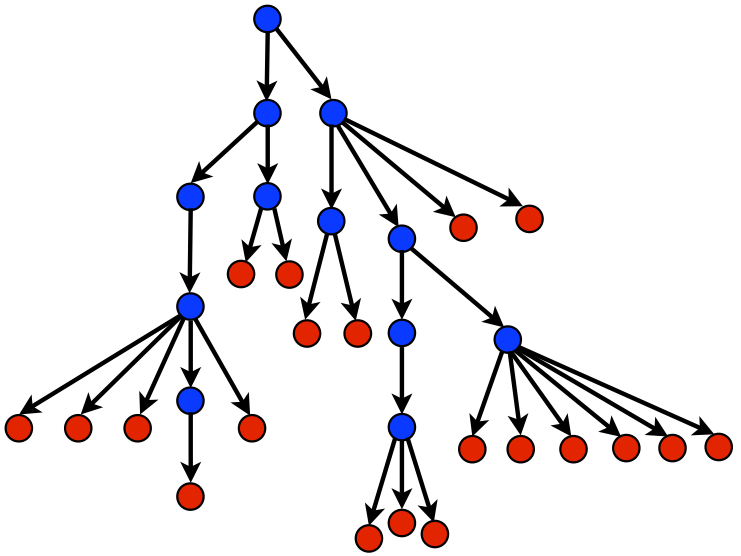
Call Stack Unwinding to Attribute Costs in Context

- Unwind when timer or hardware counter overflows
  - —measurement overhead proportional to sampling frequency rather than call frequency
- Unwind to capture context for events such as GPU kernel launches

Call path sample



Calling context tree



hpcrun: Measure CPU and/or GPU activity

- GPU profiling
  - `hpcrun -e gpu=xxx <app> ….` *xxx ∈ {nvidia,amd,opencl,level0}*
- GPU instrumentation (Intel GPU only)
  - `hpcrun -e gpu=level0,inst=count,latency <app>`
- GPU PC sampling (NVIDIA GPU only)
  - `hpcrun -e gpu=nvidia,pc <app>`
- CPU and GPU Tracing (in addition to profiling)
  - `hpcrun -e CPUTIME -e gpu=xxx -t <app>`
- Use hpcrun with job launchers
  - `jsrun -n 32 -g 1 -a 1 hpcrun -e gpu=xxx <app>`
  - `srun -n 1 -G 1 hpcrun -e gpu=xxx <app>`
  - `aprun -n 16 -N 8 -d 8 hpcrun -e gpu=xxx <app>`

Profiles: aggregated on the fly
- a calling context tree per thread
- a calling context tree per GPU stream
- instruction level measurements

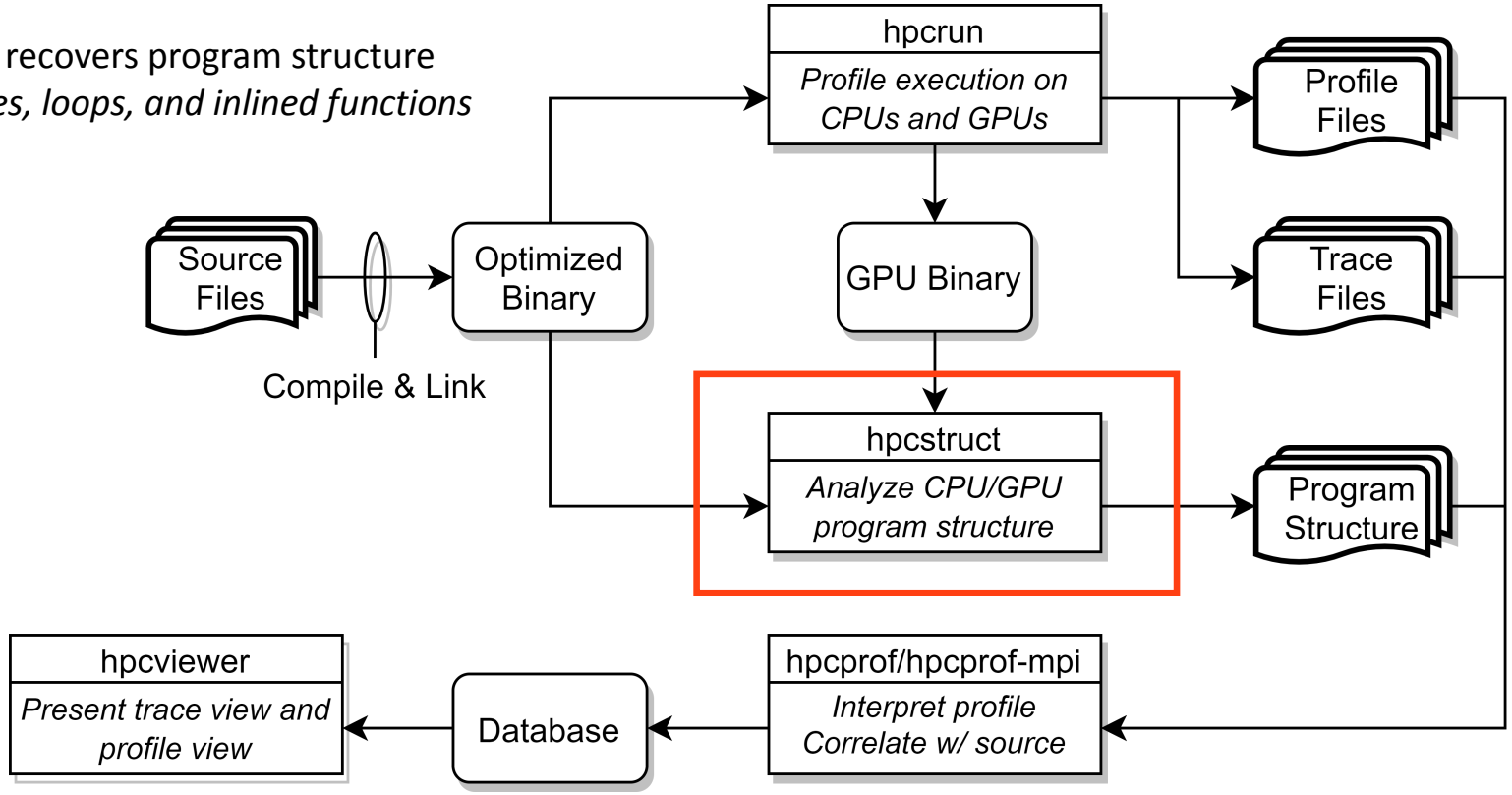
CPU traces
- trace of call stack samples

GPU traces
- trace of call stacks that initiate GPU operations

HPCToolkit's Workflow for GPU-accelerated Applications

Step 3:

- *hpcstruct* recovers program structure *about lines, loops, and inlined functions*



hpcstruct: Analyze CPU and GPU Binaries Using Multiple Threads

- Usage

```
hpcstruct [--gpucfg yes] <measurement-directory>
```

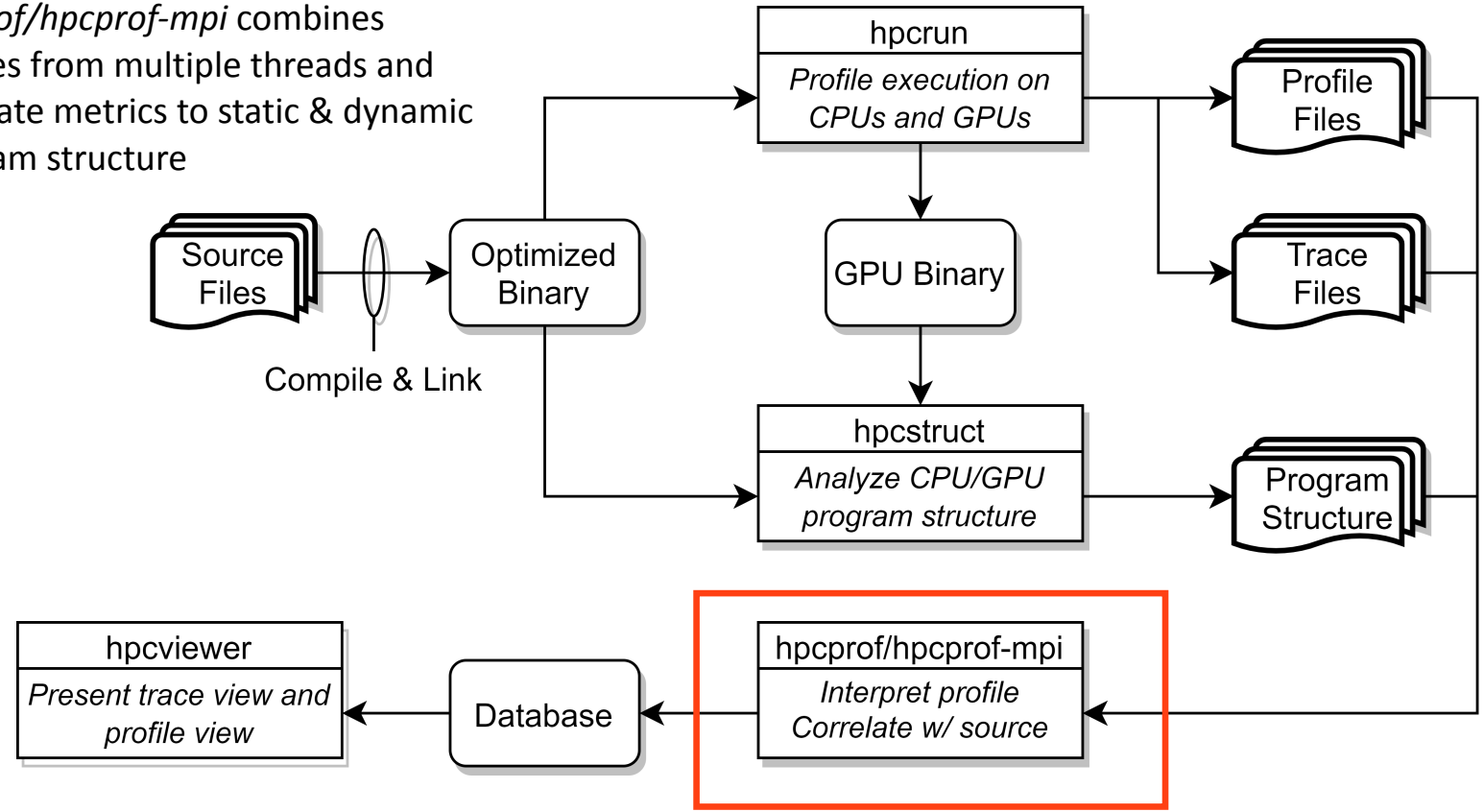
- What it does
  - Recover program structure information
    - Files, functions, inlined templates or functions, loops, source lines
  - In parallel, analyze all CPU and GPU binaries that were measured by HPCToolkit
    - —default: use size(CPU set)/2 threads
    - —analyze large application binaries with 16 threads
    - —analyze multiple small application binaries concurrently with 2 threads each
  - Cache binary analysis results for reuse when analyzing other executions

NOTE: --gpucfg yes needed only for analysis of GPU binaries when NVIDIA PC samples were collected

HPCToolkit's Workflow for GPU-accelerated Applications

Step 4:

- *hpcprof/hpcprof-mpi* combines profiles from multiple threads and correlate metrics to static & dynamic program structure



hpcprof/hpcprof-mpi: Associate Measurements with Program Structure

- Analyze data from modest executions sequentially

```
hpcprof <measurement-directory>
```

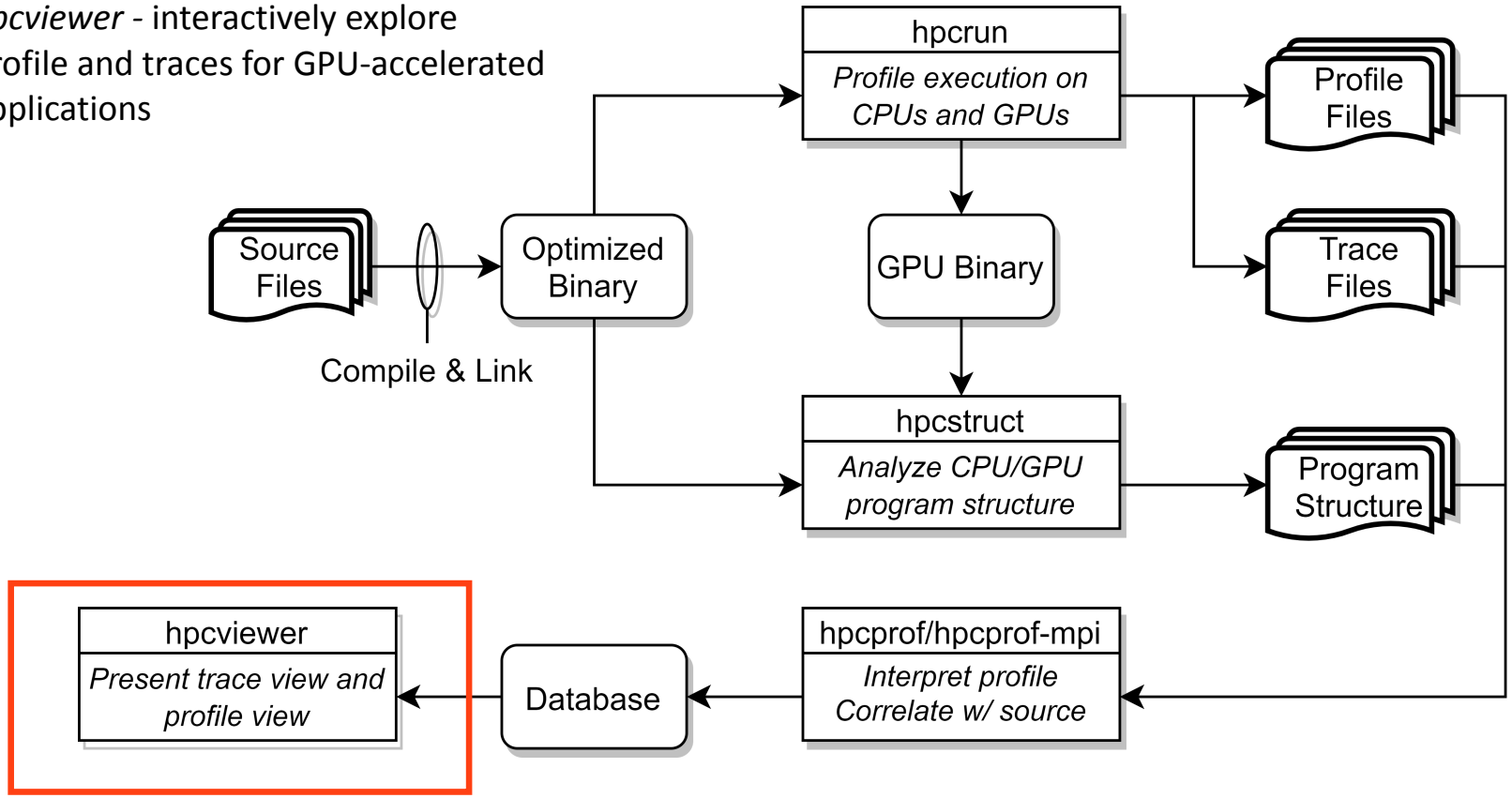
- Analyze data from large executions in parallel

```
jsrun -n 32 -a 1 hpcprof-mpi <measurement-directory>
srun -n 32 hpcprof-mpi <measurement-directory>
aprun -n 128 -N 8 hpcprof-mpi <measurement-directory>
```

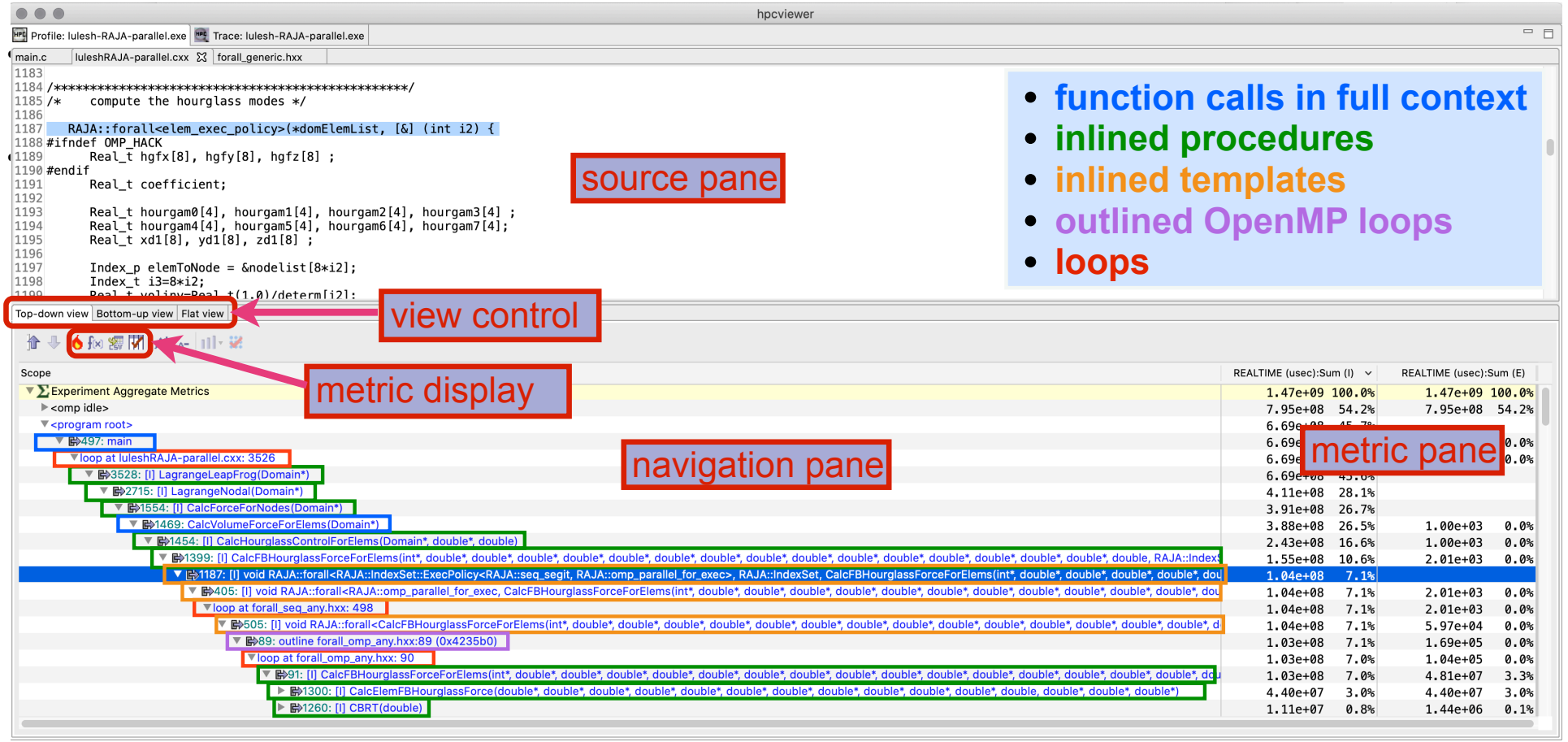
HPCToolkit's Workflow for GPU-accelerated Applications

Step 4:

- *hpcviewer* - interactively explore profile and traces for GPU-accelerated applications

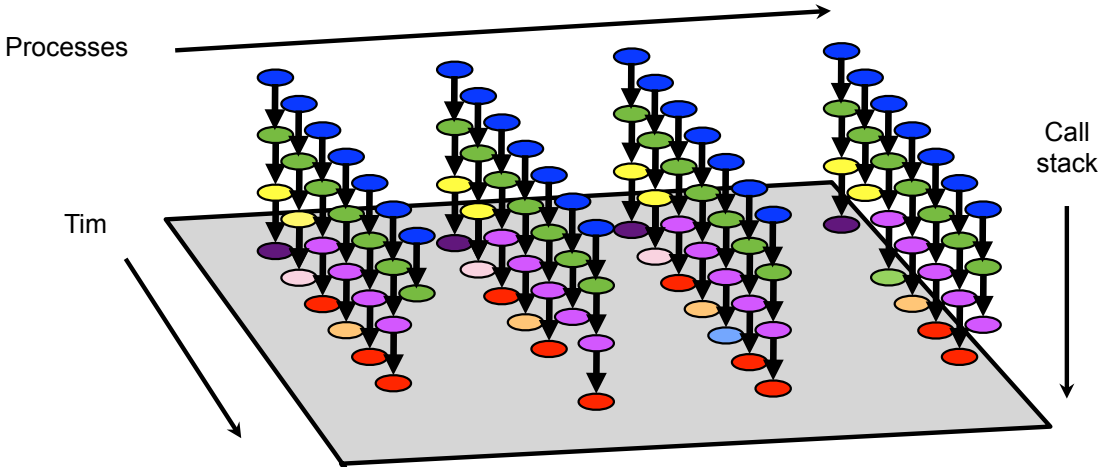


Code-centric Analysis with hpcviewer

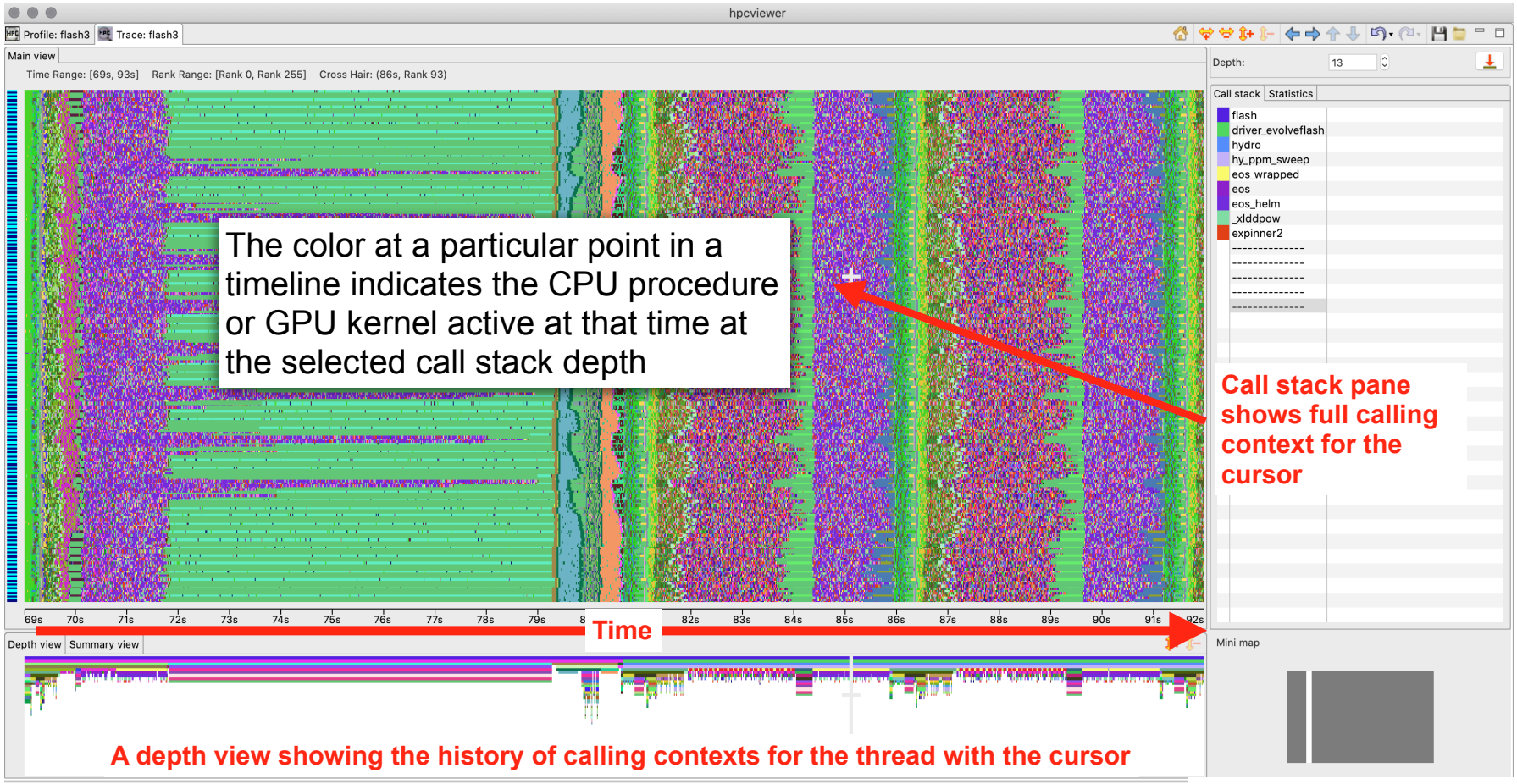


Understanding Temporal Behavior

- 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 hpcviewer



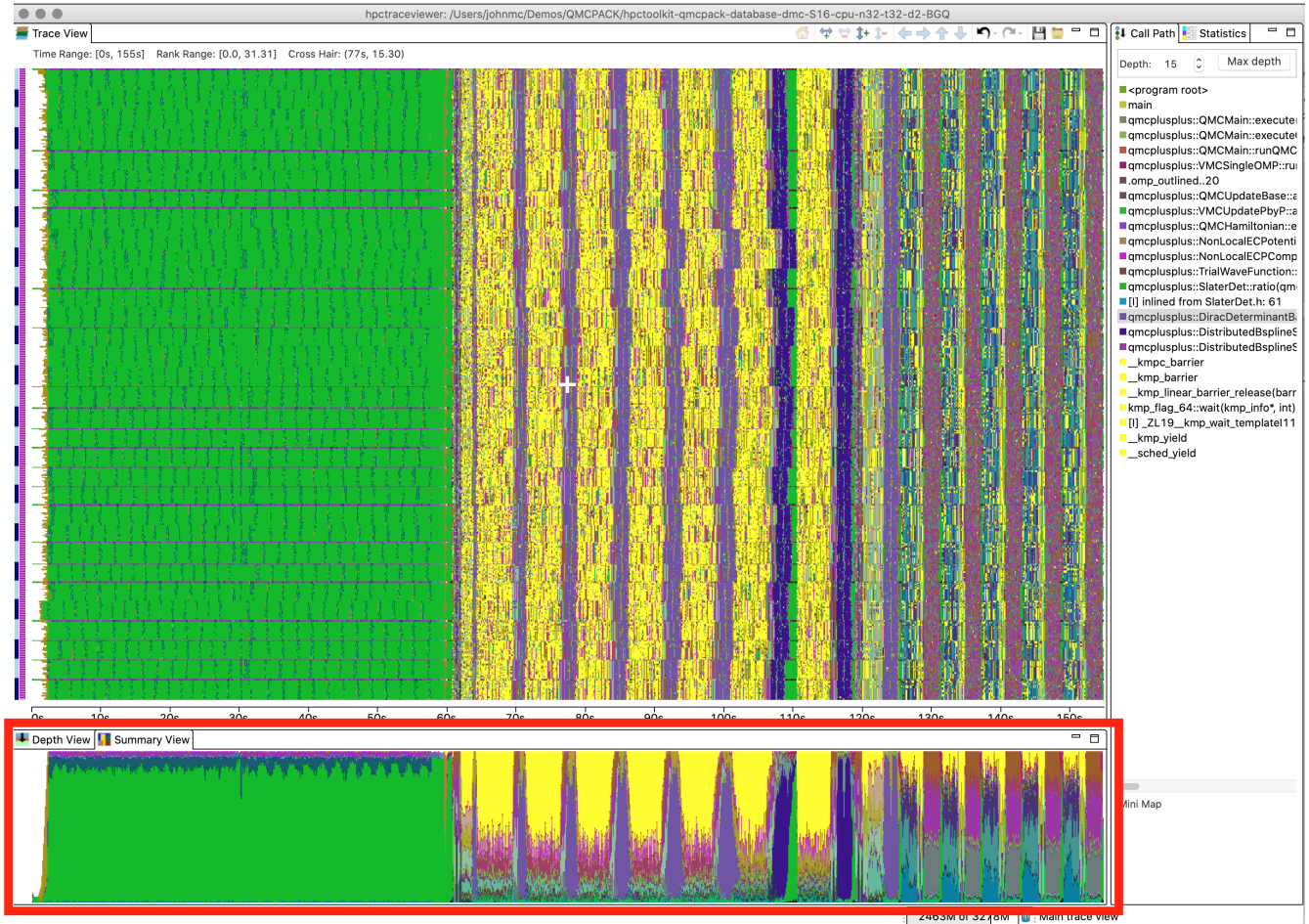
A multi-level call stack based view of execution over time

Minimap indicates part of execution trace shown

Time-centric Analysis with hpctraceviewer

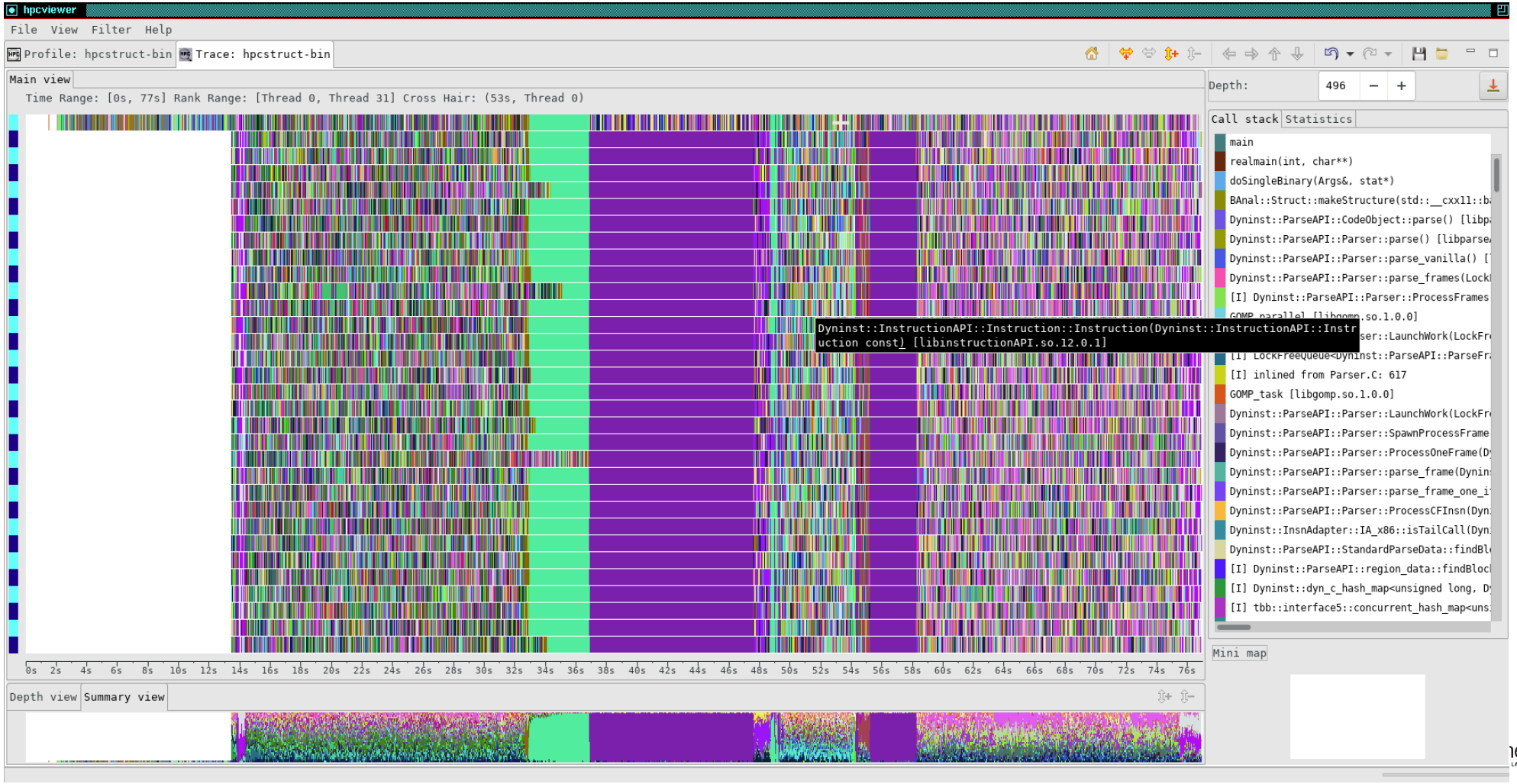
Experimental version of QMCPack

- 32 ranks
- 32 threads each



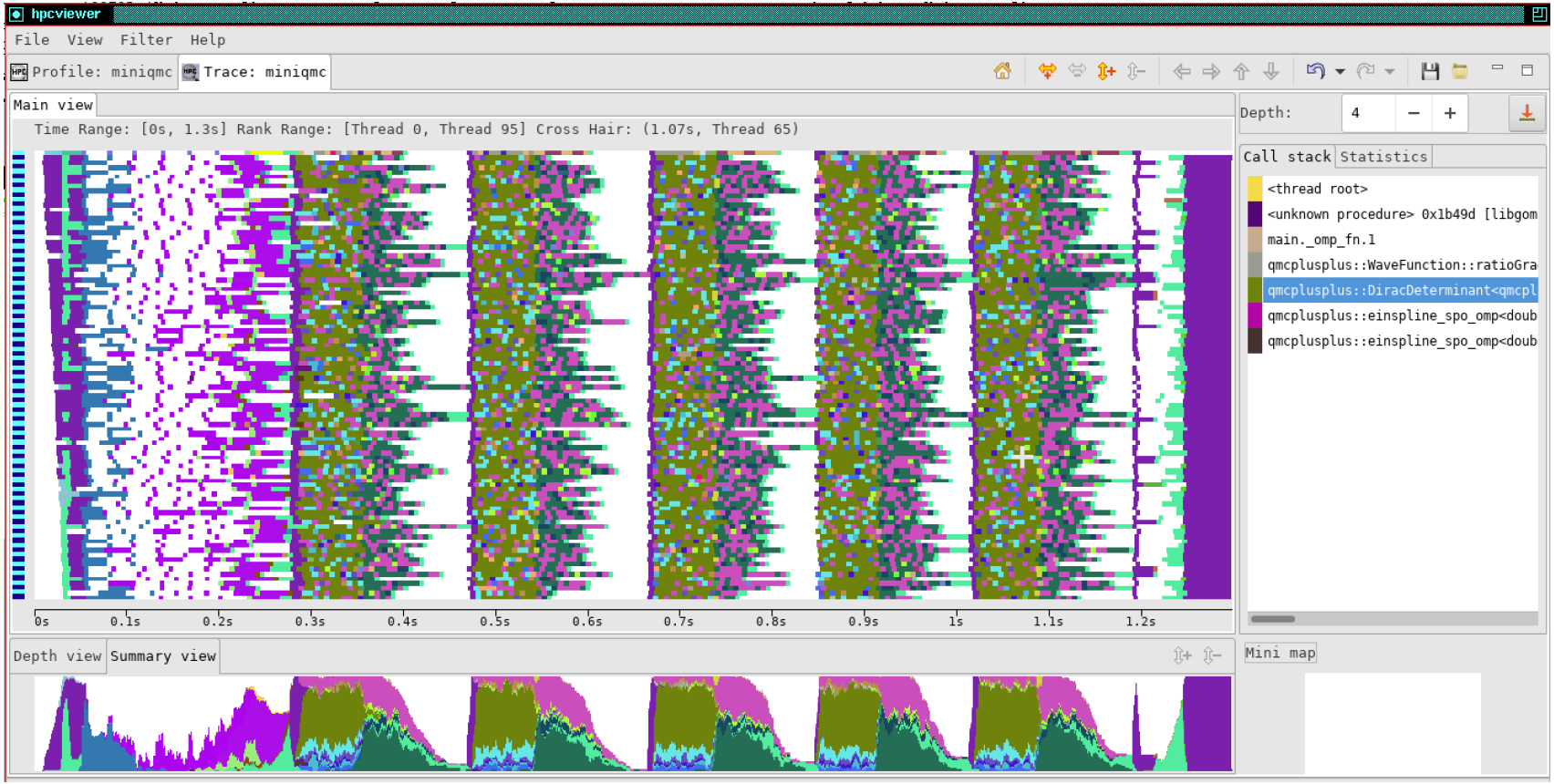
Summary view summarizes activity across threads at each point in time

hpcstruct Example: Analyze 7.7GB TensorFlow library (170MB text) in 77s



Improved Tracing to Show Blocking on CPU Threads

Miniqmc: OpenMP on 32 CPU threads

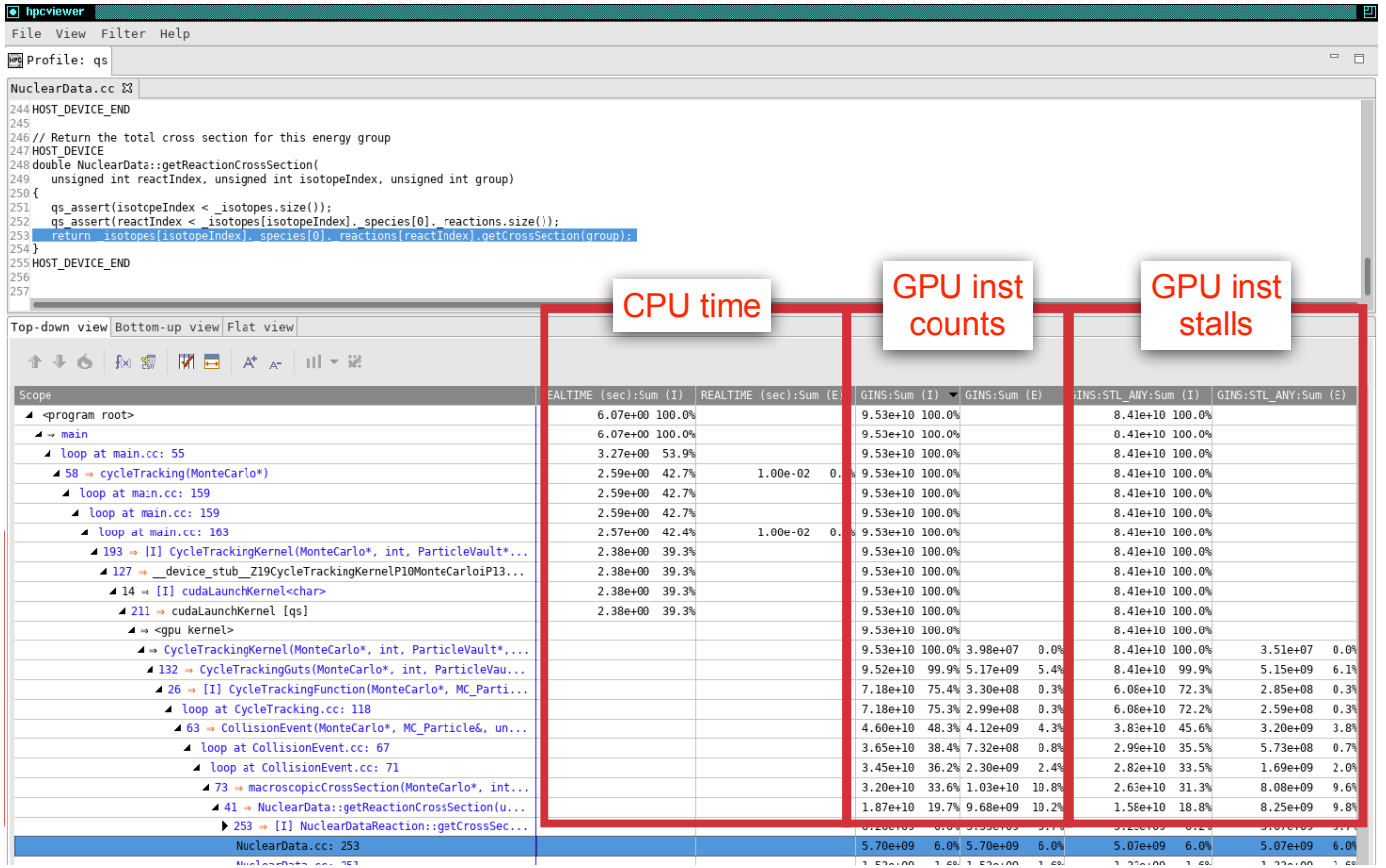


Coarse- and Fine-grain Measurement on NVIDIA GPUs: LLNL's Quicksilver

Compute Node

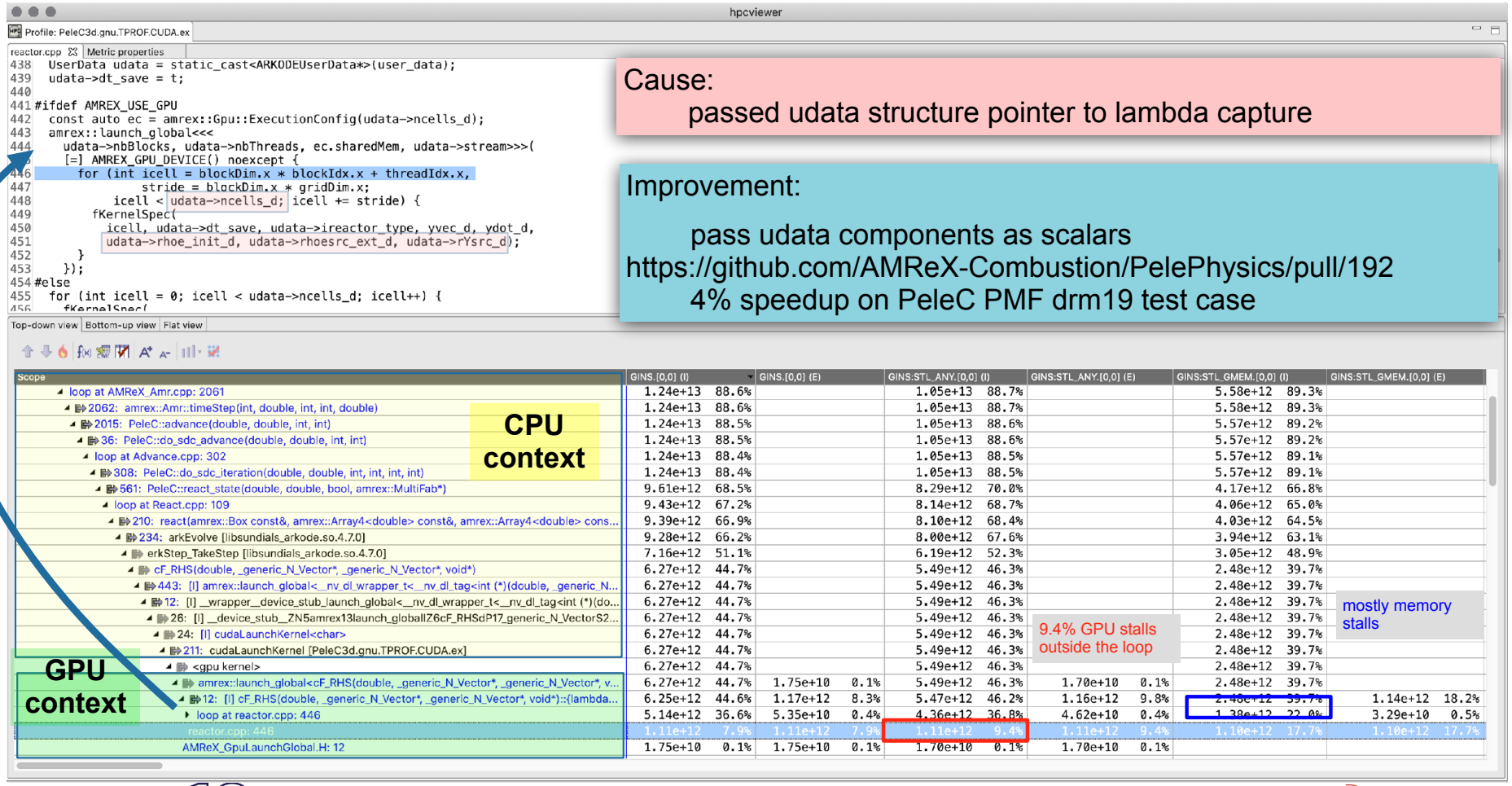
- 2xPower9 + 4xNIVIDIA GPUs

- Optimized (-O2) compilation with nvcc
- Detailed measurement and attribution using PC sampling
- Attribute information to heterogeneous calling context
- Key Metrics
  - instructions executed
  - instruction stalls and reasons
  - GPU utilization

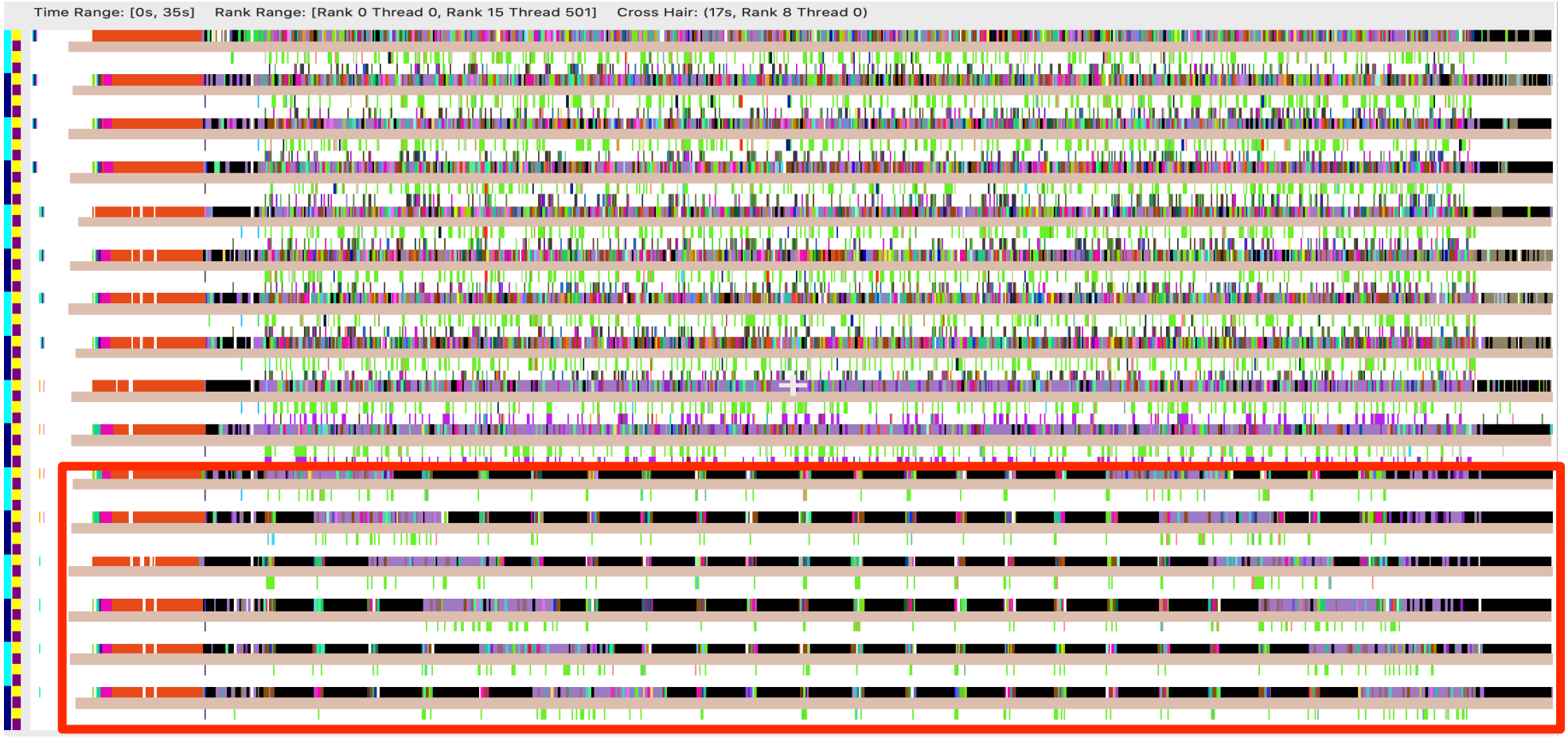


K. Zhou, M. W. Krentel, and J. Mellor-Crummey. Tools for top-down performance analysis of GPU-accelerated applications. International Conference on Supercomputing. ACM, New York, NY, USA, June, 2020.

Analysis of PeleC using PC Sampling on an NVIDIA GPU

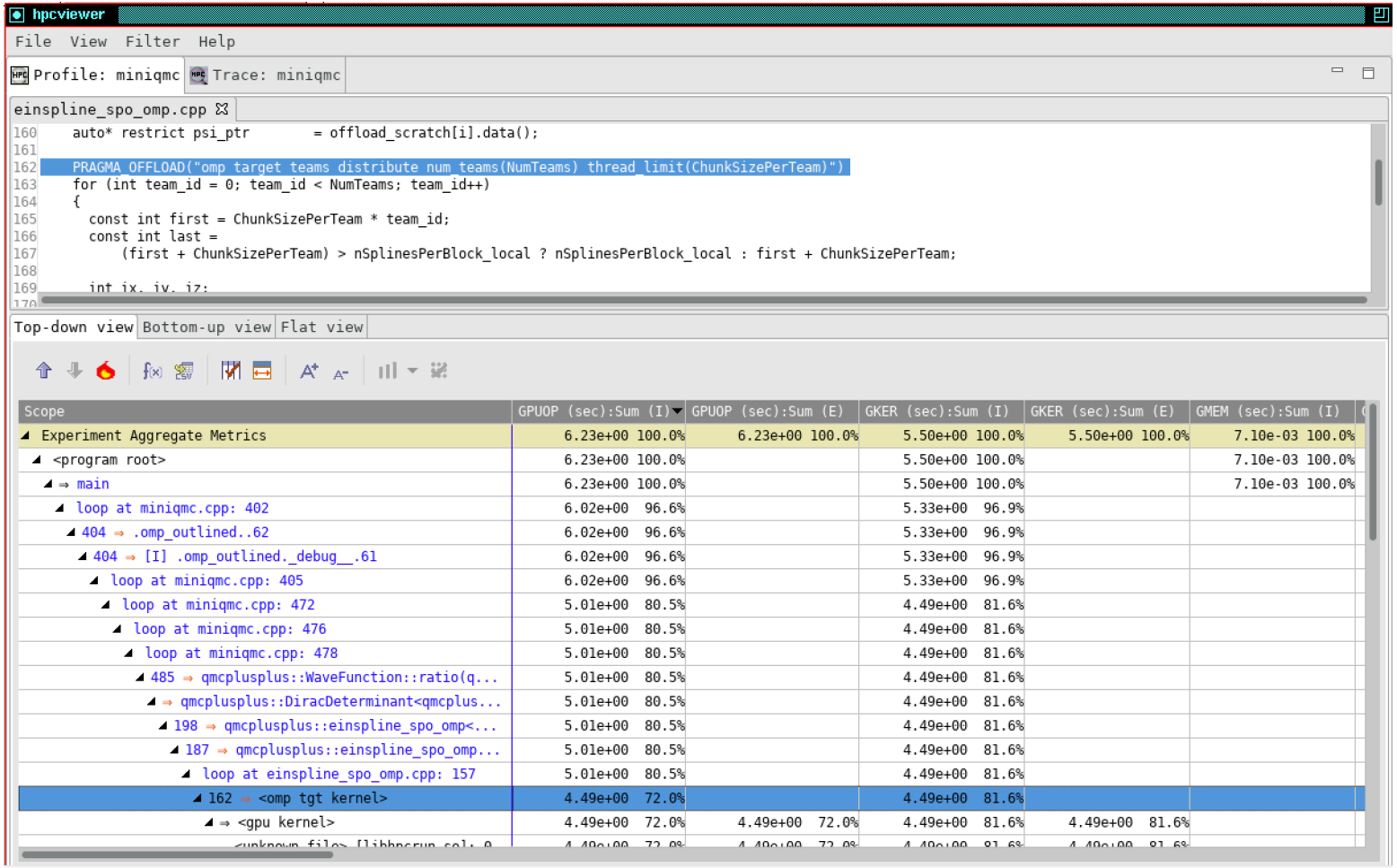


HPCToolkit Trace of WarpX (16 ranks + 16 GPUs)



GPU imbalance: significantly less GPU work on last 6 ranks

Measure and Attribute OpenMP Offloading



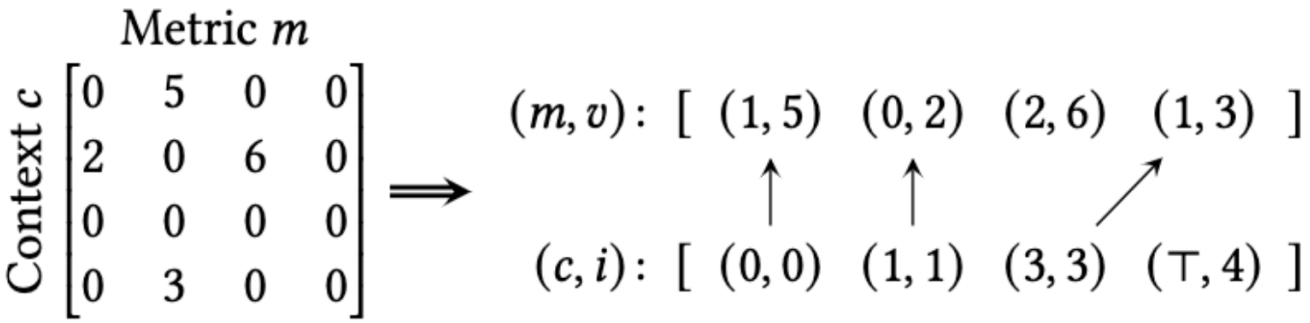
HPCToolkit Status on GPUs

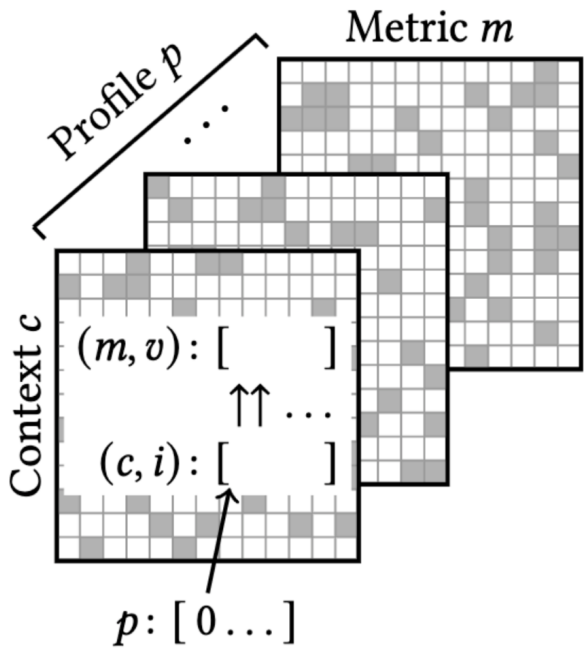
- NVIDIA
  - heterogeneous profiles, including GPU instruction-level execution and stalls using PC sampling
  - traces
- AMD
  - heterogeneous profiles; no GPU instruction-level measurements within kernels
  - measure OpenMP offloading using OMPT interface
  - traces
- Intel
  - heterogeneous profiles, including GPU instruction-level measurements with kernel instrumentation and heuristic latency attribution to instructions
  - traces

Coming Attraction: Improved Scalability of Post-mortem Analysis

- Exploit natural sparsity in performance data
  - —Reduce storage requirements, efficiently use available I/O
- Use multithreading to process performance data
  - —Reduce memory footprint and communication cost, efficiently use available compute
- Empirical results of improvements in HPCToolkit
  - —Practical benefits: process data from 1000s of nodes with <10, in minutes!

Storing Mountains of Performance Data from Extreme-Scale Executions

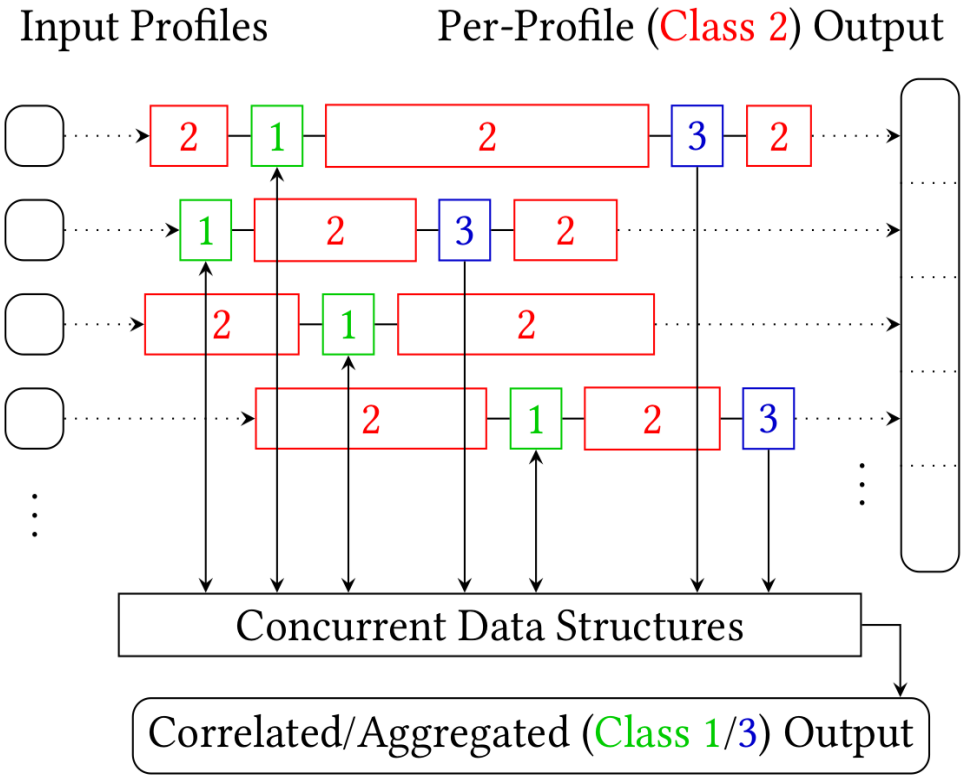


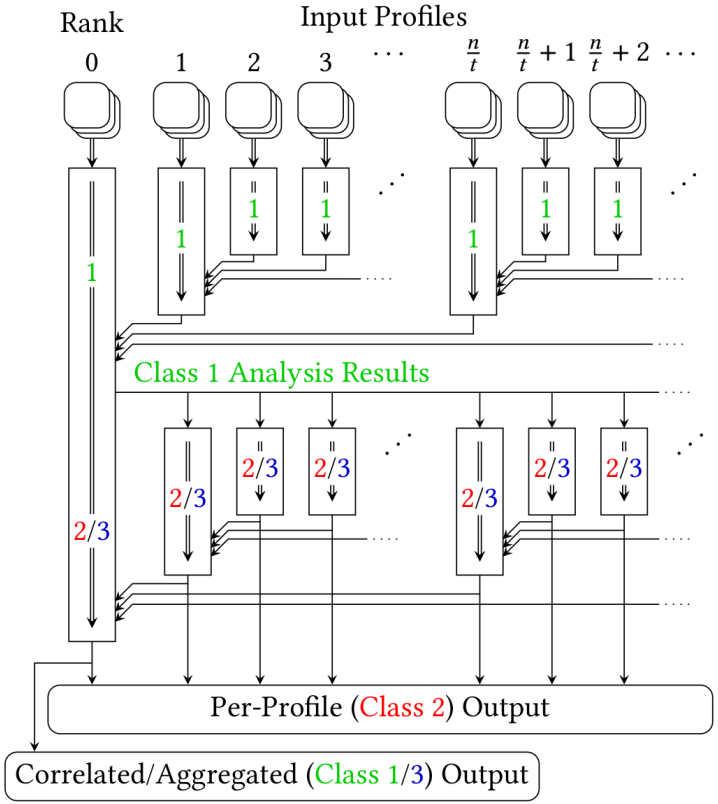


Exploit natural sparsity to reduce storage and I/O

"1254x compression: 14TB→11GB for PeleC (turbulent combustion) @ 2K threads + 2K GPUs"

Analyzing Mountains of Performance Data from Extreme-Scale Executions



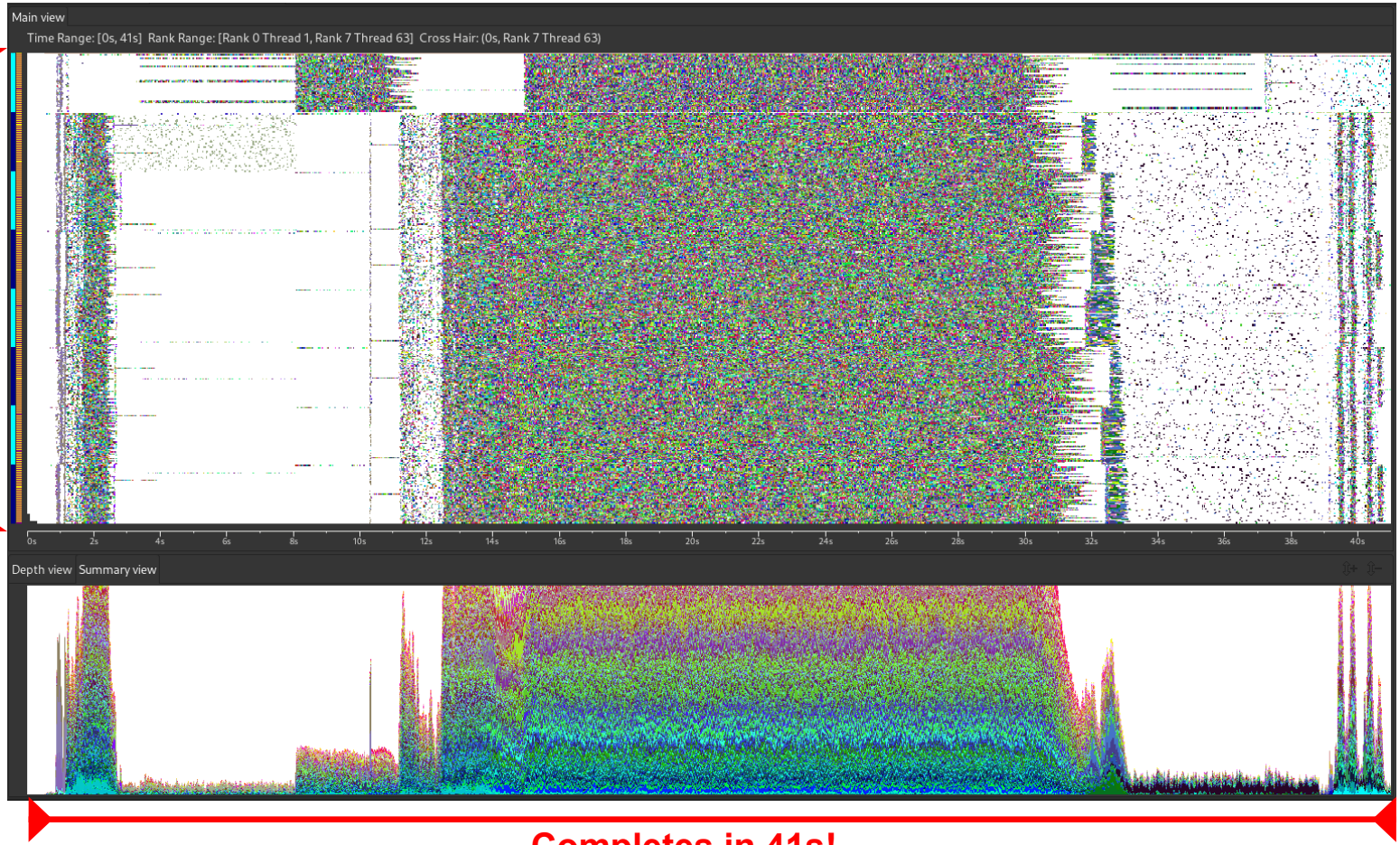


Highly-efficient multithreaded parallelism!

Scalable parallelism: multithreading + MPI

hpcprof-mpi: Analyze Measurements of LAMMPS @ 2K threads + 2K GPUs

Analysis on 8 nodes using 504 threads!



Completes in 41s!

HPCToolkit Resources

- Documentation
  - User manual
    - http://hpctoolkit.org/manual/HPCToolkit-users-manual.pdf
  - Tutorial videos
    - http://hpctoolkit.org/training.html
- Software
  - Download hpcviewer GUI binaries for your laptop, desktop, cluster, or supercomputer
    - OS: Linux, Windows, MacOS
    - Processors: x86_64, aarch64, ppc64le
    - http://hpctoolkit.org/download.html
  - Install HPCToolkit on your Linux desktop, cluster, or supercomputer using Spack
    - http://hpctoolkit.org/software-instructions.html

ARGONNE ATPESC 10 EXTREME-SCALE COMPUTING

HPCToolkit Hands-On Directions

Performance analysis of CPU and GPU-accelerated applications

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Sample Performance Databases for You to Explore

- Where can you find the databases: theta:/grand/ATPESC2022/hpctoolkit/data
  - —hpctoolkit-gamess.makefp.crusher.db
    - General Atomic and Molecular Electronic Structure System (GAMESS) is a general ab initio quantum chemistry package
    - Fortran; MPI + OpenMP offloading (Cray CCE); AMD GPUs
    - 110s; 40MB; 16 MPI ranks x (5 CPU threads + 2 GPU streams)
  - —hpctoolkit-qmcpack-database-dmc-S16-cpu-n32-t32-d2-BGQ
    - An early prototype distributed-memory implementation of QMCPACK - a many-body ab initio Quantum Monte Carlo code for computing the electronic structure of atoms, molecules, 2D nanomaterials & solids
    - C++; MPI + OpenMP; Blue Gene Q
    - 155s; 3.2GB; 32 MPI ranks x 32 threads
  - —hpctoolkit-PeleC-PMF-96GPU.d
    - PeleC is an adaptive-mesh compressible hydrodynamics code for reacting flows
    - C++; AMReX framework using CUDA ; Power9 + NVIDIA GPUs
    - 1.4GB; 96 MPI ranks x (3 threads + 5 GPU streams)
  - —hpctoolkit-PeleC3d.dpcpp.ex-skylake-gpu.d
    - C++; AMReX framework using SYCL ; Intel Skylake with integrated GPU cores
    - Instruction-level measurements within GPU kernels
    - 10s; 44MB; Single process + GPU offloading

Profiling Quicksilver with HPCToolkit on Theta-gpu

- `module swap cobalt/cobalt-knl cobalt/cobalt-gpu  # if cobalt/cobalt-gpu is loaded`
- `ssh thetagpusn1`
- `qsub -I -q single-gpu -t 60 -n 1 --attrs filesystems=grand -A  ATPESC2022`
- `source /grand/ATPESC2022/hpctoolkit/scripts/setup-proxy.sh`
- `cd /grand/ATPESC2022/usr/${LOGNAME}`
- `git clone https://github.com/hpctoolkit/hpctoolkit-tutorial-examples`
- `cd hpctoolkit-tutorial-examples/examples/gpu/quicksilver`
- `source setup-env/theta-gpu.sh`
- `make build`
- `make run`
- `make run-pc`
- `exit  # your compute node`
- `exit  # thetagpusn1`
- `cd /grand/ATPESC2022/usr/${LOGNAME}`
- `cd hpctoolkit-tutorial-examples/examples/gpu/quicksilver`
- `module load hpctoolkit`
- `hpcviewer  hpctoolkit-qs-gpu-cuda.d`
- `hpcviewer  hpctoolkit-qs-gpu-cuda-pc.d`

Profiling AMG2013 with HPCToolkit on Theta

- `module swap cobalt/cobalt-gpu cobalt/cobalt-knl  # if cobalt/cobalt-gpu is loaded`
- `cd /grand/ATPESC2022/usr/${LOGNAME}`
- `git clone https://github.com/hpctoolkit/hpctoolkit-tutorial-examples`
- `cd hpctoolkit-tutorial-examples/examples/cpu/mpi+openmp/amg2013`
- `export HPCTOOLKIT_TUTORIAL_RESERVATION=<queue name>`
- `export HPCTOOLKIT_TUTORIAL_PROJECTID=ATPESC2022`
- `source setup-env/theta.sh`
- `make build`
- `make run`
- # wait for $COBALT_JOBID.done to appear in your directory
- Alternatives
  - `make analyze`
  - `make analyze-parallel`
- # wait for $COBALT_JOBID.done to appear in your directory
- Alternatives
  - `make view`
  - `hpcviewer hpctoolkit-amg2013.d`