

# A Community-Driven Portable Profiler at Scale

## HPCToolkit

**John Mellor-Crummey**  
**Rice University**

# DOE's GPU-Accelerated Exascale Platforms



- Frontier compute nodes (OLCF)
  - 1 AMD EPYC “Trento” CPU
  - 4 AMD MI250X GPUs
  - 4 Slingshot 11 endpoints
  - Unified memory architecture



- Aurora compute nodes (ALCF)
  - 2 Intel Xeon “Sapphire Rapids” processors
  - 6 Intel Data Center GPU Max 1500
  - 8 Slingshot 11 endpoints
  - Unified memory architecture



- El Capitan compute nodes (LLNL)
  - 4 AMD MI300A APU
  - 4 Slingshot 11 endpoints
  - Unified memory architecture

# Outline

Introduction to HPCToolkit performance tools

- Overview of HPCToolkit components and their workflow

- HPCToolkit's graphical user interfaces

Analyzing the performance of GPU-accelerated codes with HPCToolkit

- Slides: Exawind (AMReX)

- Slides: LAMMPS at Exascale (Kokkos)

- Demo: GAMESS (OpenMP)

Hands-on after lunch

- Explore available performance databases for a set of applications

- Collect and explore some measurements for some prepared examples

# Linux Foundation's HPCToolkit Performance Tools

- Collect profiles and traces of unmodified parallel CPU and GPU-accelerated applications
- Understand where an application spends its time and why
  - call path profiles associate metrics with application source code contexts
    - analyze instruction-level performance within GPU kernels and attribute it to your source code
  - hierarchical traces to understand execution dynamics
- Parallel programming models
  - across nodes: MPI, SHMEM, UPC++, ...
  - within nodes: OpenMP, Kokkos, RAJA, HIP, DPC++, Sycl, CUDA, OpenACC, ...
- Languages
  - C, C++, Fortran, Python, ...
- Hardware
  - CPU cores and GPUs within a node
    - CPU: x86\_64, Power, ARM
    - GPU: NVIDIA, AMD, Intel
  -

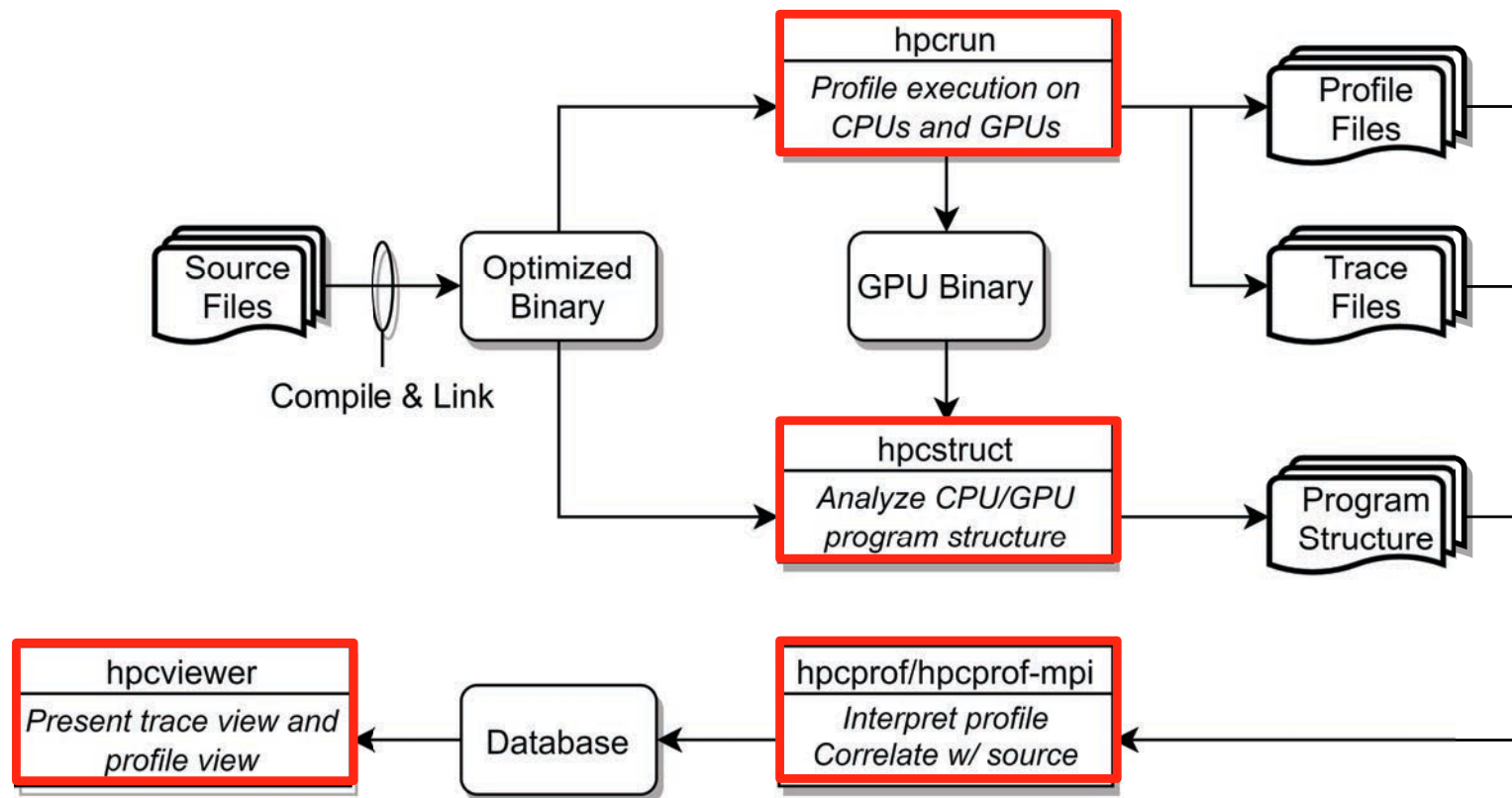
# Why HPCToolkit?

- 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
- Unlike vendor tools works with a wide range of CPUs and GPUs

# How does HPCToolkit Differ from Vendor Tools?

- Intel VTune: designed for analysis of performance on a single node
- NVIDIA Nsight Systems and AMD ROCm Systems
  - tracing of CPU and GPU streams
  - AMD visualizes directly with Perfetto
  - Nsight systems supports parallel analysis of measurement data with Dask
    - analyzing on more than one node requires setting up your own Dask cluster
- NVIDIA Nsight Compute and AMD ROCm Compute
  - detailed measurement of kernels with counters and execution replay
  - very slow measurement
  - flat display of measurements within GPU kernels
- HPCToolkit
  - supports more scalable tracing than vendor tools
    - measure exascale executions across many GPUs and nodes
  - highly scalable, parallel post-mortem analysis
  - detailed reconstruction of estimates for calling context profiles within GPU kernels

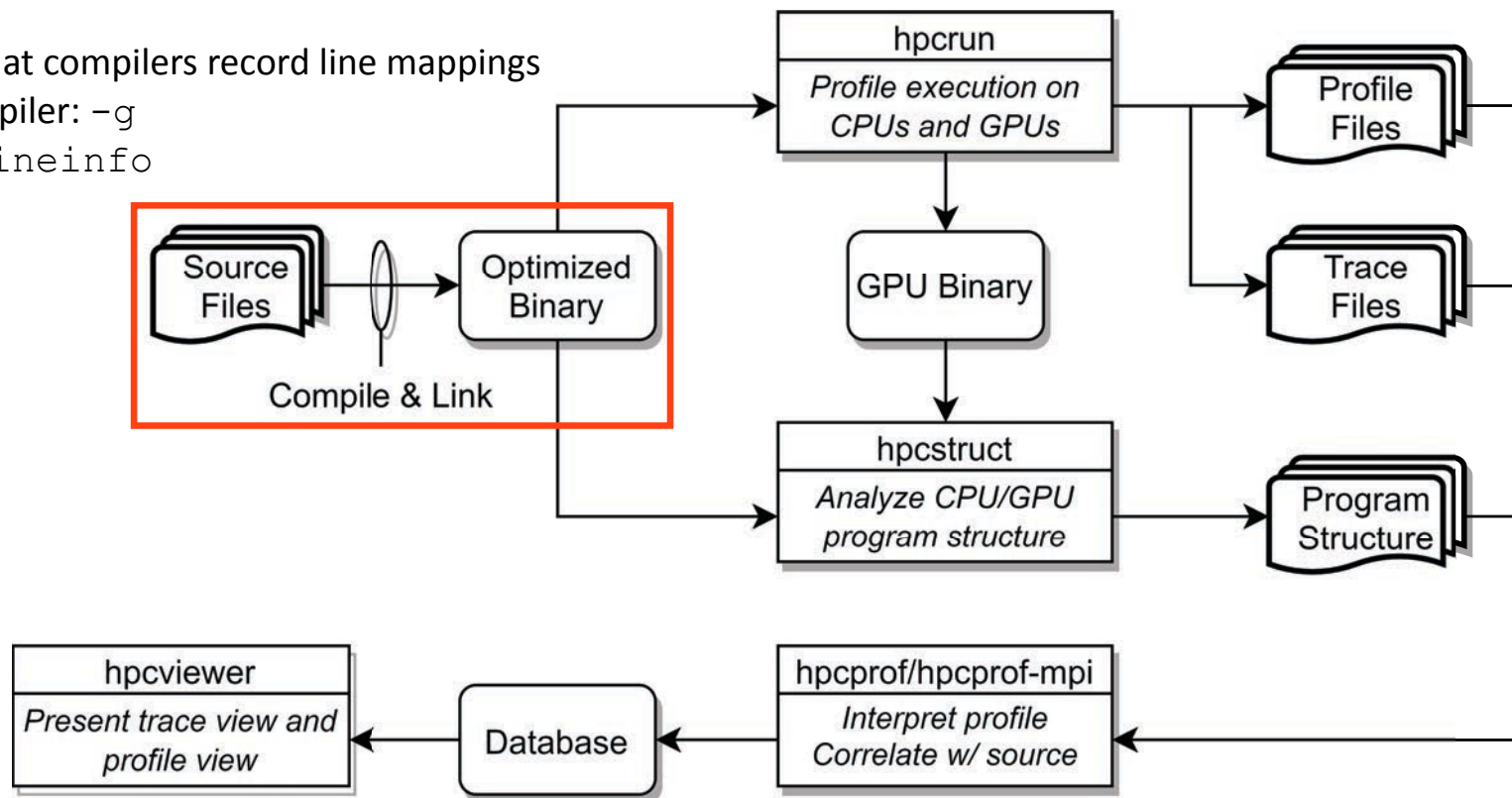
# HPCToolkit's Workflow for GPU-accelerated Applications



# HPCToolkit's Workflow for GPU-accelerated Applications

Step 1:

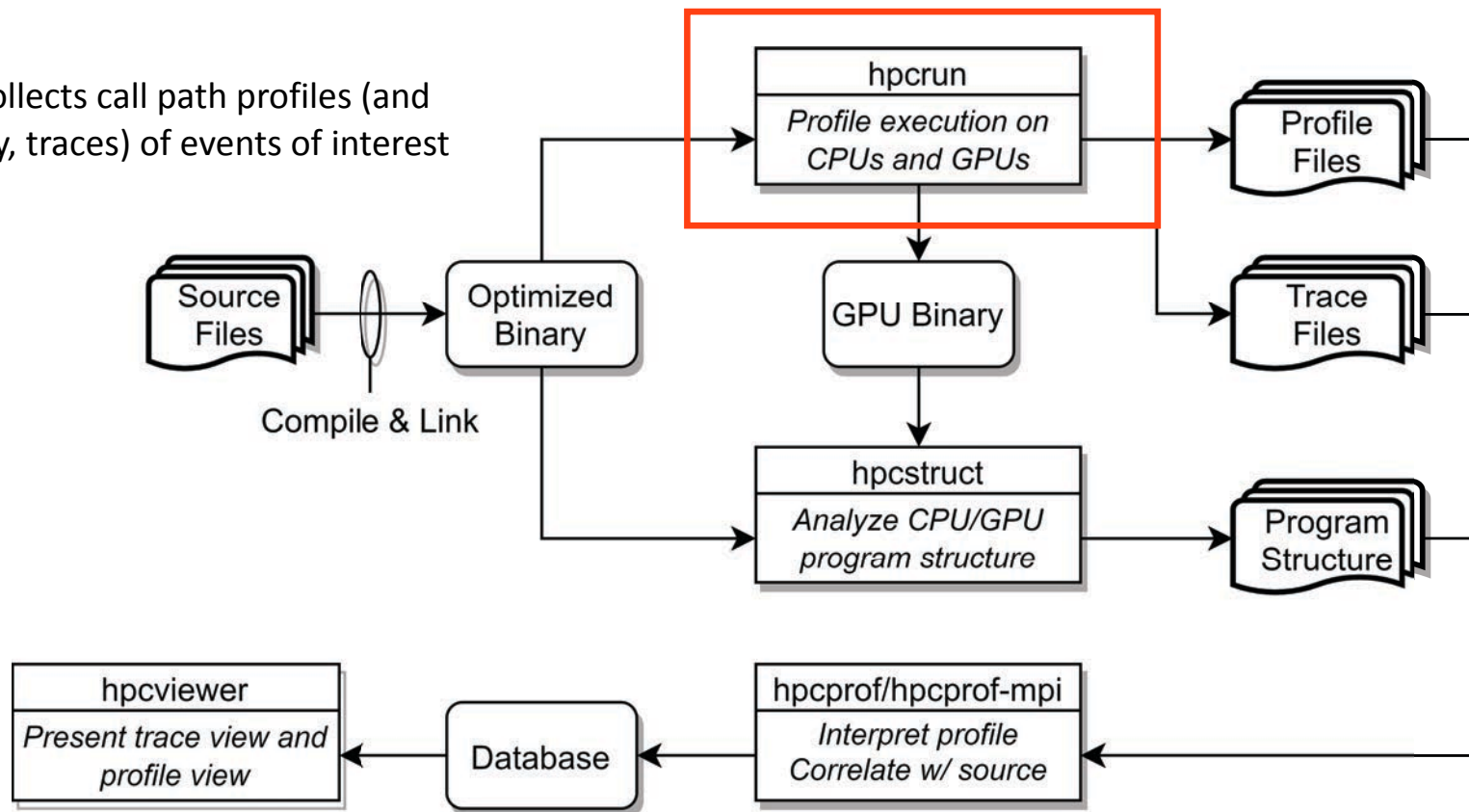
- Ensure that compilers record line mappings
- host compiler: `-g`
- `nvcc: -lineinfo`



# HPCToolkit's Workflow for GPU-accelerated Applications

Step 2:

- *hpcrun* collects call path profiles (and optionally, traces) of events of interest



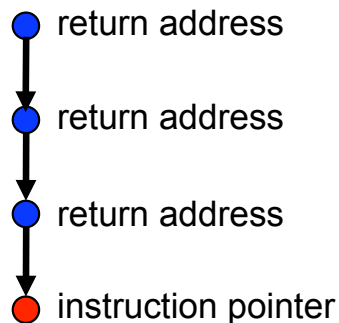
# Measurement of CPU and GPU-accelerated Applications

- Sampling using Linux timers and hardware counter overflows on the CPU
- Callbacks when GPU operations are launched and (sometimes) completed
- Event stream for GPU operations
- Program Counter (PC) samples within kernels on AMD, Intel, and NVIDIA GPUs
- Binary instrumentation of GPU kernels on Intel GPUs for instruction-level measurements

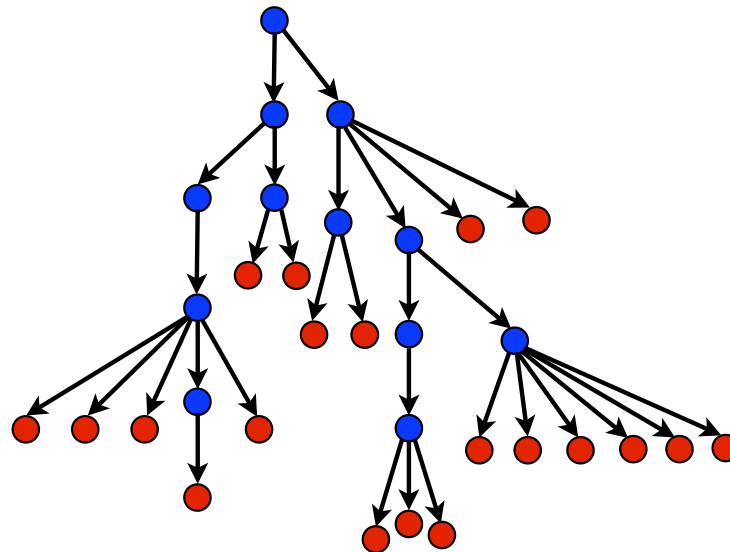
# Call Stack Unwinding to Attribute Costs in Context

- 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



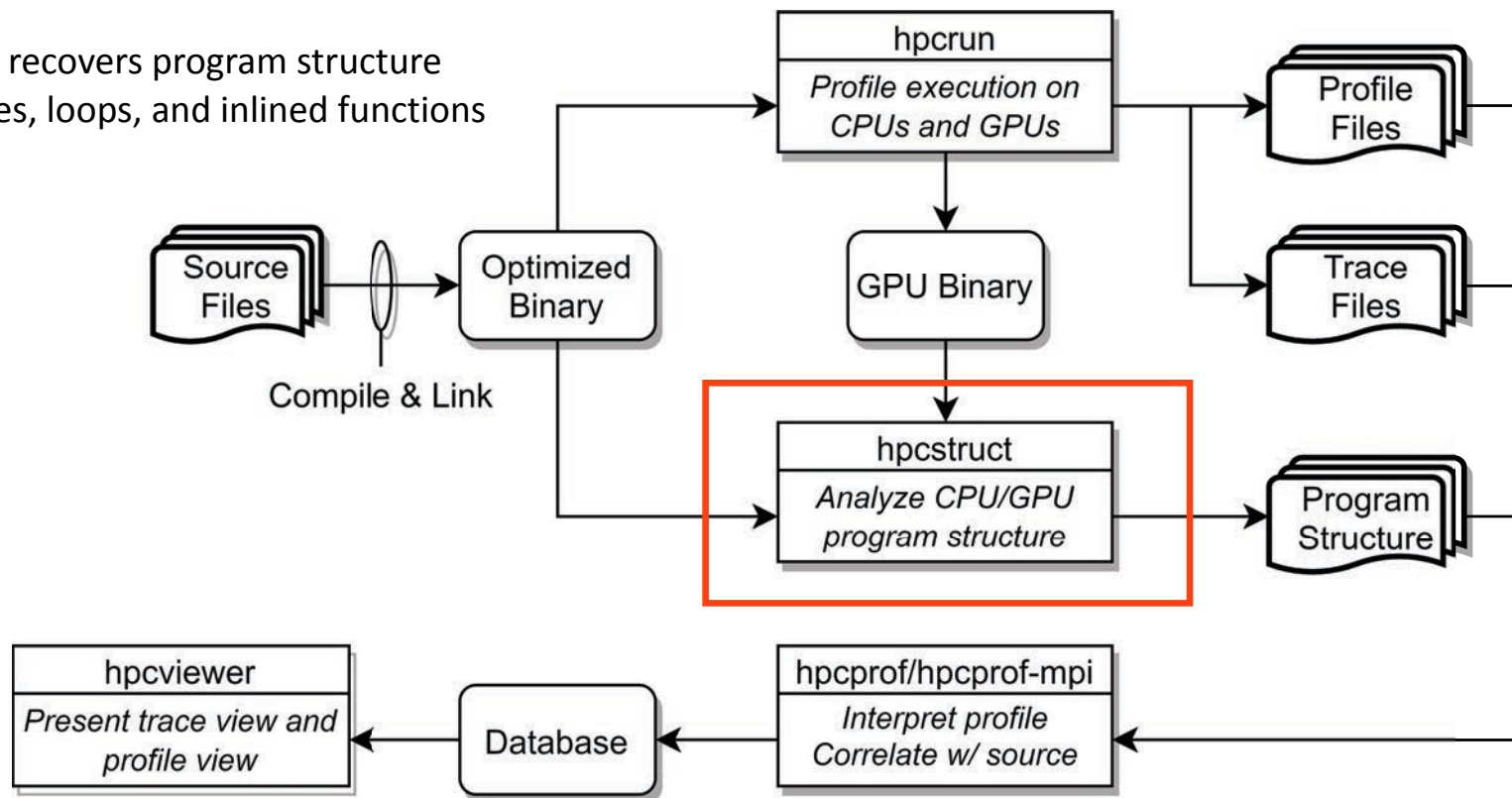
# hpcrun: Measure CPU and/or GPU activity

- GPU profiling  
—hpcrun -e gpu=**xxx** <app> ... **xxx** ∈ {*cuda, rocm, opencl, level0*}
- GPU PC sampling  
—hpcrun -e gpu=**yyy**,pc <app> **yyy** ∈ {*cuda, rocm, level0*}
- CPU and GPU Tracing (in addition to profiling)  
—hpcrun -e CPUTIME -e gpu=**xxx** **-tt** <app>
- Use hpcrun with MPI on Polaris or Aurora  
—mpiexec -n <ranks> ... hpcrun -e gpu=**xxx** <app>

# 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

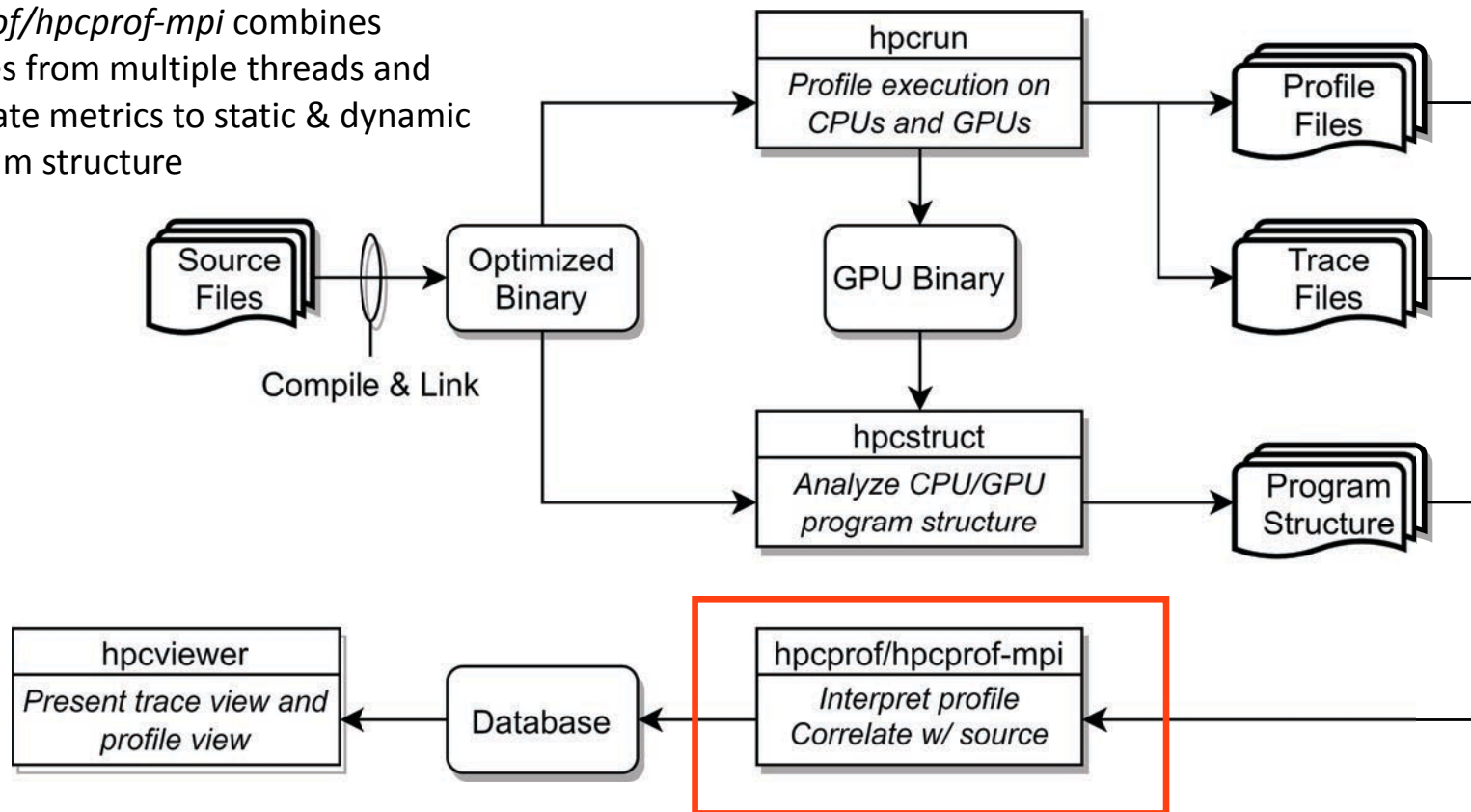
- Recover program structure information
  - Files, functions, inlined templates or functions, loops, source lines
- In parallel, analyze all CPU and GPU binaries that were measured by HPCToolkit
  - analyze each binary with threads proportional to size of program text and symbol table
- Cache binary analysis results for reuse when analyzing other executions

NOTE: `--gpucfg yes` needed only for analysis of GPU binaries for interpreting PC samples

# 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 with multithreading (moderate scale)

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

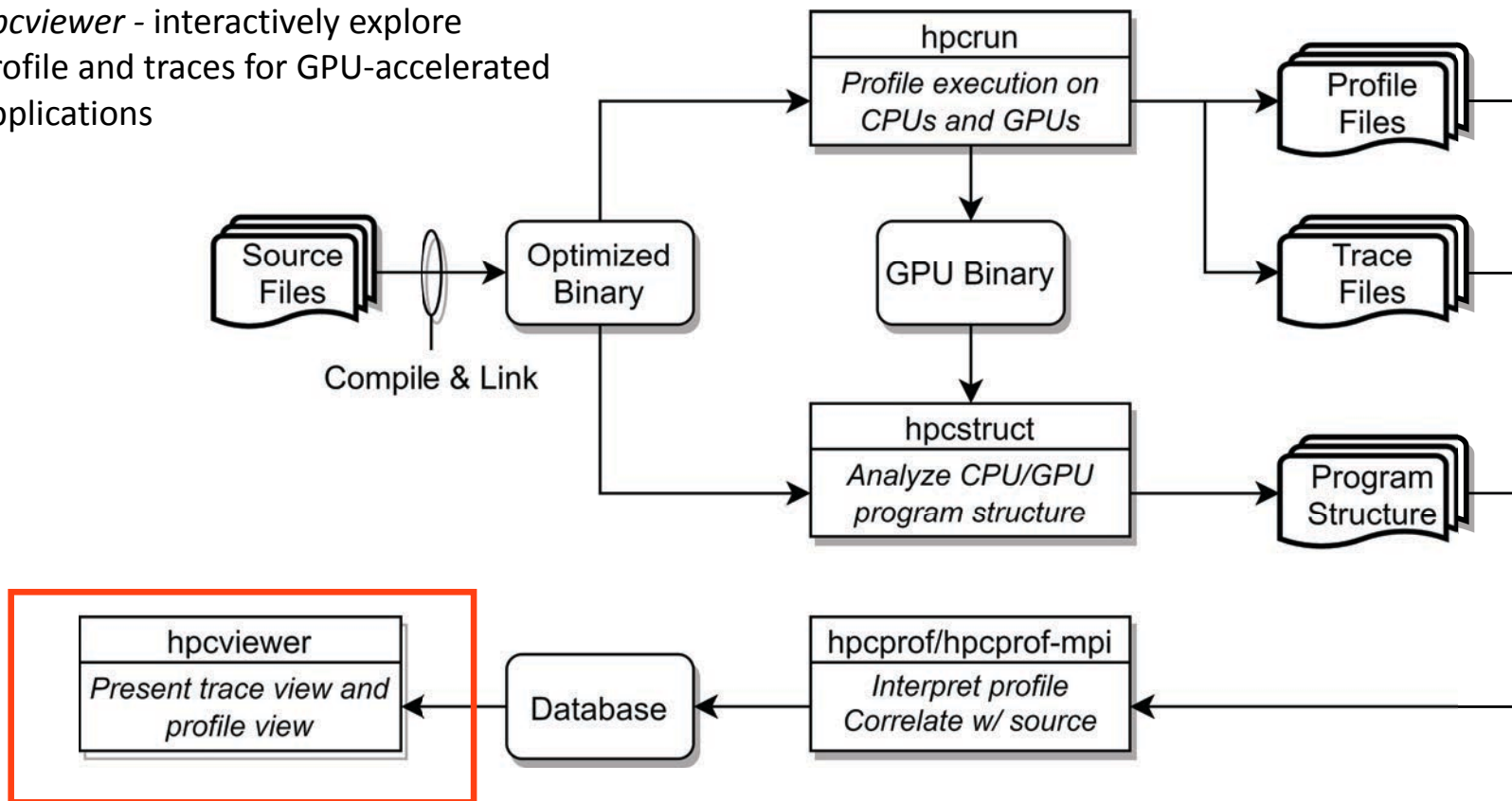
- Analyze data from large executions with distributed-memory parallelism + multithreading (large scale)

```
mpiexec -n ${NODES} --ppn 1 -depth=128 \  
hpcprof-mpi <measurement-directory>
```

# HPCToolkit's Workflow for GPU-accelerated Applications

Step 4:

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

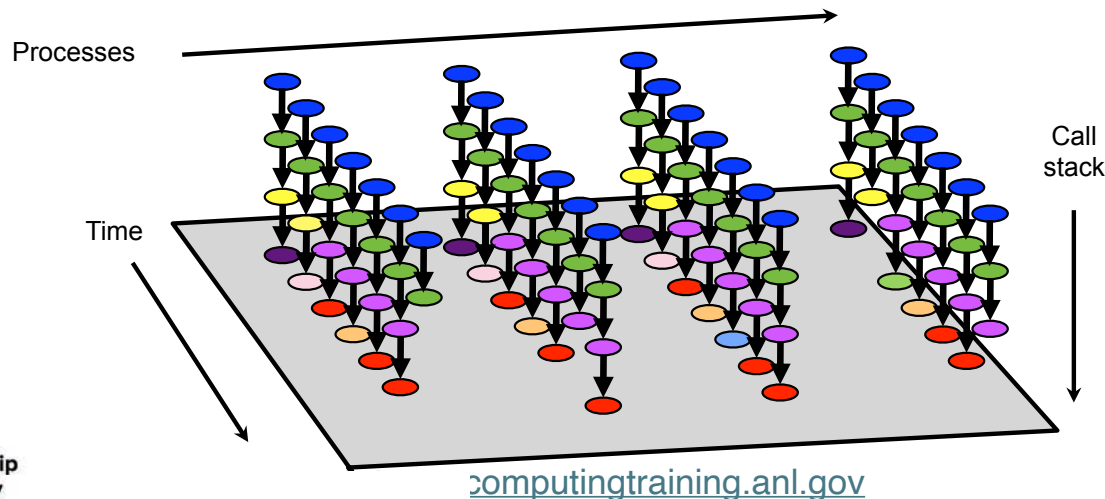


- **function calls in full context**
- **inlined procedures**
- **inlined templates**
- **outlined OpenMP loops**
- **loops**

[extremecomputingtraining.anl.gov](http://extremecomputingtraining.anl.gov)

# Understanding Temporal Behavior

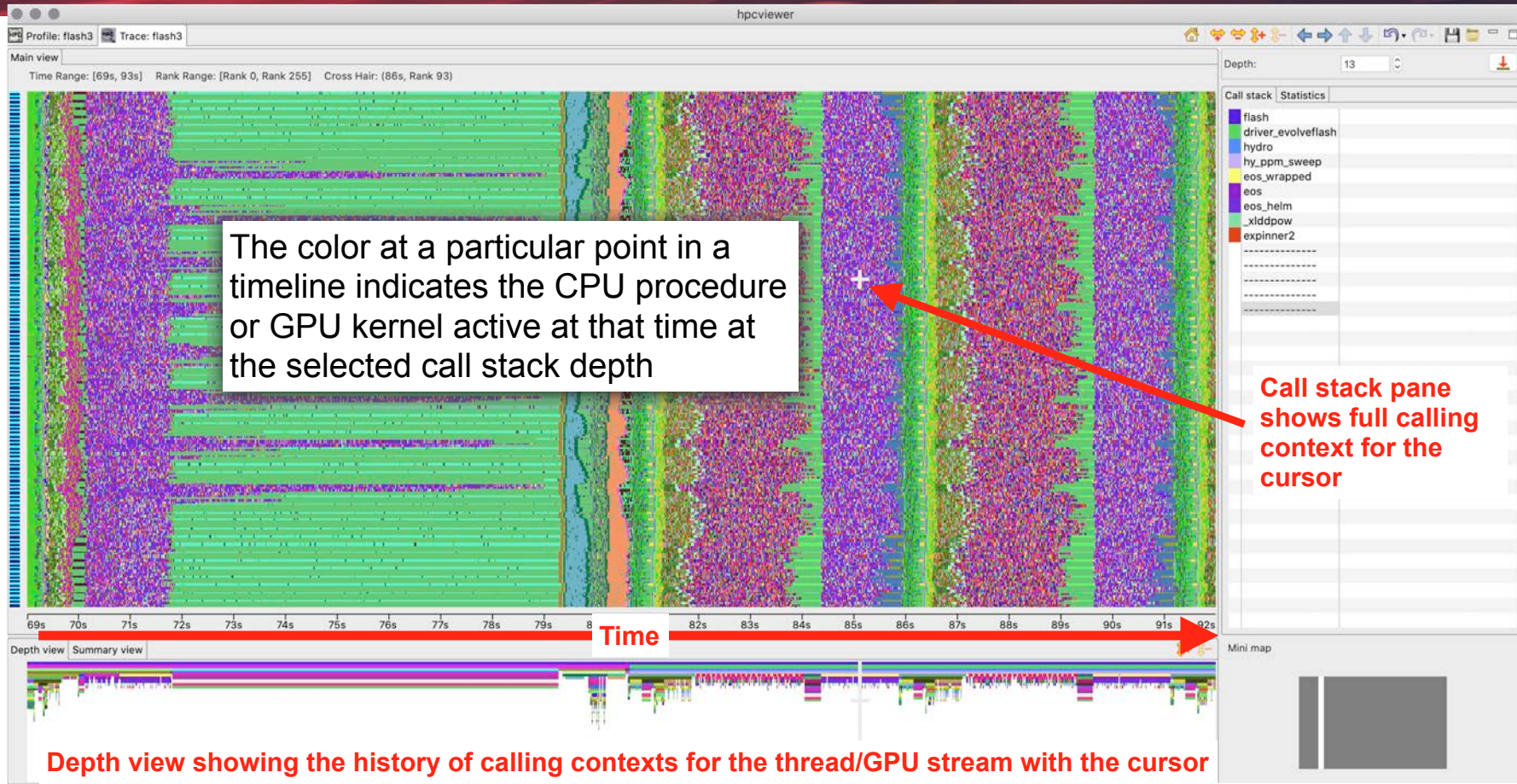
- Profiling compresses out the temporal dimension
  - Temporal patterns, e.g. serial sections and dynamic load imbalance are invisible in profiles
- What can we do? Trace call path samples
  - N times per second, take a call path sample of each thread
  - Organize the samples for each thread along a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



[computingtraining.anl.gov](http://computingtraining.anl.gov)

# Time-centric Analysis with hpcviewer

MPI ranks, OpenMP Threads, GPU streams



# Case Studies

- ExaWind
- GAMESS (OpenMP)
- Quicksilver (CUDA)
- LAMMPS (Kokkos) at exascale

# ExaWind: Wakes from Three Turbines over Time

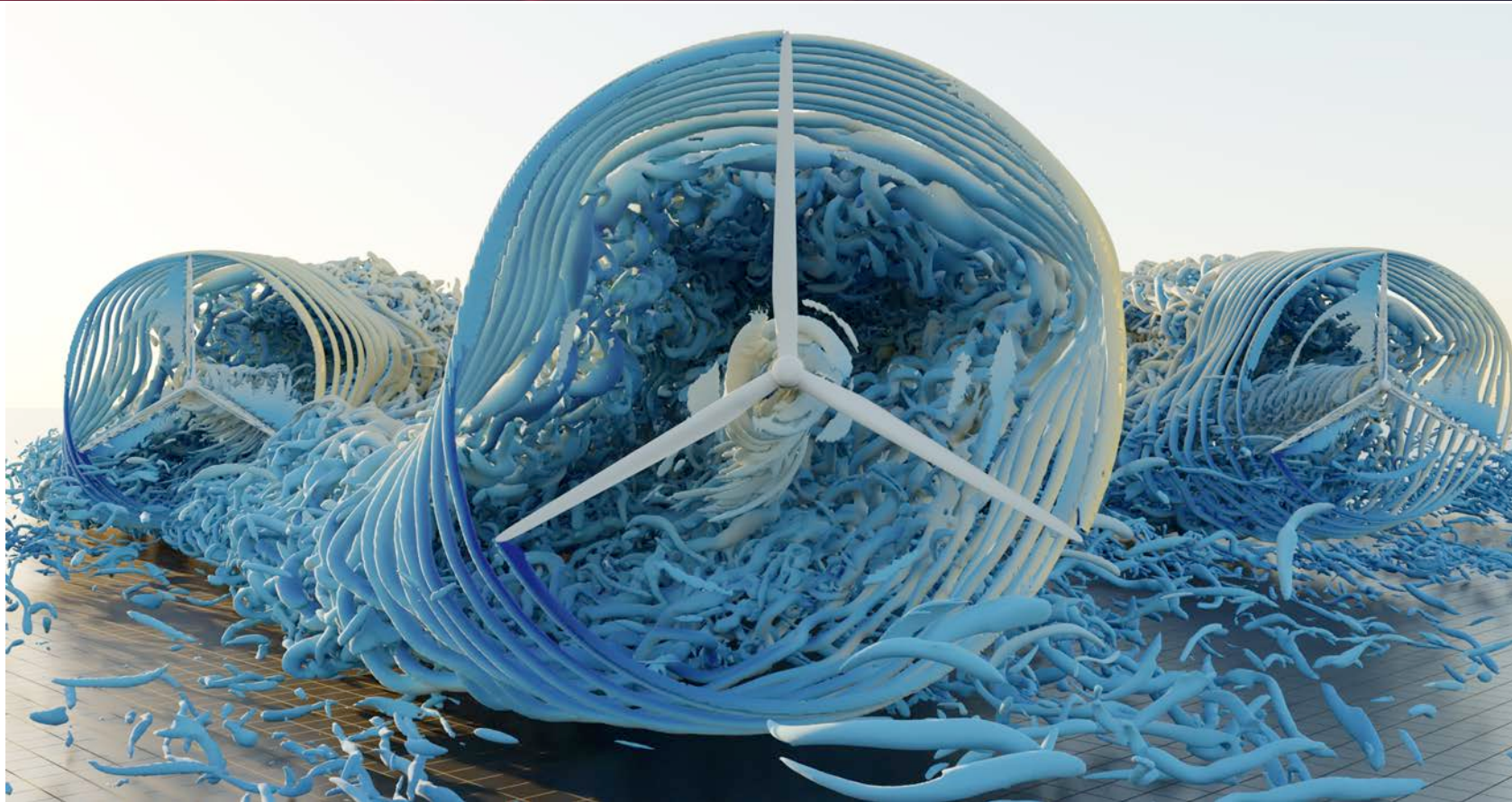


Figure credit: Jon Rood, NREL

# ExaWind: Visualization of a Wind Farm Simulation

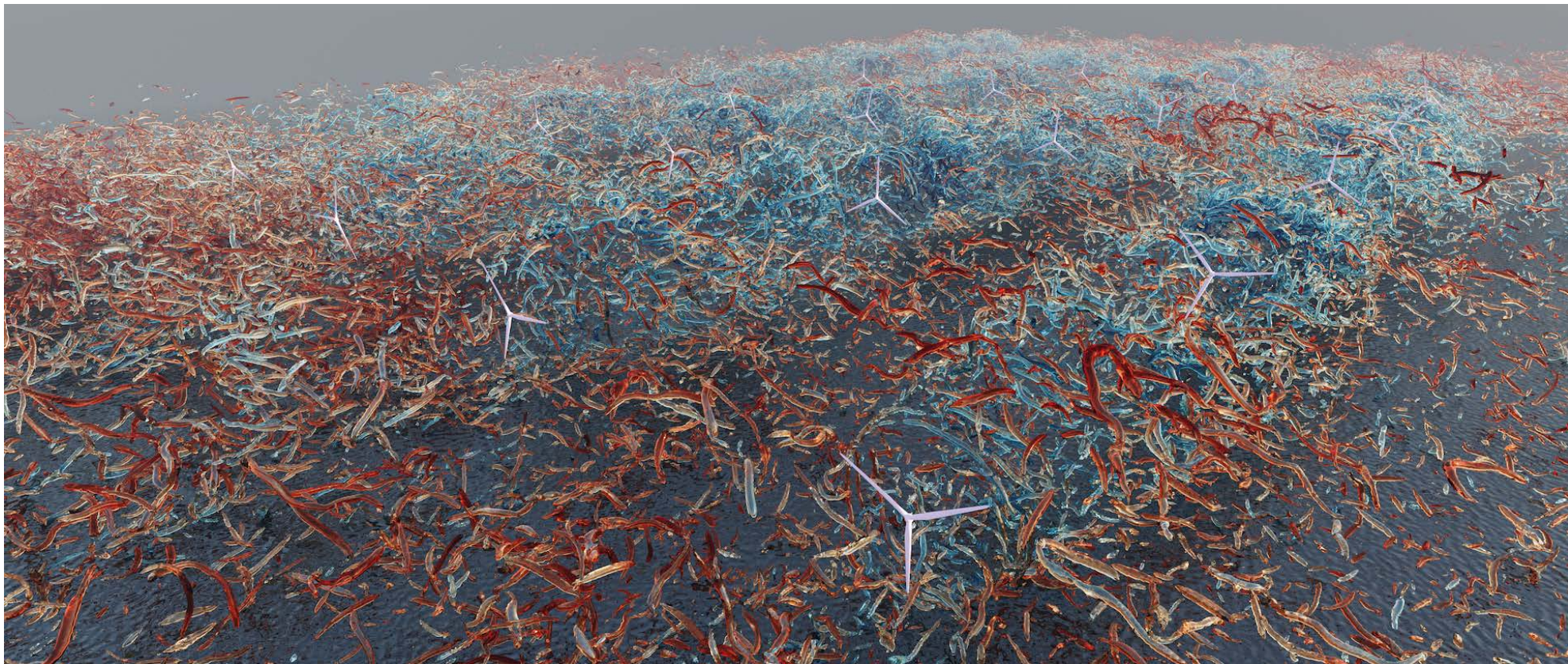


Figure credit: Jon Rood, NREL

# ExaWind: Execution Traces on Frontier Collected with HPCToolkit

Traces on roughly ~70K MPI ranks for ~17minutes

Before: MPI waiting (bad), shown in red

After: MPI overhead negligible\*

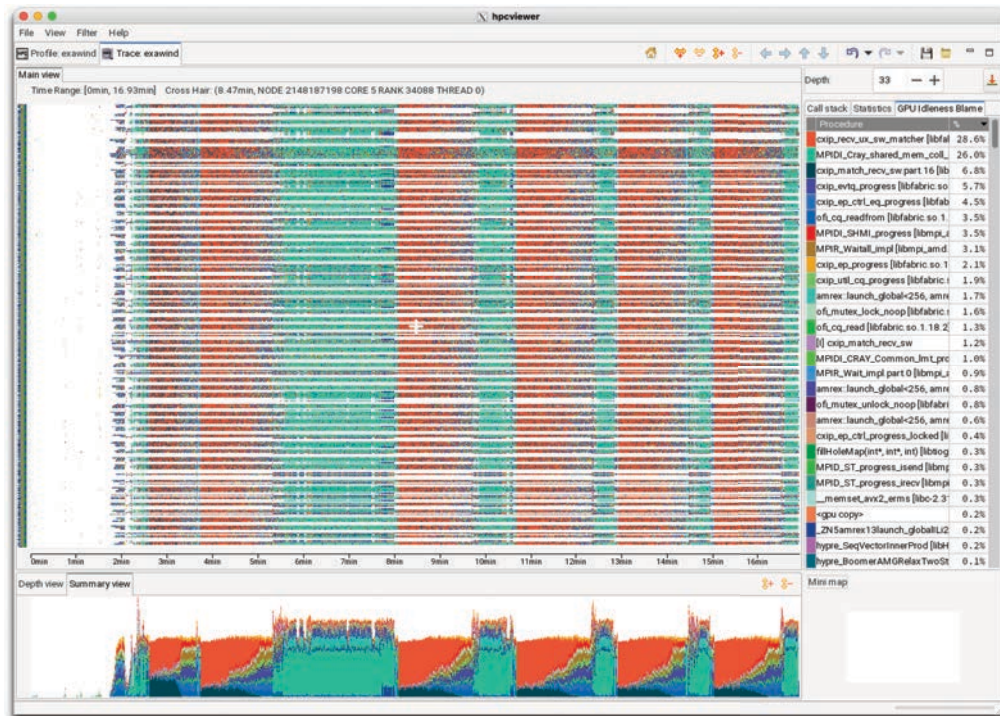


Figure credits: Jon Rood, NREL

\*replaced non-blocking send/recv with ialltoallv

# ExaWind Testimonials for HPCToolkit

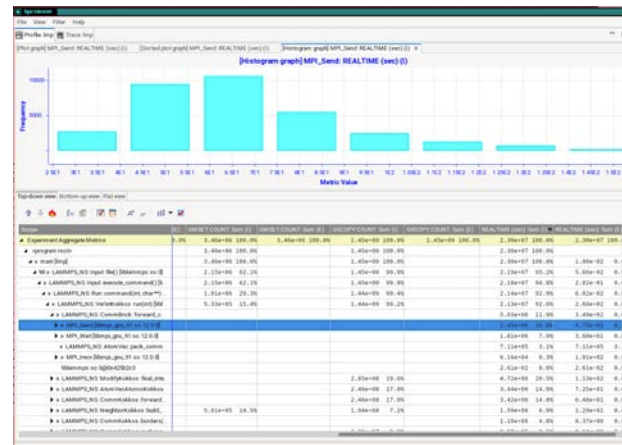
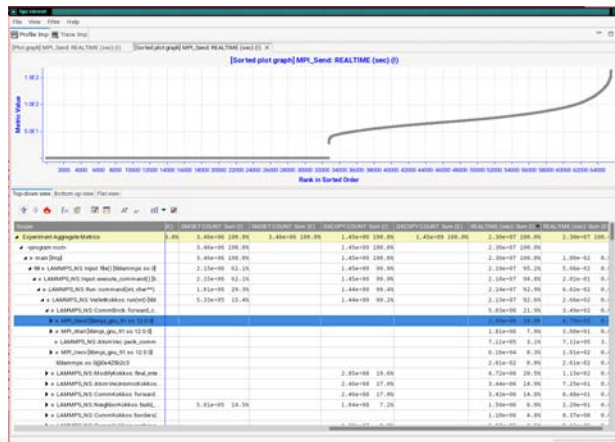
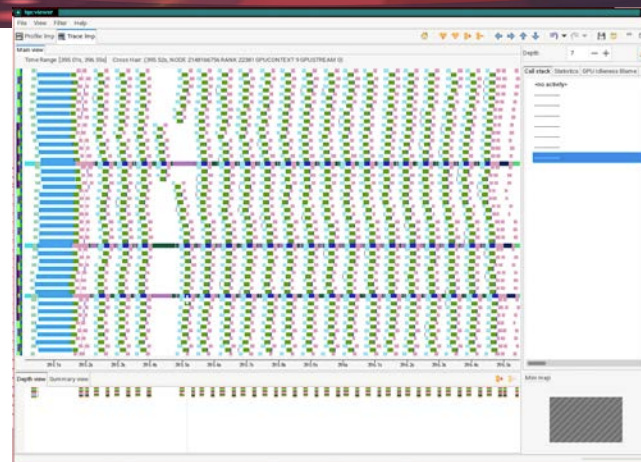
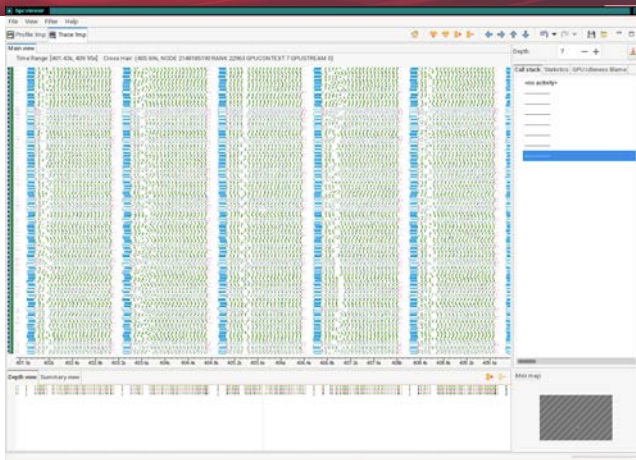
*I just wanted to mention we've been using HPCToolkit a lot for our ExaWind application on Frontier, which is **a hugely complicated code**, and **your profiler is one of the only ones we've found that really lets us easily instrument and then browse what our application is doing at runtime including GPUs**. As an example, during a recent hackathon we had, we **improved our large scale performance by 24x** by understanding our code better with HPCToolkit and **running it on 1000s of nodes while profiling**. We also recently improved upon this by 10% for our total runtime.*

*- Jon Rood NREL (5/31/2024)*

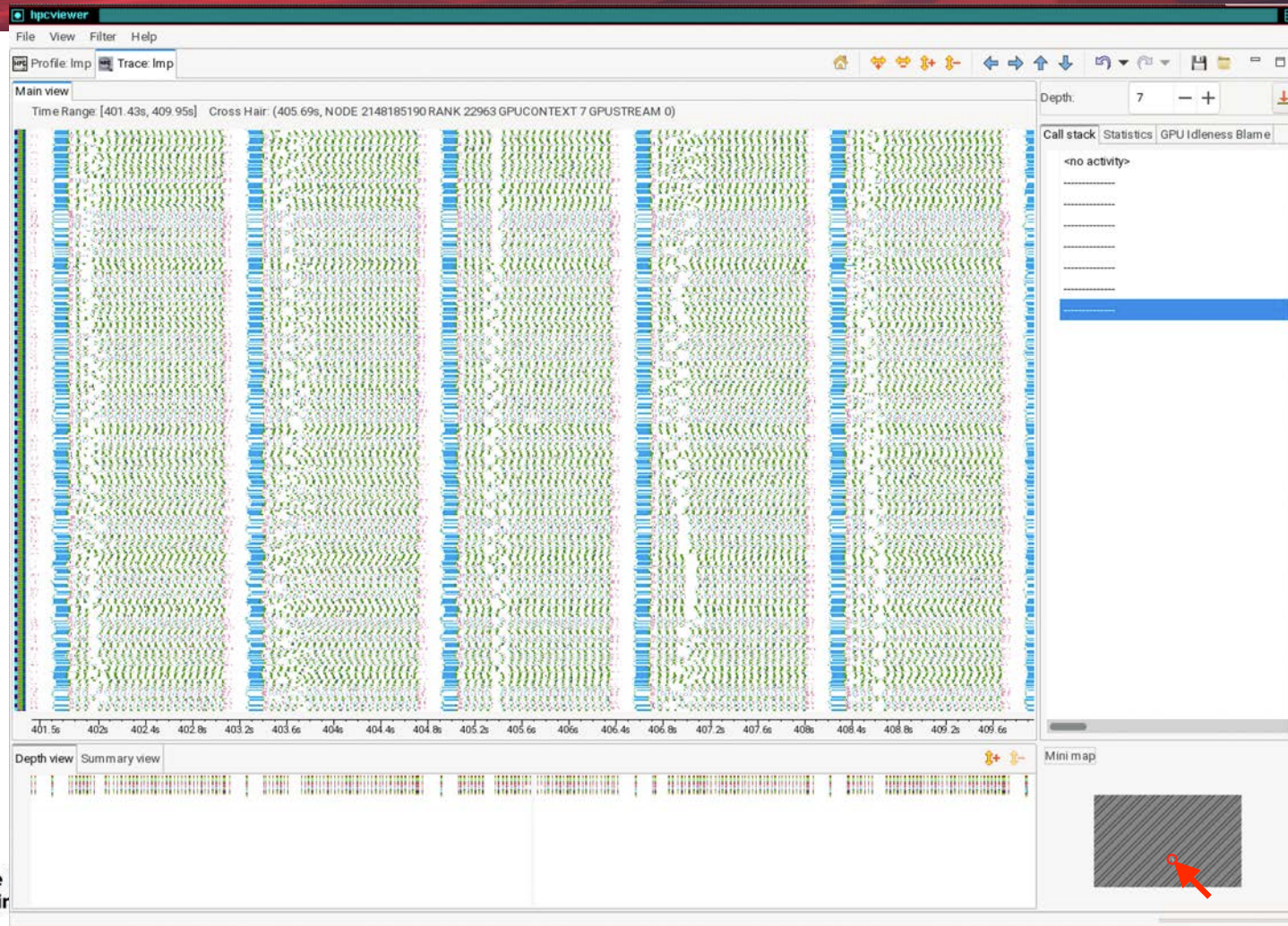
*One big thing for us is that we can't overstate how complicated ExaWind is in general, and how complicated it is to build, so finding out that **HPCToolkit could easily profile our entire application without a ton of instrumentation during the build process, and be able to profile it on a huge amount of Frontier with line numbers and visualizing the trace was really amazing to us**.*

*- Jon Rood NREL (6/3/2024)*

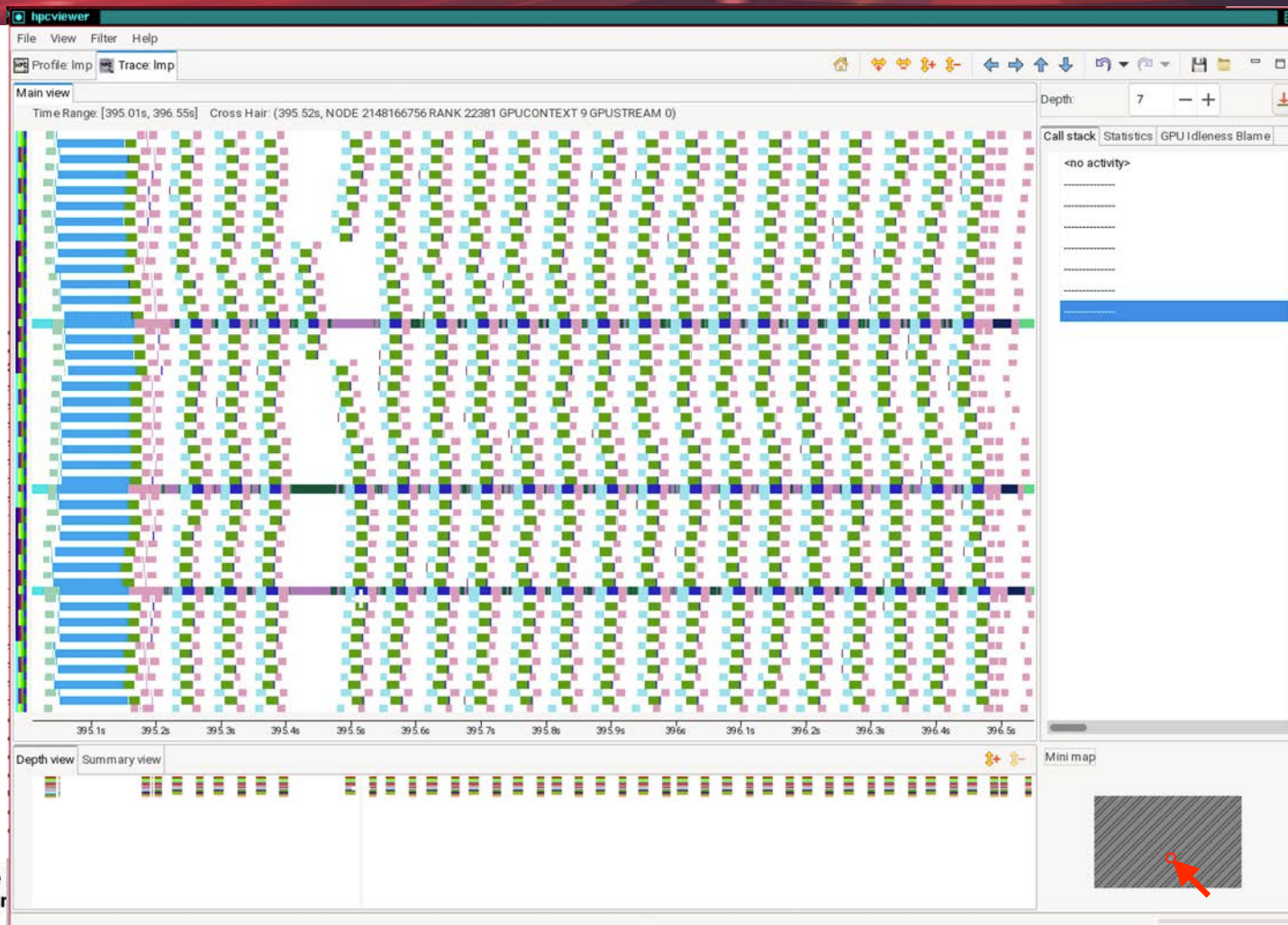
## LAMMPS on Frontier: Executions with Kernel Duration of Milliseconds



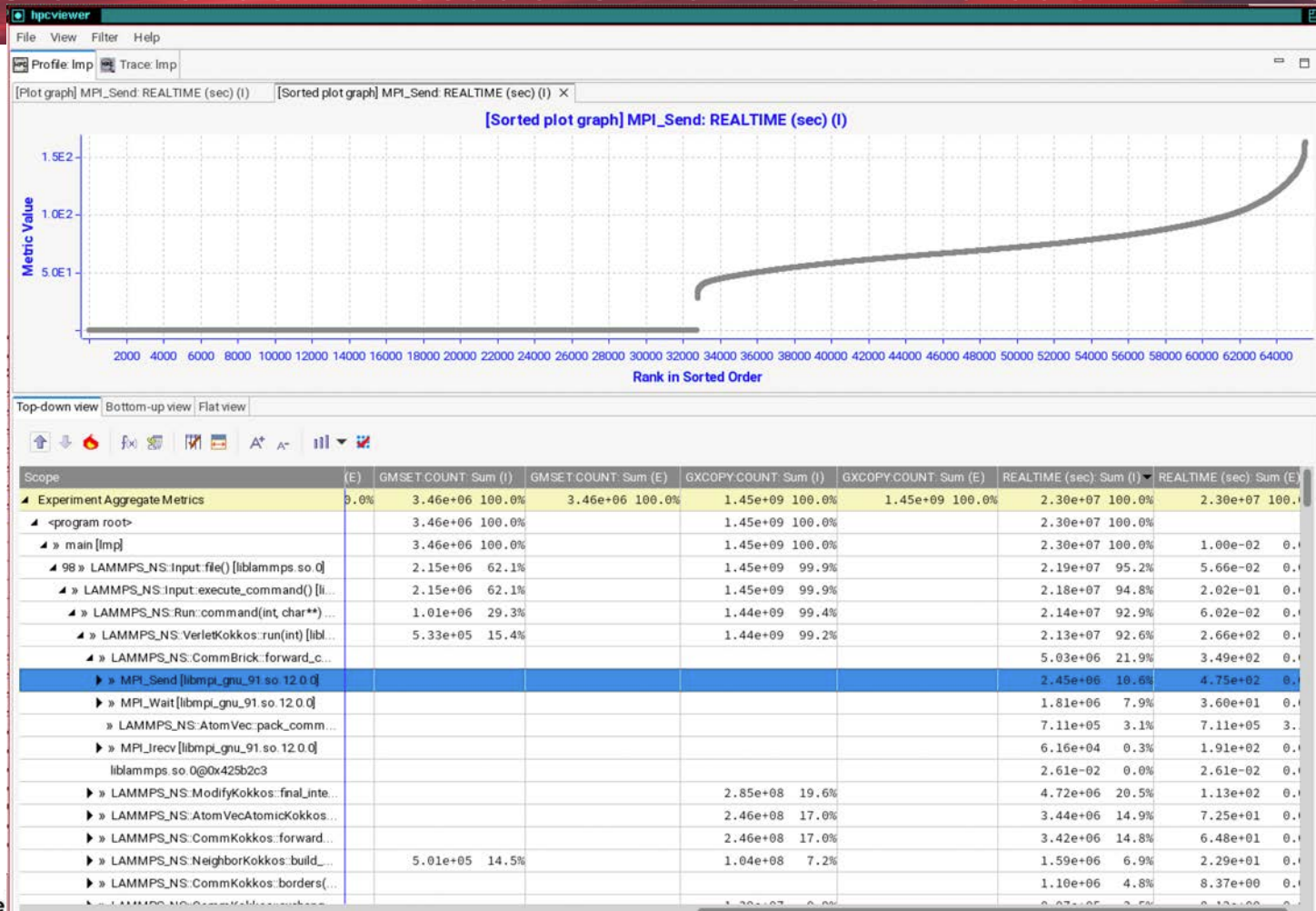
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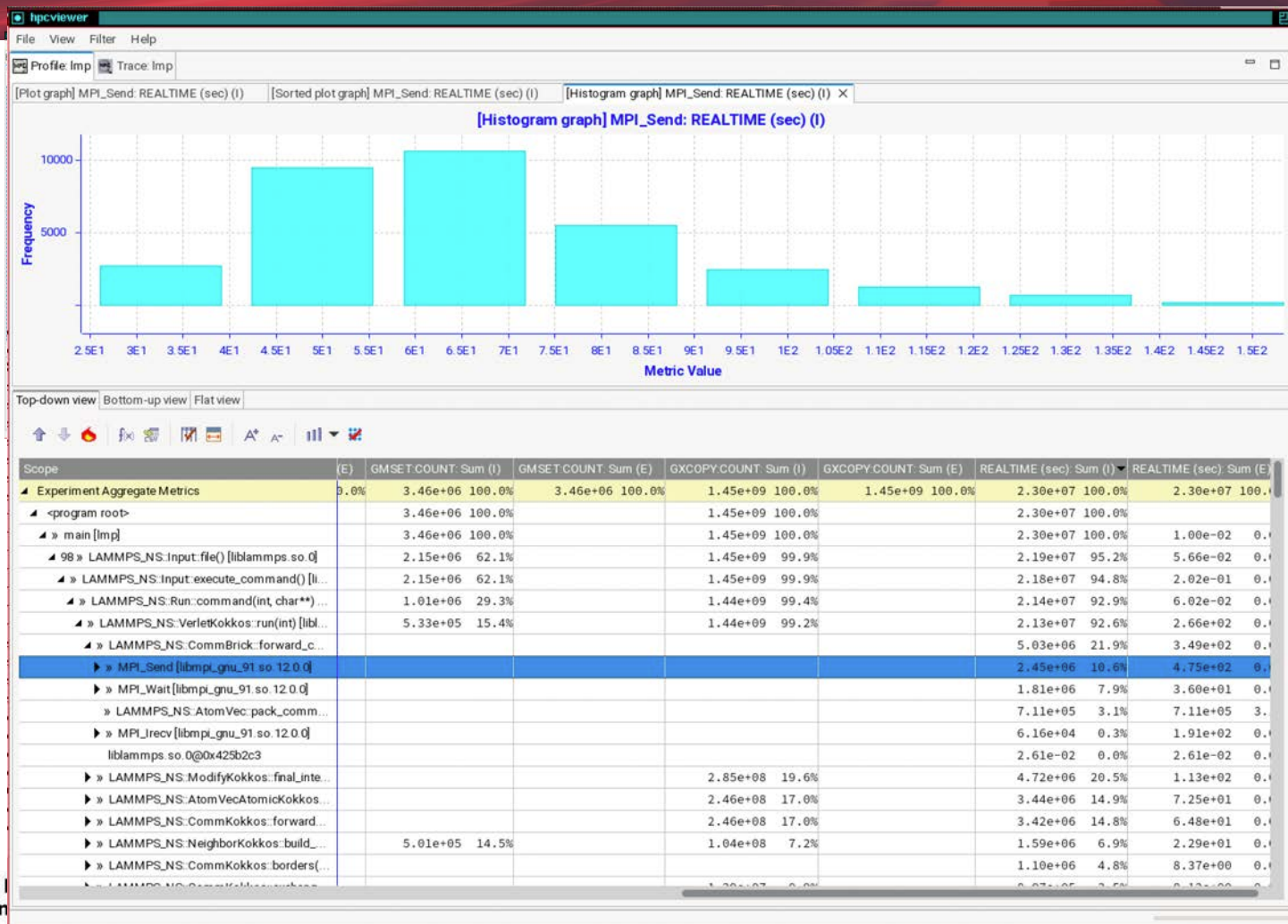
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# LAMMPS on Frontier: Executions with Kernel Duration of Milliseconds

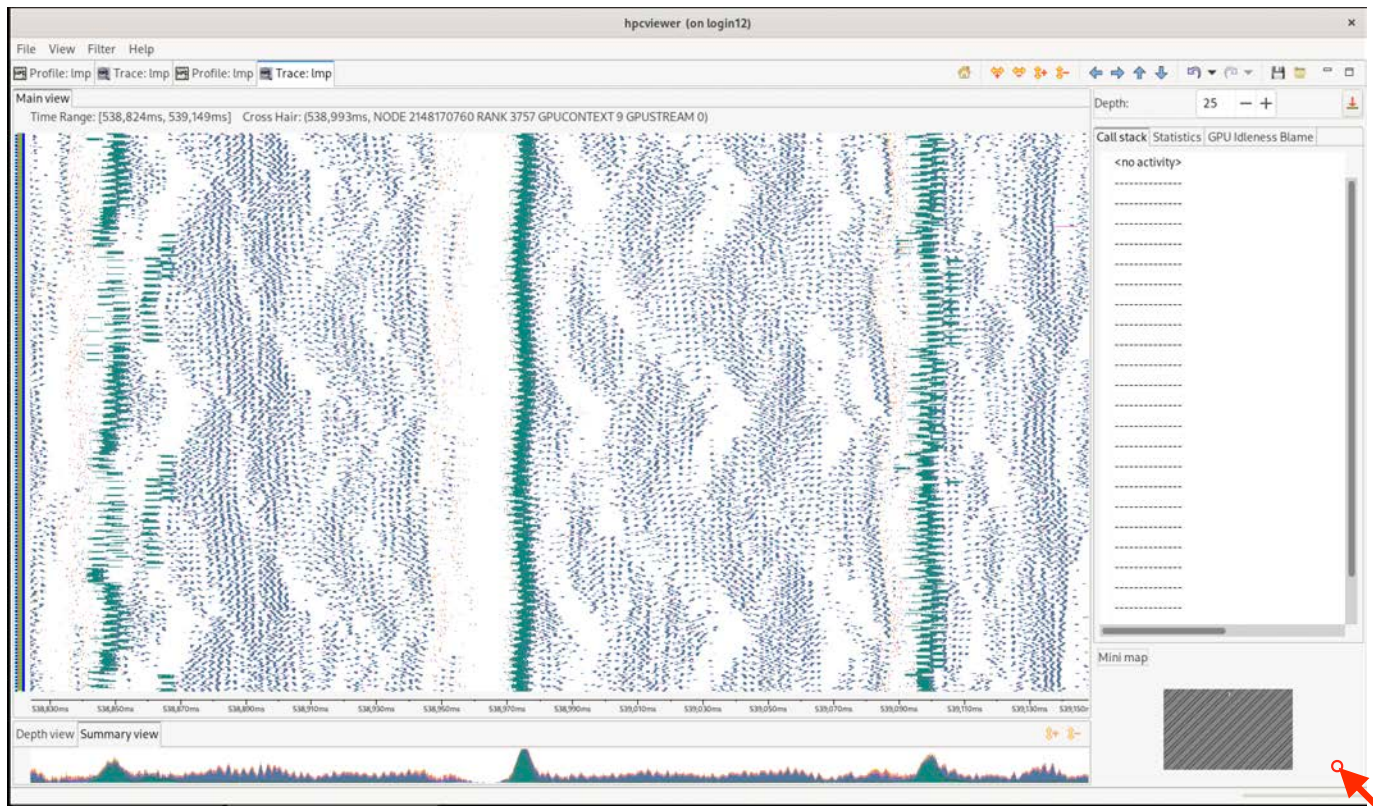


# LAMMPS on Frontier: Executions with Kernel Duration of Milliseconds



# LAMMPS on Frontier: 8K nodes, 64K MPI ranks + 64K GPU tiles

Kernel duration of microseconds



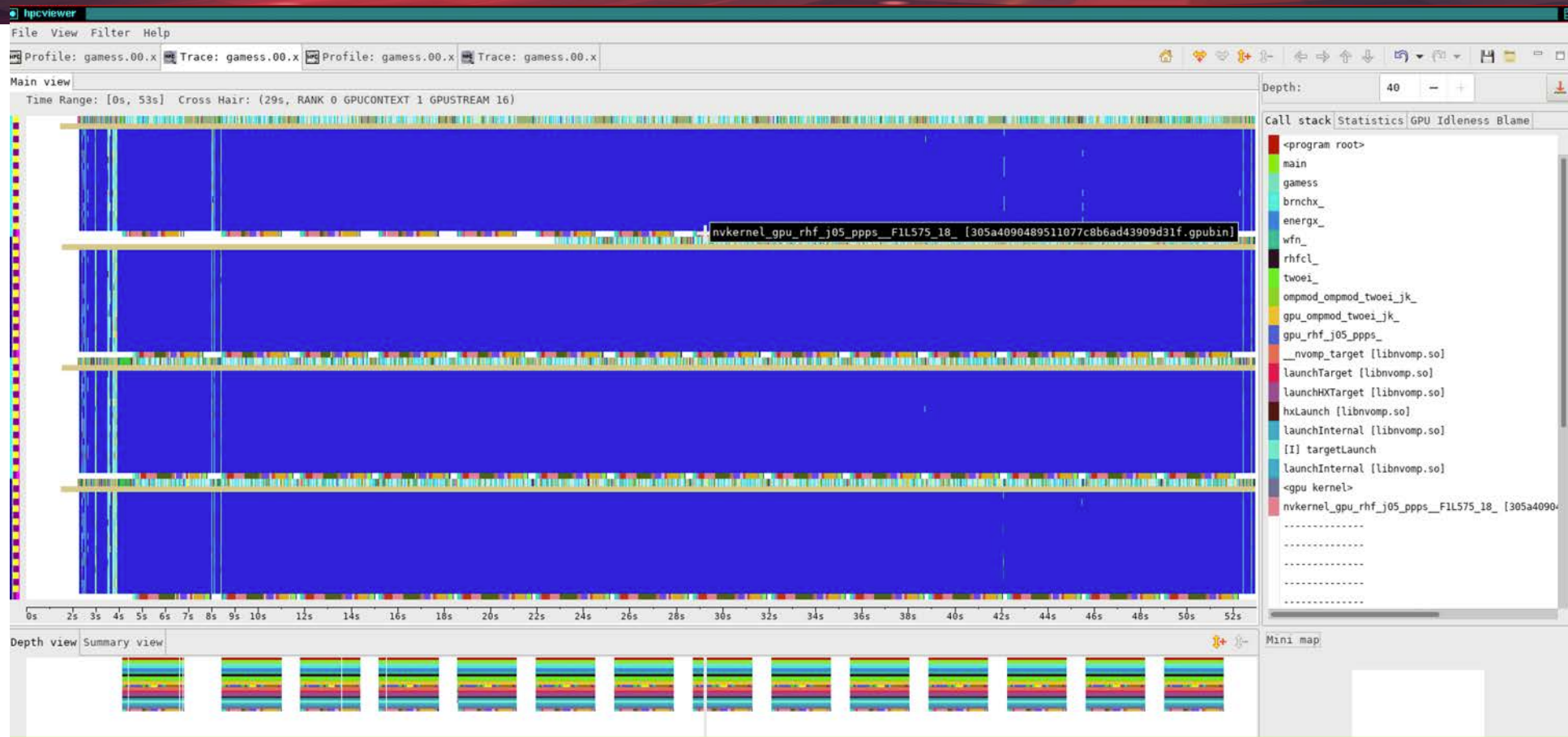
# Case Study: GAMESS

- General Atomic and Molecular Electronic Structure System (GAMESS)
  - general *ab initio* quantum chemistry package
- Calculates the energies, structures, and properties of a wide range of chemical systems
- Experiments
  - GPU-accelerated nodes at a prior Perlmutter hackathon
    - Single node with 4 GPUs
    - Five nodes with 20 GPUs

## Perlmutter node at a glance

AMD Milan CPU  
4 NVIDIA A100 GPUs  
256 GB memory

# Time-centric Analysis: GAMESS 4 ranks, 4 GPUs on Perlmutter



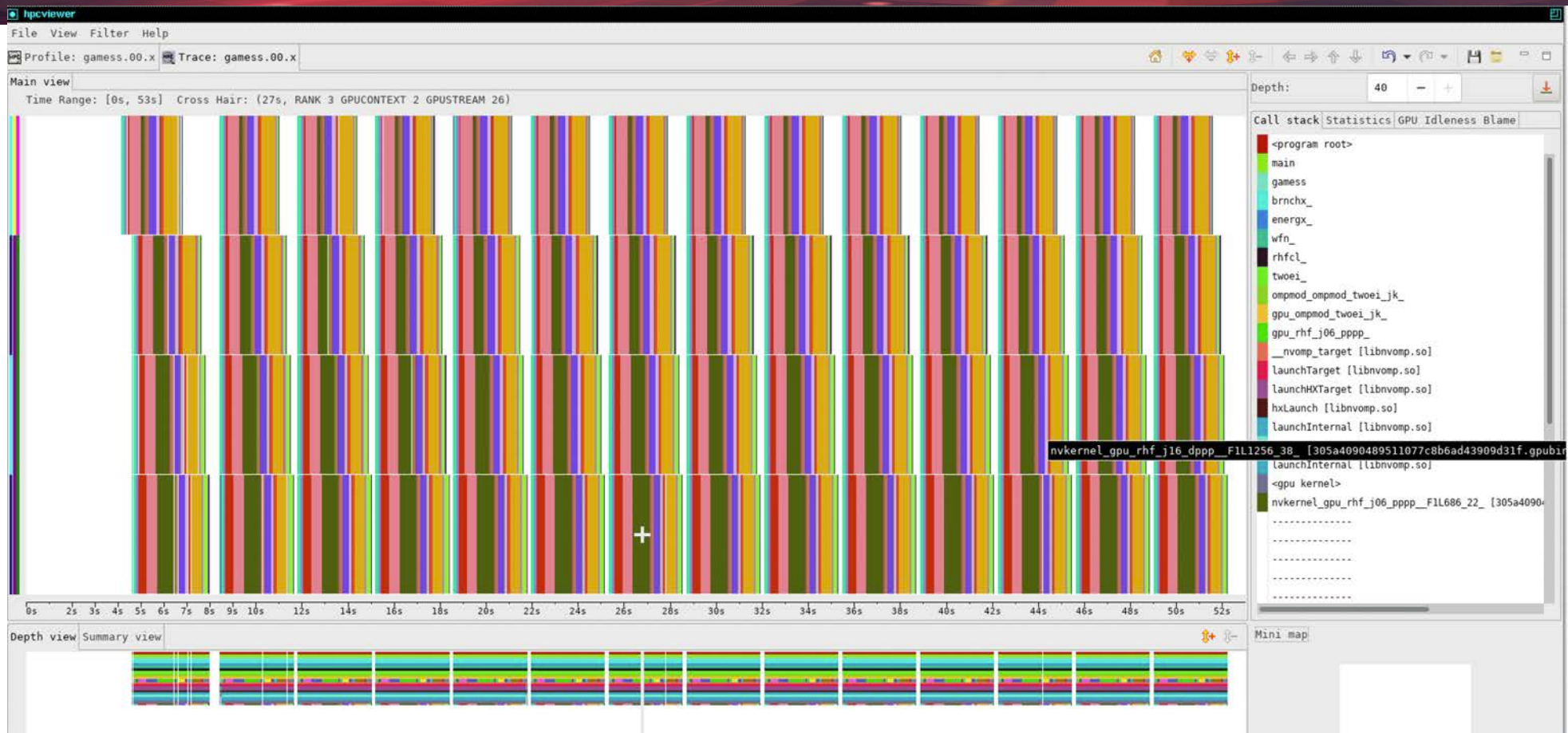
GAMESS original

All CPU threads and GPU streams

The screenshot shows the hpcviewer application interface. The main window displays a GPU usage timeline for a game named 'game00'. The timeline is a horizontal bar chart with a color-coded legend on the left. The x-axis represents time in seconds, ranging from 0s to 52s. The y-axis represents the GPU usage, with a 'Depth view' and 'Summary view' at the bottom. A 'Select rank to display' dialog box is open in the center, showing a table of ranks and threads. The dialog box has a 'Filter' field set to 'GPU' and a 'Regular expression' checkbox. The table lists four ranks, each with a checked checkbox and a description: RANK 0 GPUCONTEXT 1 GPSTREAM 16, RANK 1 GPUCONTEXT 2 GPSTREAM 26, RANK 2 GPUCONTEXT 2 GPSTREAM 26, and RANK 3 GPUCONTEXT 2 GPSTREAM 26. The dialog box has 'Cancel' and 'OK' buttons. On the right side of the main window, there is a 'Call stack' panel showing a list of functions: <thread root>, threadPoolEntryPoint [libnvomp.so], hxiExecuteHostTreeBarrierWithTasks [libnvomp.so], [I] executeHostTreeBarrier, [I] waitNeighborThreads, hxAddressWait [libnvomp.so], and syscall [libc-2.31.so]. The 'Depth' field is set to 40. The 'Mini map' panel at the bottom right shows a small overview of the timeline.

## All CPU threads and GPU streams

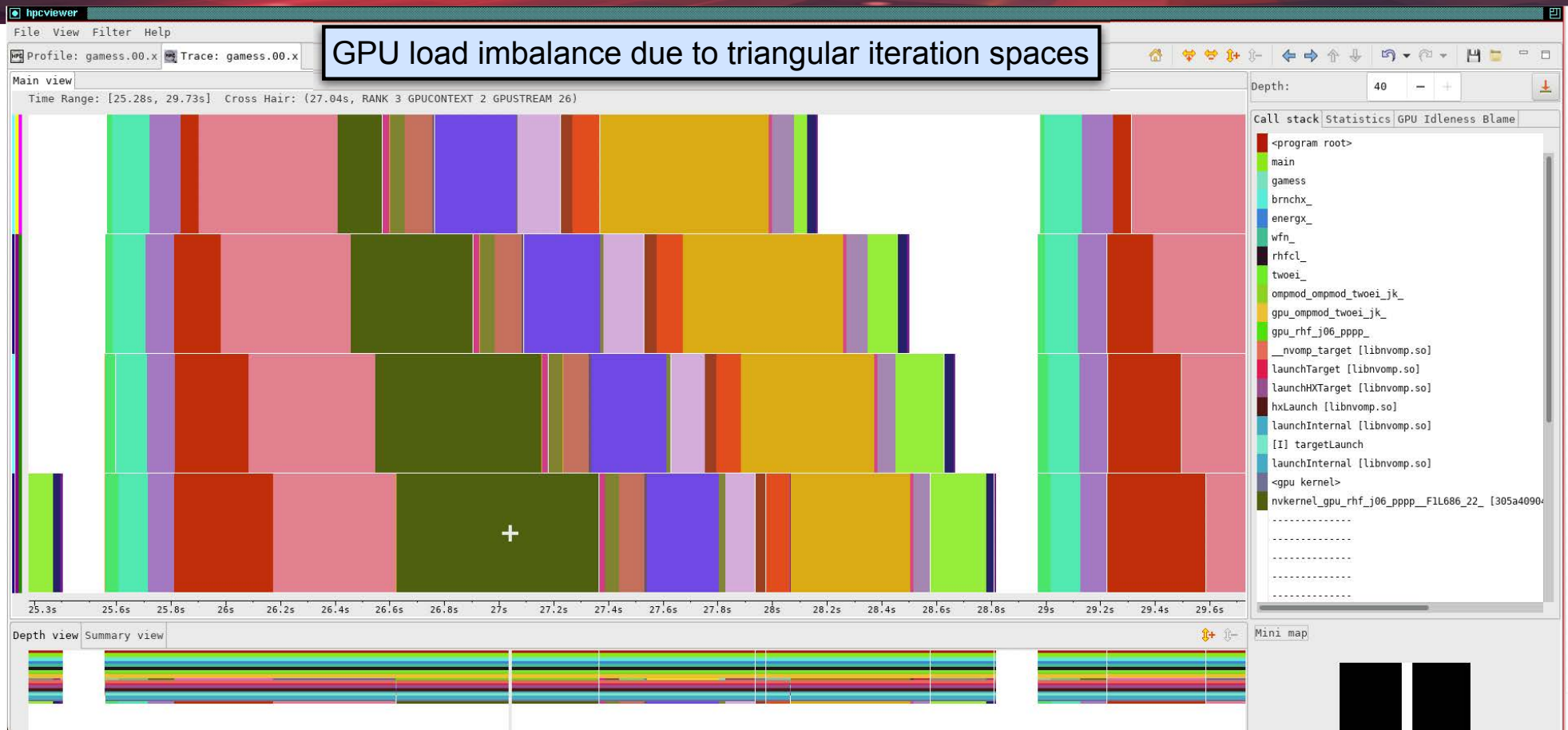
## Time-centric Analysis: GAMESS 4 ranks, 4 GPUs on Perlmutter



# GAMESS original

## All GPU streams, whole execution

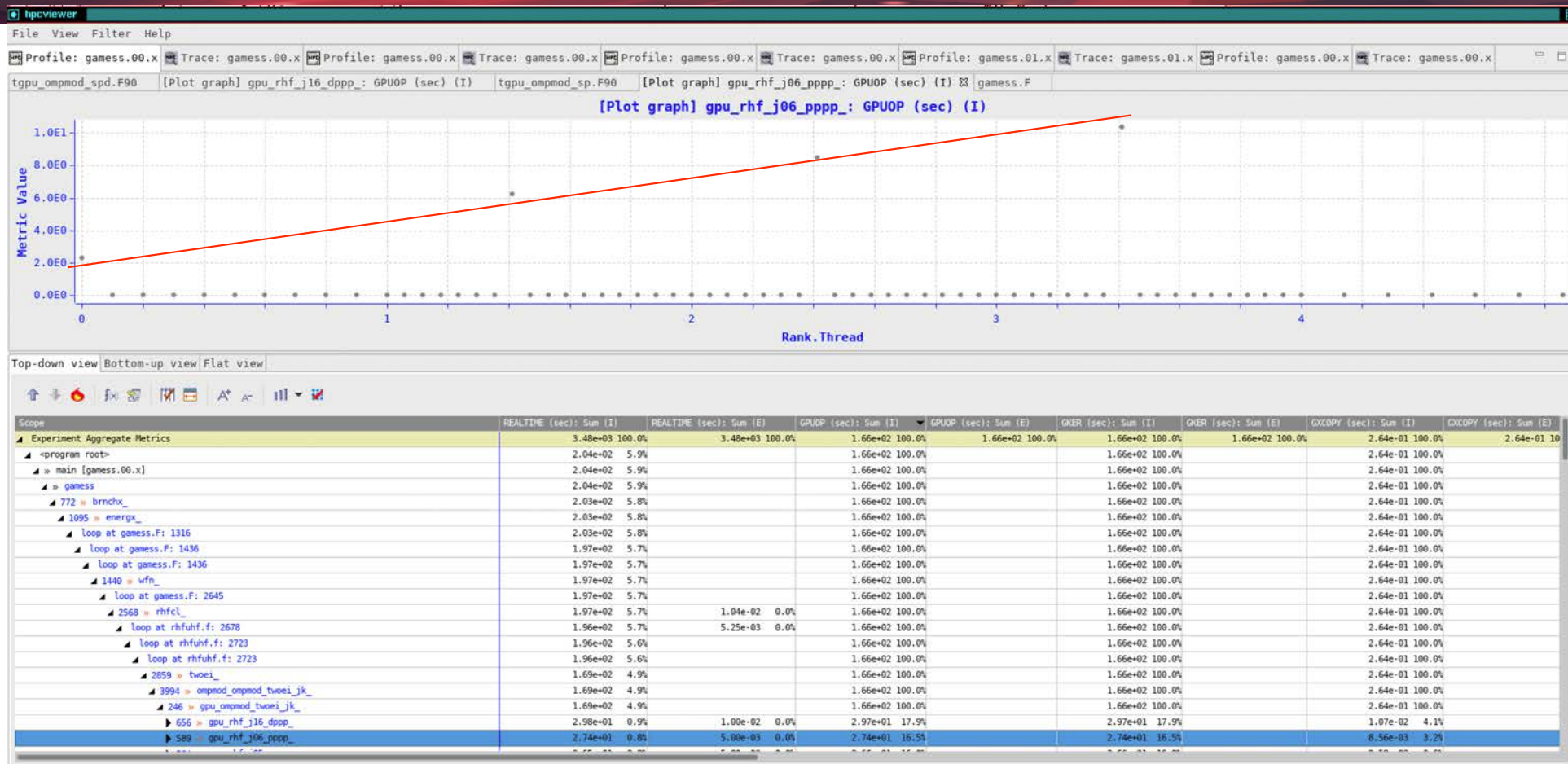
# Time-centric Analysis: GAMESS 4 ranks, 4 GPUs on Perlmutter



GAMESS original

GPU streams: 1 iteration

# Time-centric Analysis: GAMESS 4 ranks, 4 GPUs on Perlmutter



GAMESS original

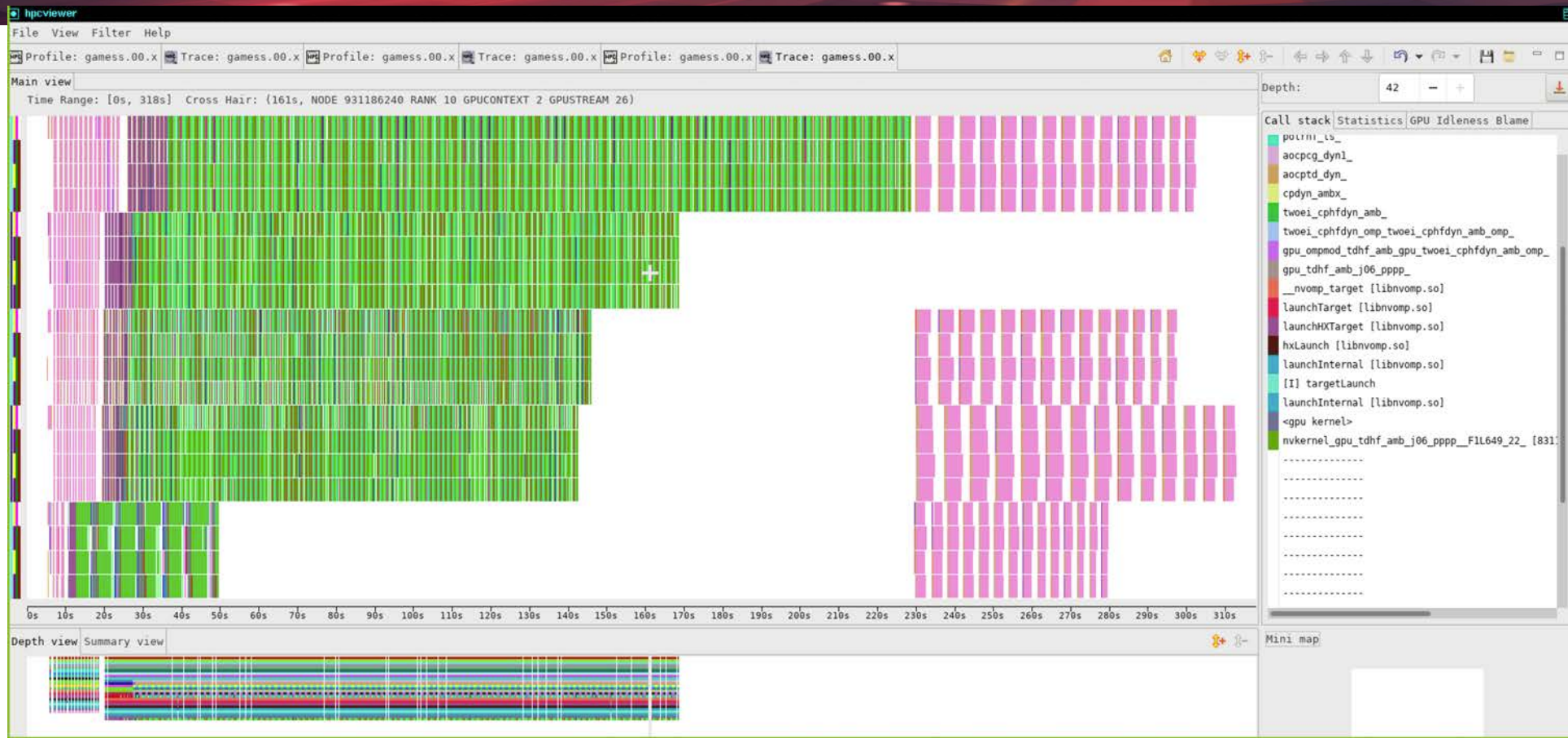
# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter



GAMESS improved

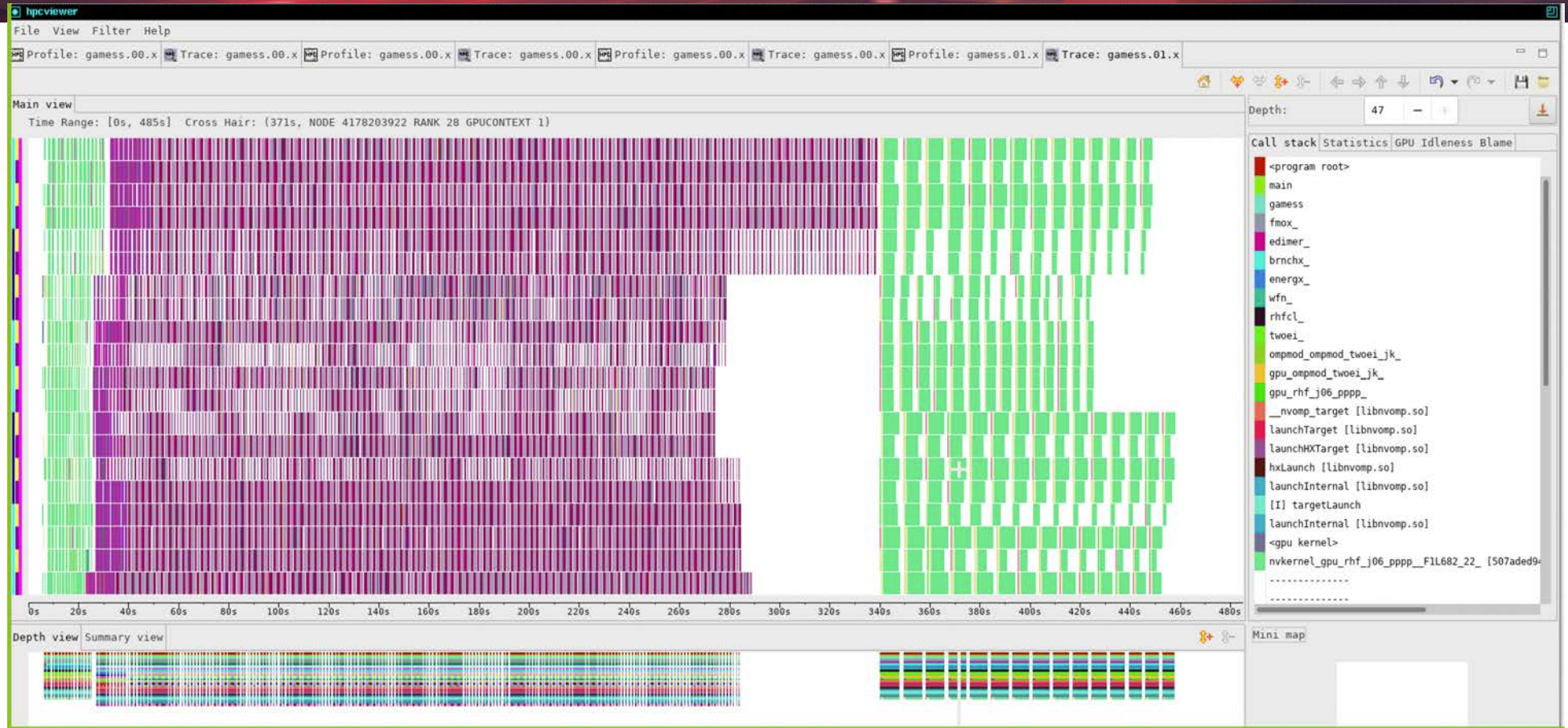
CPU Threads and GPU Streams

# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter



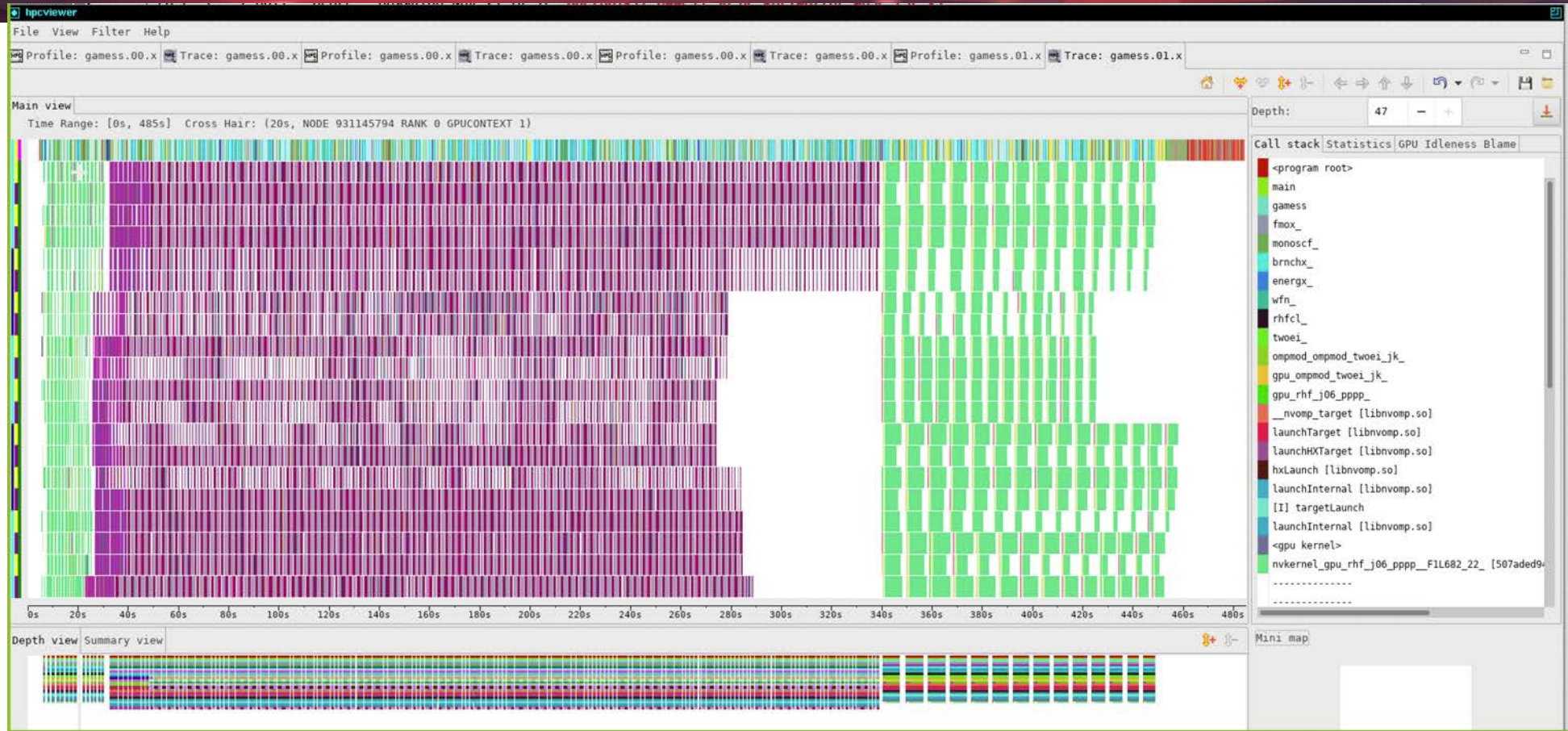
GAMESS improved

# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter



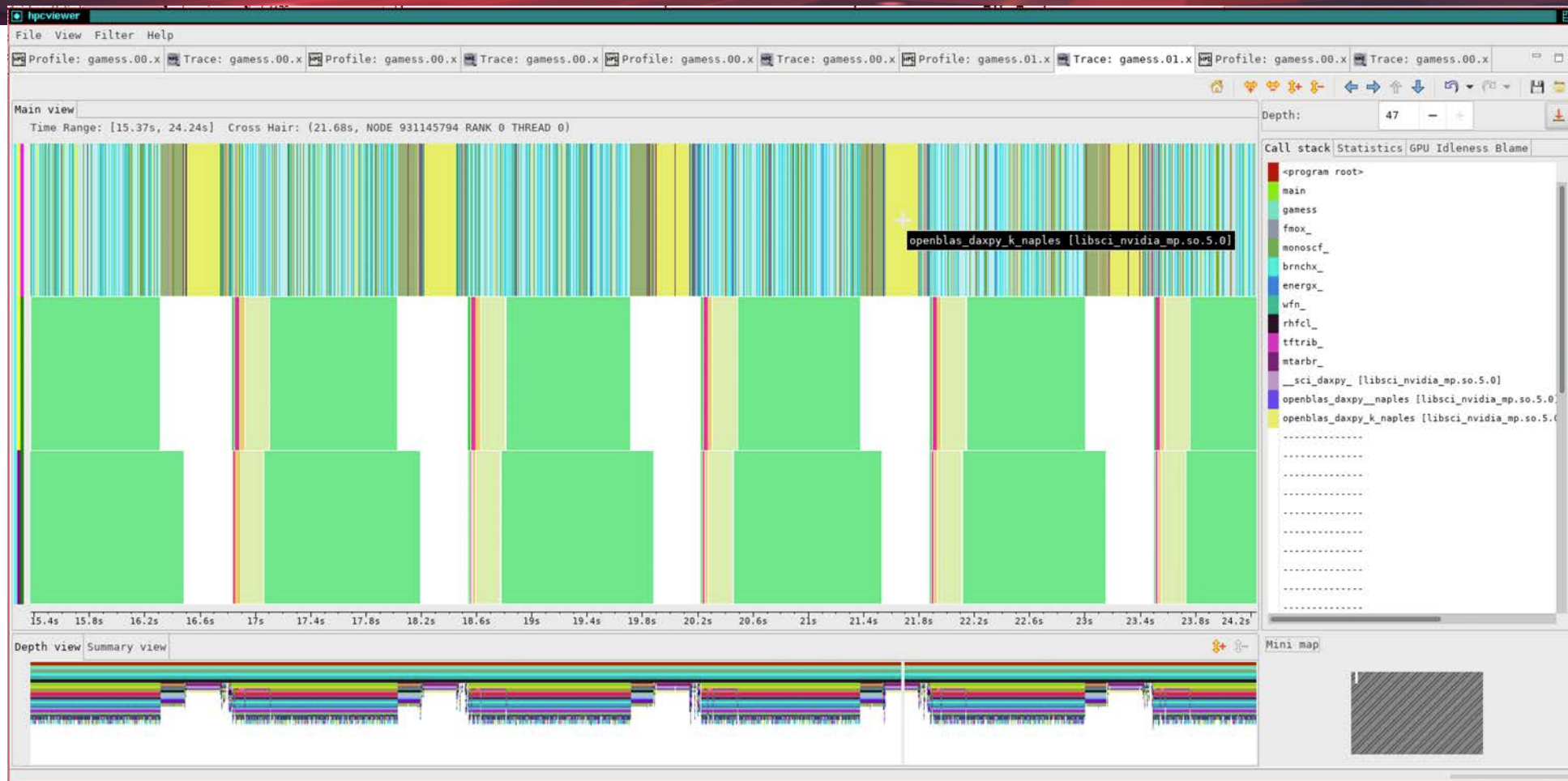
GAMESS improved with better manual distribution of work in input

# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter



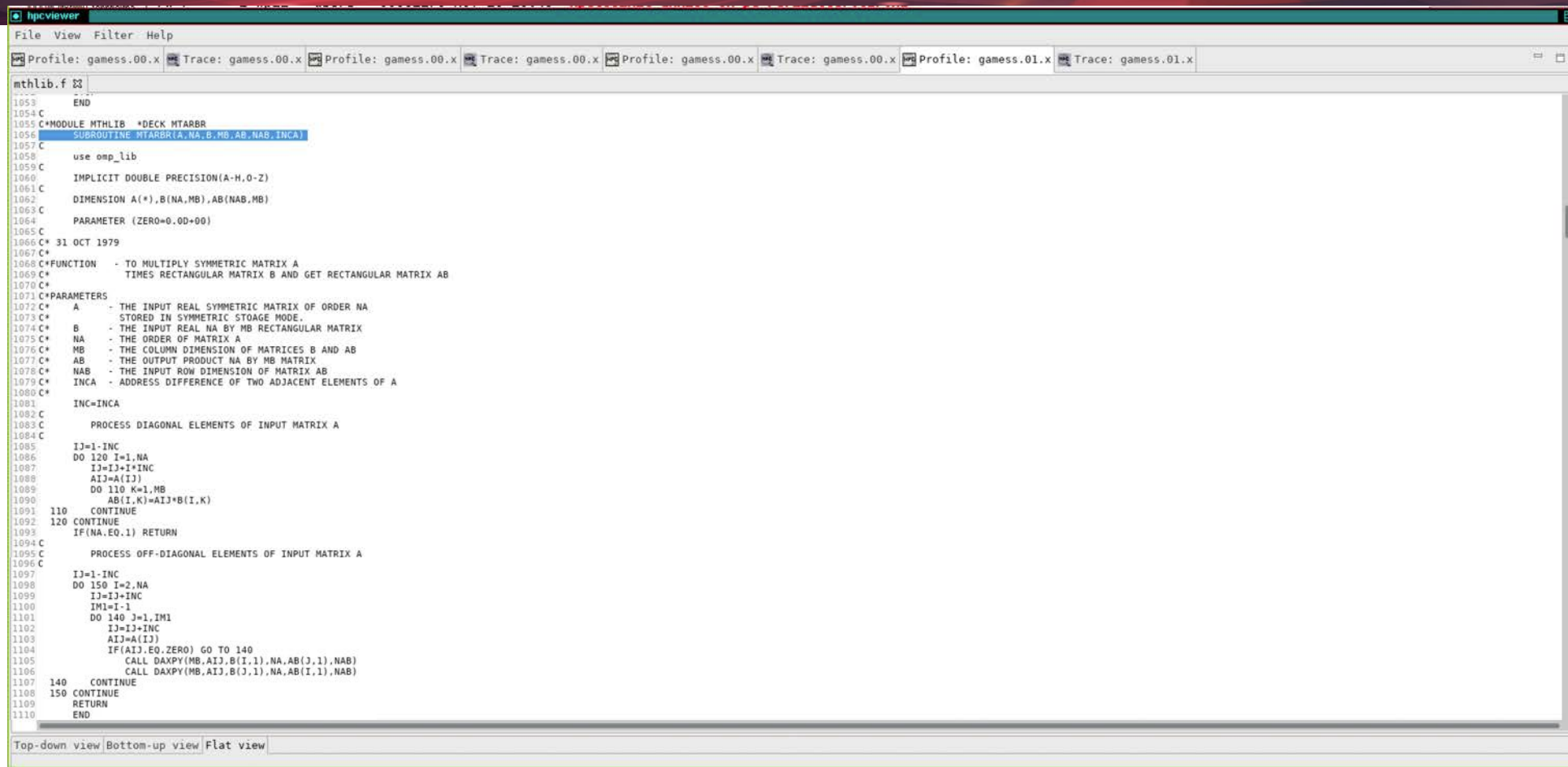
GAMESS improved adding Rank 0 Thread 0 to GPU streams

# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter



1 CPU Stream, 2 GPU Streams: 6 Iterations

# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter

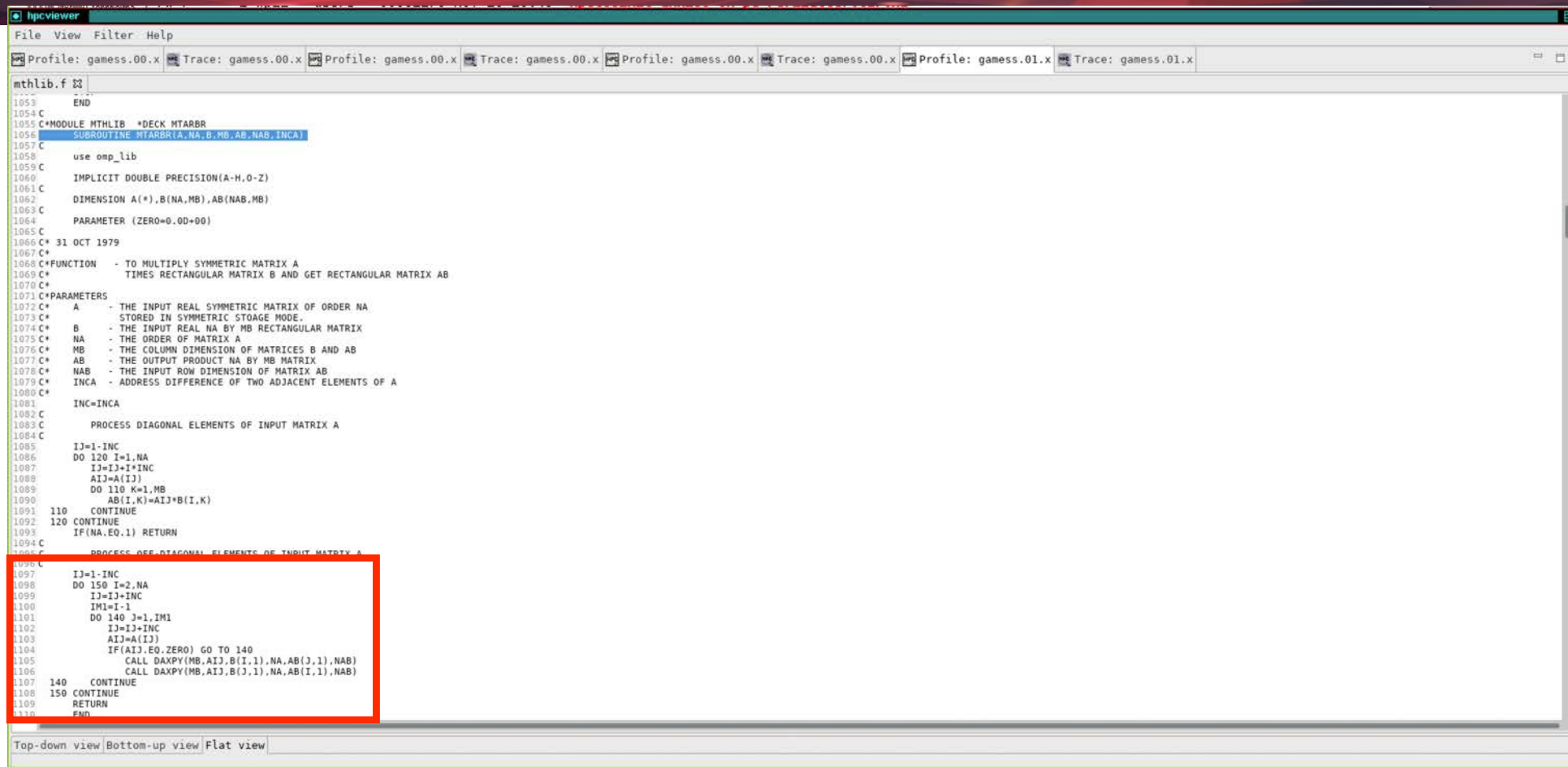


```
File View Filter Help
Profile: gamess.00.x Trace: gamess.00.x Profile: gamess.00.x Trace: gamess.00.x Profile: gamess.00.x Trace: gamess.00.x Profile: gamess.01.x Trace: gamess.01.x

mthlib.f
1053 END
1054 C
1055 C*MODULE MTHLIB *DECK MTARBR
1056 SUBROUTINE MTARBR(A,NA,B,MB,AB,NAB,INCA)
1057 C
1058 use omp_lib
1059 C
1060 IMPLICIT DOUBLE PRECISION(A-H,O-Z)
1061 C
1062 DIMENSION A(*),B(NA,MB),AB(NAB,MB)
1063 C
1064 PARAMETER (ZERO=0.0D+00)
1065 C
1066 C* 31 OCT 1979
1067 C*
1068 C*FUNCTION - TO MULTIPLY SYMMETRIC MATRIX A
1069 C* TIMES RECTANGULAR MATRIX B AND GET RECTANGULAR MATRIX AB
1070 C*
1071 C*PARAMETERS
1072 C* A - THE INPUT REAL SYMMETRIC MATRIX OF ORDER NA
1073 C* STORED IN SYMMETRIC STORAGE MODE.
1074 C* B - THE INPUT REAL NA BY MB RECTANGULAR MATRIX
1075 C* NA - THE ORDER OF MATRIX A
1076 C* MB - THE COLUMN DIMENSION OF MATRICES B AND AB
1077 C* AB - THE OUTPUT PRODUCT NA BY MB MATRIX
1078 C* NAB - THE INPUT ROW DIMENSION OF MATRIX AB
1079 C* INCA - ADDRESS DIFFERENCE OF TWO ADJACENT ELEMENTS OF A
1080 C*
1081 INC=INCA
1082 C
1083 C PROCESS DIAGONAL ELEMENTS OF INPUT MATRIX A
1084 C
1085 IJ=1-INC
1086 DO 120 I=1,NA
1087 IJ=IJ+INC
1088 AIJ=A(IJ)
1089 DO 110 K=1,MB
1090 ABI(K)=AIJ*B(I,K)
1091 110 CONTINUE
1092 120 CONTINUE
1093 IF(NA.EQ.1) RETURN
1094 C
1095 C PROCESS OFF-DIAGONAL ELEMENTS OF INPUT MATRIX A
1096 C
1097 IJ=1-INC
1098 DO 150 I=2,NA
1099 IJ=IJ+INC
1100 IM1=I-1
1101 DO 140 J=1,IM1
1102 IJ=IJ+INC
1103 AIJ=A(IJ)
1104 IF(AIJ.EQ.ZERO) GO TO 140
1105 CALL DAXPY(MB,AIJ,B(I,1),NA,AB(J,1),NAB)
1106 CALL DAXPY(MB,AIJ,B(J,1),NA,AB(I,1),NAB)
1107 140 CONTINUE
1108 150 CONTINUE
1109 RETURN
1110 END

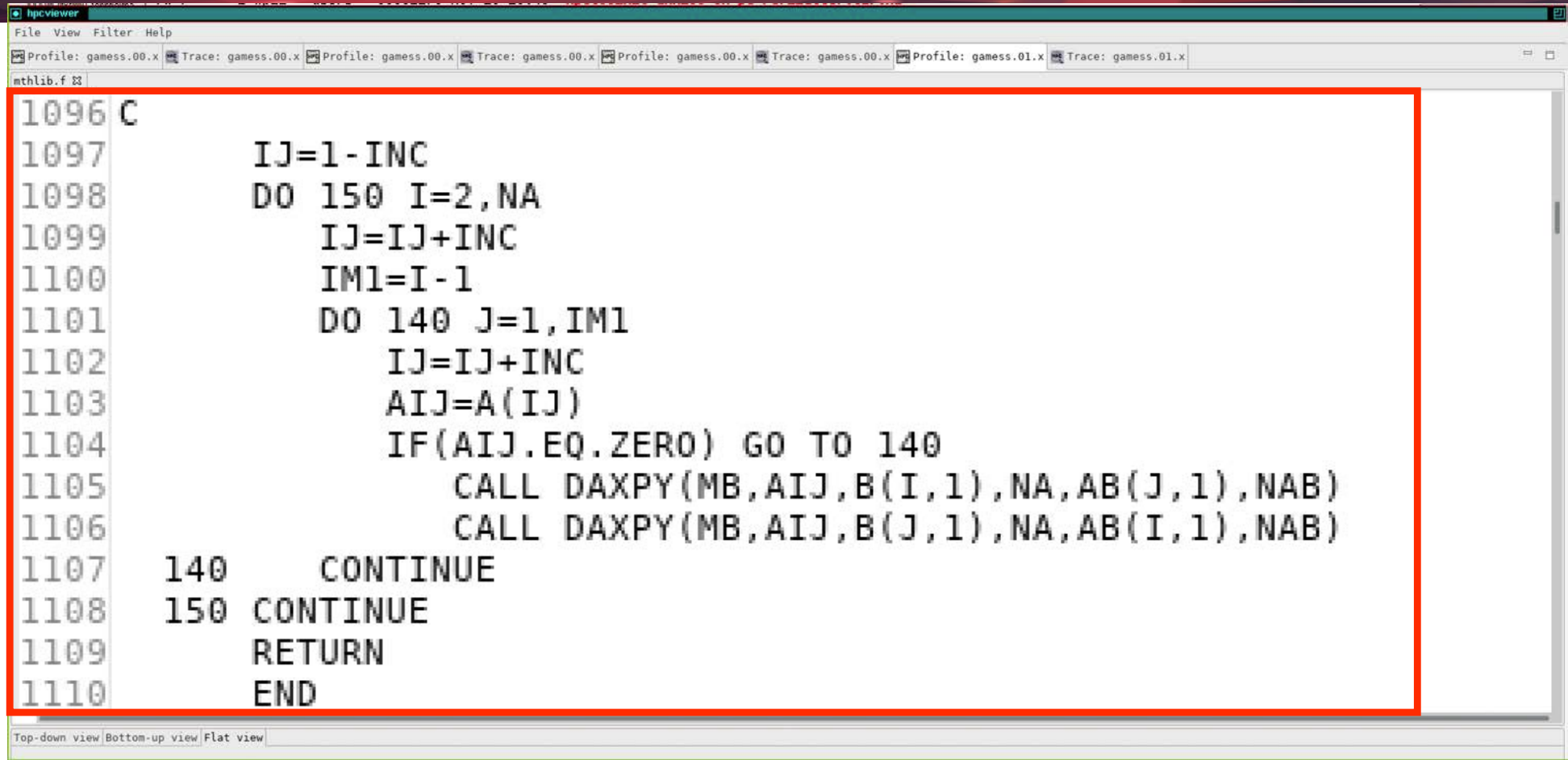
Top-down view Bottom-up view Flat view
```

# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter



```
mthlib.f
END
1053 C
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1105 CALL DAXPY(MB,AIJ,B(I,1),NA,AB(J,1),NAB)
1106 CALL DAXPY(MB,AIJ,B(J,1),NA,AB(I,1),NAB)
1107 140 CONTINUE
1108 150 CONTINUE
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1110 END
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# Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter



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1096 C
1097     IJ=1-INC
1098     DO 150 I=2,NA
1099         IJ=IJ+INC
1100         IM1=I-1
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1102             IJ=IJ+INC
1103             AIJ=A(IJ)
1104             IF(AIJ.EQ.ZERO) GO TO 140
1105                 CALL DAXPY(MB,AIJ,B(I,1),NA,AB(J,1),NAB)
1106                 CALL DAXPY(MB,AIJ,B(J,1),NA,AB(I,1),NAB)
1107 140     CONTINUE
1108 150 CONTINUE
1109     RETURN
1110     END
```

# Case Study: Quicksilver

- Proxy application that represents some elements of LLNL's Mercury workload
- Solves a simplified dynamic Monte Carlo particle transport problem
  - Attempts to replicate memory access patterns, communication patterns, and branching or divergence of Mercury for problems using multigroup cross sections
- Parallelization: MPI, OpenMP, and CUDA
- Performance Issues
  - load imbalance (for canned example)
  - latency bound table look-ups
  - a highly branchy/divergent code path
  - poor vectorization potential

# Quicksilver: Detailed analysis within a Kernel using PC Sampling

The screenshot displays the hpcviewer application interface. The top pane shows the source code for `CollisionEvent.cc`, with lines 73-85 highlighted. The bottom pane shows a performance analysis table with columns for various metrics and a tree view on the left.

**Source Code (CollisionEvent.cc):**

```
69 int uniqueNumber = monteCarlo->materialDatabase->mat[globalMatIndex]._iso[isoIndex]._gid;
70 int numReacts = monteCarlo->nuclearData->getNumberReactions(uniqueNumber);
71 for (int reactIndex = 0; reactIndex < numReacts; reactIndex++)
72 {
73     currentCrossSection -= macroscopicCrossSection(monteCarlo, reactIndex, mc_particle.domain, mc_particle.cell,
74             isoIndex, mc_particle.energy_group);
75     if (currentCrossSection < 0)
76     {
77         selectedIso = isoIndex;
78         selectedUniqueNumber = uniqueNumber;
79         selectedReact = reactIndex;
80         break;
81     }
82 }
83 }
84 qs_assert(selectedIso != -1);
85
```

**Performance Analysis Table:**

|                                                                        | GINs: Sum (I)   | GINs: Sum (E) | GINs:STL_ANY: Sum (I) | GINs:STL_ANY: Sum (E) | GINs:STL_IFET: Sum (I) | GINs:STL_IFET: Sum (E) | GINs:STL_IDEP: |
|------------------------------------------------------------------------|-----------------|---------------|-----------------------|-----------------------|------------------------|------------------------|----------------|
| 14 » [1] cudaLaunchKernel<char>                                        | 1.30e+11 100.0% |               | 1.19e+11 100.0%       |                       | 5.27e+09 100.0%        |                        | 9.34e+         |
| 211 » cudaLaunchKernel [qs]                                            | 1.30e+11 100.0% |               | 1.19e+11 100.0%       |                       | 5.27e+09 100.0%        |                        | 9.34e+         |
| » <gpu kernel>                                                         | 1.30e+11 100.0% |               | 1.19e+11 100.0%       |                       | 5.27e+09 100.0%        |                        | 9.34e+         |
| » CycleTrackingKernel(MonteCarlo*, int, ParticleVault*, ParticleVau... | 1.30e+11 100.0% | 4.08e+07 0.0% | 1.19e+11 100.0%       | 3.62e+07 0.0%         | 5.27e+09 100.0%        | 2.11e+07 0.4%          | 9.34e+         |
| 132 » CycleTrackingGuts(MonteCarlo*, int, ParticleVault*, Particle...  | 1.30e+11 100.0% | 9.03e+09 7.0% | 1.19e+11 100.0%       | 9.01e+09 7.6%         | 5.24e+09 99.5%         | 8.98e+06 0.2%          | 9.32e+         |
| 26 » [1] CycleTrackingFunction(MonteCarlo*, MC_Particle&, int, P...    | 8.36e+10 64.4%  | 4.12e+08 0.3% | 7.25e+10 61.1%        | 3.65e+08 0.3%         | 5.21e+09 98.9%         | 1.02e+08 1.9%          | 9.25e+         |
| » loop at CycleTracking.cc: 118                                        | 8.35e+10 64.3%  | 3.76e+08 0.3% | 7.25e+10 61.1%        | 3.34e+08 0.3%         | 5.21e+09 98.8%         | 9.90e+07 1.9%          | 9.24e+         |
| 63 » CollisionEvent(MonteCarlo*, MC_Particle&, unsigned int) [...]     | 5.20e+10 40.1%  | 4.99e+09 3.8% | 4.44e+10 37.4%        | 4.02e+09 3.4%         | 3.85e+09 73.1%         | 4.89e+08 9.3%          | 6.37e+         |
| » loop at CollisionEvent.cc: 67                                        | 4.09e+10 31.5%  | 8.15e+08 0.6% | 3.42e+10 28.8%        | 6.54e+08 0.6%         | 3.54e+09 67.1%         | 1.27e+08 2.4%          | 5.67e+         |
| » loop at CollisionEvent.cc: 71                                        | 3.85e+10 29.6%  | 2.70e+09 2.1% | 3.22e+10 27.1%        | 2.06e+09 1.7%         | 3.27e+09 62.0%         | 2.28e+08 4.3%          | 5.33e+         |
| 73 » macroscopicCrossSection(MonteCarlo*, int, int, int, 1...          | 3.58e+10 27.5%  | 1.22e+10 9.4% | 3.01e+10 25.4%        | 9.85e+09 8.3%         | 3.04e+09 57.7%         | 1.79e+09 33.9%         | 4.60e+         |
| 41 » NuclearData::getReactionCrossSection(unsigned int, u...           | 2.09e+10 16.1%  | 1.09e+10 8.4% | 1.79e+10 15.1%        | 9.42e+09 7.9%         | 1.26e+09 23.8%         | 6.68e+08 12.7%         | 2.19e+         |
| 253 » [I] NuclearDataReaction::getCrossSection(unsigned ...            | 6.89e+09 5.3%   | 3.77e+09 2.9% | 5.86e+09 4.9%         | 3.32e+09 2.8%         | 2.25e+08 4.3%          | 8.24e+07 1.6%          | 8.86e+         |
| NuclearData.cc: 253                                                    | 6.28e+09 4.8%   | 6.28e+09 4.8% | 5.66e+09 4.8%         | 5.66e+09 4.8%         | 4.76e+08 9.0%          | 4.76e+08 9.0%          | 6.11e+         |
| NuclearData.cc: 251                                                    | 1.85e+09 1.4%   | 1.85e+09 1.4% | 1.64e+09 1.4%         | 1.64e+09 1.4%         | 8.12e+07 1.5%          | 8.12e+07 1.5%          | 2.47e+         |
| NuclearData.cc: 248                                                    | 1.61e+09 1.2%   | 1.61e+09 1.2% | 1.18e+09 1.0%         | 1.18e+09 1.0%         | 1.10e+08 2.1%          | 1.10e+08 2.1%          | 3.62e+         |
| 252 » [I] qs_vector<NuclearDataSpecies>::operator[](int)               | 1.29e+09 1.0%   | 1.29e+09 1.0% | 1.14e+09 1.0%         | 1.14e+09 1.0%         | 7.37e+04 0.0%          | 7.37e+04 0.0%          | 1.24e+         |
| NuclearData.cc: 252                                                    | 1.12e+09 0.9%   | 1.12e+09 0.9% | 9.48e+08 0.8%         | 9.48e+08 0.8%         | 3.44e+05 0.0%          | 3.44e+05 0.0%          | 2.50e+         |
| 252 » [I] qs_vector<NuclearDataReaction>::size() const                 | 9.41e+08 0.7%   | 9.41e+08 0.7% | 8.17e+08 0.7%         | 8.17e+08 0.7%         |                        |                        | 4.63e+         |

# Quicksilver: Detailed analysis within a Kernel using PC Sampling

```
Scope
  ▲ 14 » [I] cudaLaunchKernel<char>
    ▲ 211 » cudaLaunchKernel [qs]
      ▲ » <gpu kernel>
        ▲ » CycleTrackingKernel(MonteCarlo*, int, ParticleVault*, ParticleVau...
          ▲ 132 » CycleTrackingGuts(MonteCarlo*, int, ParticleVault*, Particle...
            ▲ 26 » [I] CycleTrackingFunction(MonteCarlo*, MC_Particle&, int, P...
              ▲ loop at CycleTracking.cc: 118
                ▲ 63 » CollisionEvent(MonteCarlo*, MC_Particle&, unsigned int) [...
                  ▲ loop at CollisionEvent.cc: 67
                    ▲ loop at CollisionEvent.cc: 71
                      ▲ 73 » macroscopicCrossSection(MonteCarlo*, int, int, int, i...
                        ▲ 41 » NuclearData::getReactionCrossSection(unsigned int, u...
                          ▶ 253 » [I] NuclearDataReaction::getCrossSection(unsigned ...
                            NuclearData.cc: 253
                            NuclearData.cc: 251
                            NuclearData.cc: 248
                          ▶ 252 » [I] qs_vector<NuclearDataSpecies>::operator[](int)
                            NuclearData.cc: 252
                          ▶ 252 » [I] qs_vector<NuclearDataReaction>::size() const
                          ▶ 252 » [I] qs_vector<NuclearDataReaction>::operator[](int)
```

# HPCToolkit Resources

- Documentation
  - User manual for HPCToolkit: <https://hpctoolkit.gitlab.io/hpctoolkit>
  - Cheat sheet: <https://gitlab.com/hpctoolkit/hpctoolkit/-/wikis/HPCToolkit-cheat-sheet>
  - Tutorial videos
    - <http://hpctoolkit.org/training.html>
    - recorded demo of GPU analysis of Quicksilver: <https://youtu.be/vixa3hGDuGg>
    - recorded tutorial presentation including demo with GPU analysis of GAMESS: <https://vimeo.com/781264043>
- 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
    - <https://hpctoolkit.gitlab.io/hpctoolkit/users/spack.html>

# Some Hpcviewer Tips

# Information for Using Hpcviewer

- Filtering GPU traces
  - Can use the filter menu to select what execution traces you want to see
    - cpu only, gpu, a mix
    - type a string or a regular expression in the chooser select or unselect the new set
    - only traces that exceed a minimum number of samples
- Filtering GPU calling context tree nodes to hide clutter
  - hide individual CCT nodes: e.g. lines that have no source code mapping library@0x0f450
  - hide subtrees: MPI implementation, implementation of CUDA primitives
- When inspecting GPU activity, be aware that hpcviewer has two modes
  - expose GPU traces or not
    - means: when displaying GPU trace lines, don't just show GPU activity if the time in the middle of a pixel is in a GPU operation. instead, show the first (if any) GPU operation between the time in the middle of the pixel and the middle of the next pixel
    - why? GPU activity is so short, it may be hard to find if we don't "expose" where it is
    - downside: makes the GPU appear more active than it is
      - can correct the statistics by turning the mode off
  - mode can be selected from <File>:<Preferences>:<Traces>

# Hands-on Examples

# Two Kinds of Hands-on Examples

- **Pre-collected databases to explore**
  - gain experience using hpctoolkit's hpcviewer graphical user interface to analyze performance data
- **Hands-on examples**
  - build, run, and view several codes to get the full experience
    - hpcrun: measure an application as it executes
    - hpcstruct: recover program structure information for mapping measurements to source code
    - hpcprof: combine measurements with program structure information
    - hpcviewer: explore profiles and traces

# Performance Databases to Explore

- **On an aurora login node**

```
% qsub -I -l select=2,walltime=1:00:00,place=scatter -l  
filesystems=flare -A gpu_hack -q gpu_hack_prio -X
```

- **On an aurora compute node**

```
% module use /soft/perftools/hpctoolkit/modulefiles  
% module load hpctoolkit  
% cd /flare/ATPESC2026/EXAMPLES/hpctoolkit/DONT-COPY/data  
% ls  
  
    arborx    gamess    minitest    pelelmex    quicksilver
```

NOTE: all of the databases in these directories end with the suffix “.d”. For the gamess examples, the hpctoolkit databases are one directory deeper, i.e. in subdirectories that begin with a number.

# More about the Available Performance Databases

See [/flare/gpu\\_hack/hpctoolkit/data](/flare/gpu_hack/hpctoolkit/data) for each of the following

- quicksilver: Monte Carlo particle transport proxy application (**C++ + CUDA**)
  - hpctoolkit-qs-gpu-cuda.d - profile and trace on 4 CPUs + 4 GPUs
  - hpctoolkit-qs-gpu-cuda-pc.d - instruction-level measurements within kernels using PC sampling
  - **EXERCISES**
- pelelmex: Adaptive mesh hydrodynamics simulation code for low Mach number reacting flows (**C++ + AMReX**)
  - pelelmex.db -a large trace with load imbalance from 2025 NERSC hackathon run on 16 CPUs + 16 GPU
- gamess: General Atomic and Molecular Electronic Structure System (**Fortran + OpenMP**)
  - 1.singlegroup-unbalanced/hpctoolkit-gamess-1n-chol-noDS.d
  - 2.singlegroup-balanced/hpctoolkit-gamess-1n-chol-fix\_load\_balance\_noDS.d/
  - 3.multigroup-unbalanced-mtarbr/hpctoolkit-gamess-5n.d/
  - 4.multigroup-balanced/hpctoolkit-gamess-5n-manualbalance.d/
  - 5.multigroup-unbalanced-pc/hpctoolkit-gamess-5n-pc.d/
  - 6.scale/hpctoolkit-gamess-22n-test.d/
- arborx (**C++ + Kokkos**)
- minitest (**SYCL and OpenMP TARGET**)

# Hands-on Tutorial Examples on Aurora

```
% cd /flare/ATPESC2026/usr/${USER}
% cp -r /flare/ATPESC2026/EXAMPLES/hpctoolkit/hpctoolkit-hands-on .
% cd hpctoolkit-hands-on
% ls
    pcstruct  minitest  opensn  README
    sourceme-get-compute-node.sh  sourceme-on-compute-node.sh
```

For your chosen example

1. cd to the example directory
  2. source setup-env/aurora.sh # custom for each example
  3. make build # build the code
  4. make run # measure and analyze code performance  
this will produce a directory <something>.db
  5. View the performance data with hpcviewer
    - a. remotely from your laptop using an hpcviewer that you downloaded
    - b. make view
- REQUIREMENTS:
1. you connected to aurora using an X11 desktop
  2. you run "make view" on a login node



# Downloading, Installing, and Using Hpcviewer Graphical User Interface on Your Laptop

# Hpcviewer Graphical User Interface on Your Laptop

Prepare to explore performance data on your laptop

- Download and install hpcviewer
- See <https://hpctoolkit.org/download.html>

Select the right one for your laptop: MacOS (Apple Silicon, Intel), Windows, Linux

- User manual for hpcviewer: <https://hpctoolkit.gitlab.io/hpctoolkit>

# Viewing Performance Data

- Copy a performance database directory to your laptop and open it locally
- Open a performance database on a remote system

Note: using a HPCViewer with a remote system presumes that hpcserver has already been installed on the remote system

- hpcserver has been installed on Aurora
- you can download and install hpcserver on your local cluster as well (ask in Slack for directions)

# Configuring Hpcviewer Remote Access

Run hpcviewer

From the file menu, select “Open remote database”

Fill in the hostname/IP address: [aurora.alcf.anl.gov](https://aurora.alcf.anl.gov)

Fill in your username on Aurora

Fill in the remote installation directory for hpcviewer’s server:

`/soft/perftools/hpctoolkit/hpcserver/1.4.0`

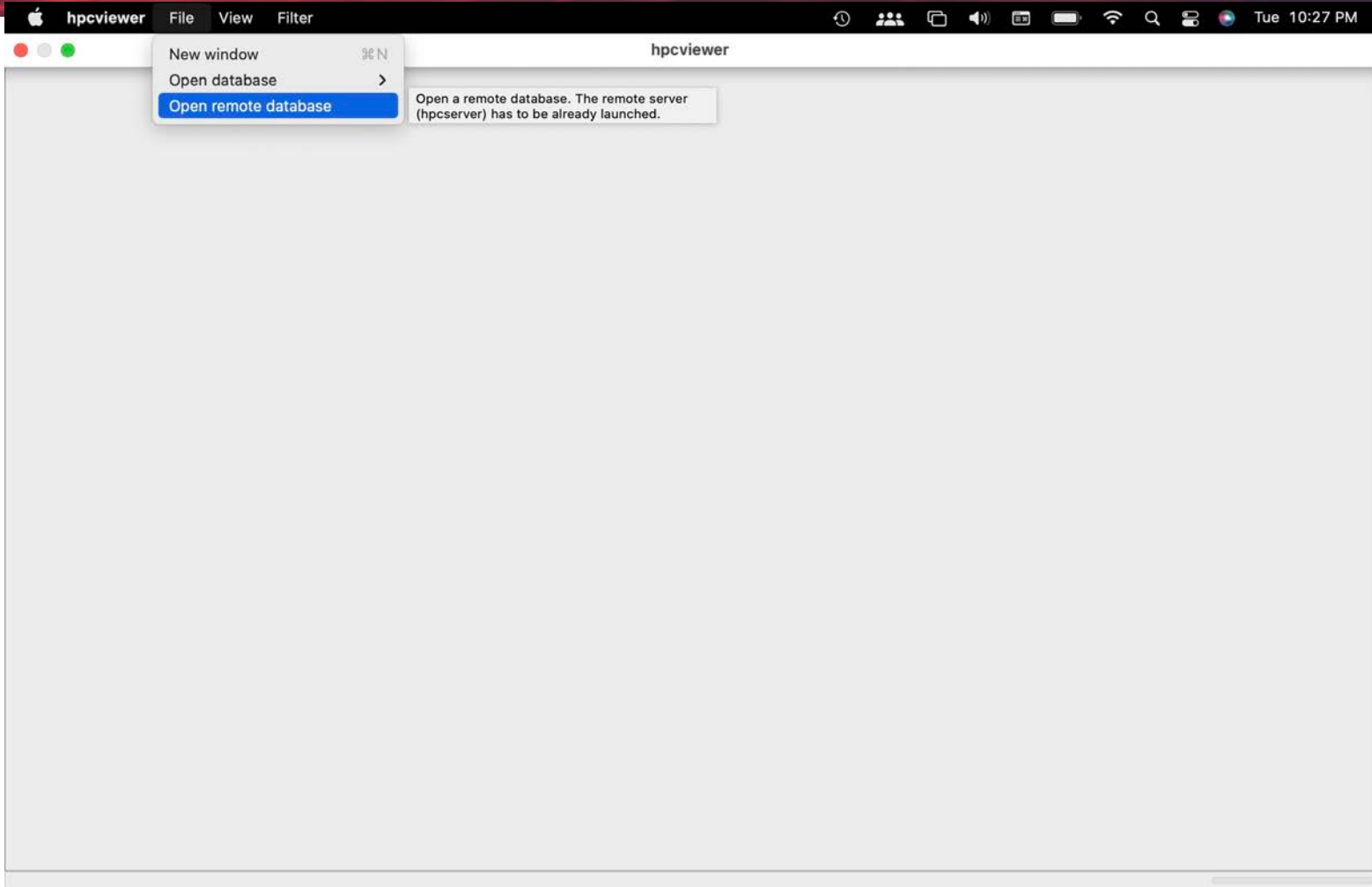
Select the authentication method: “Use password”

Click “OK”

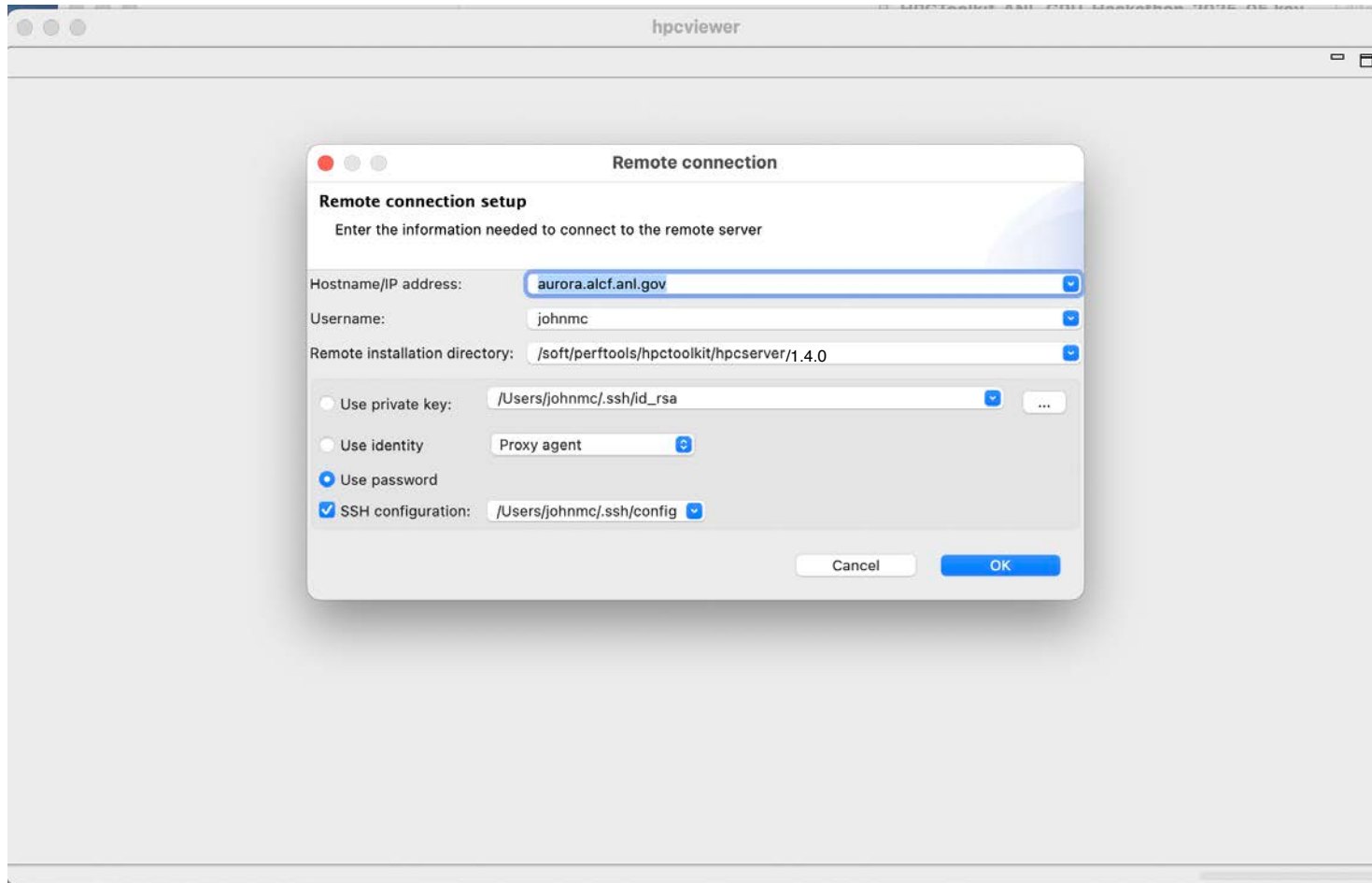
Authenticate using your token as you normally do

Navigate to a database with the file chooser in `/flare/ATPESC2026/EXAMPLES/hpctoolkit/DONT-COPY/data`

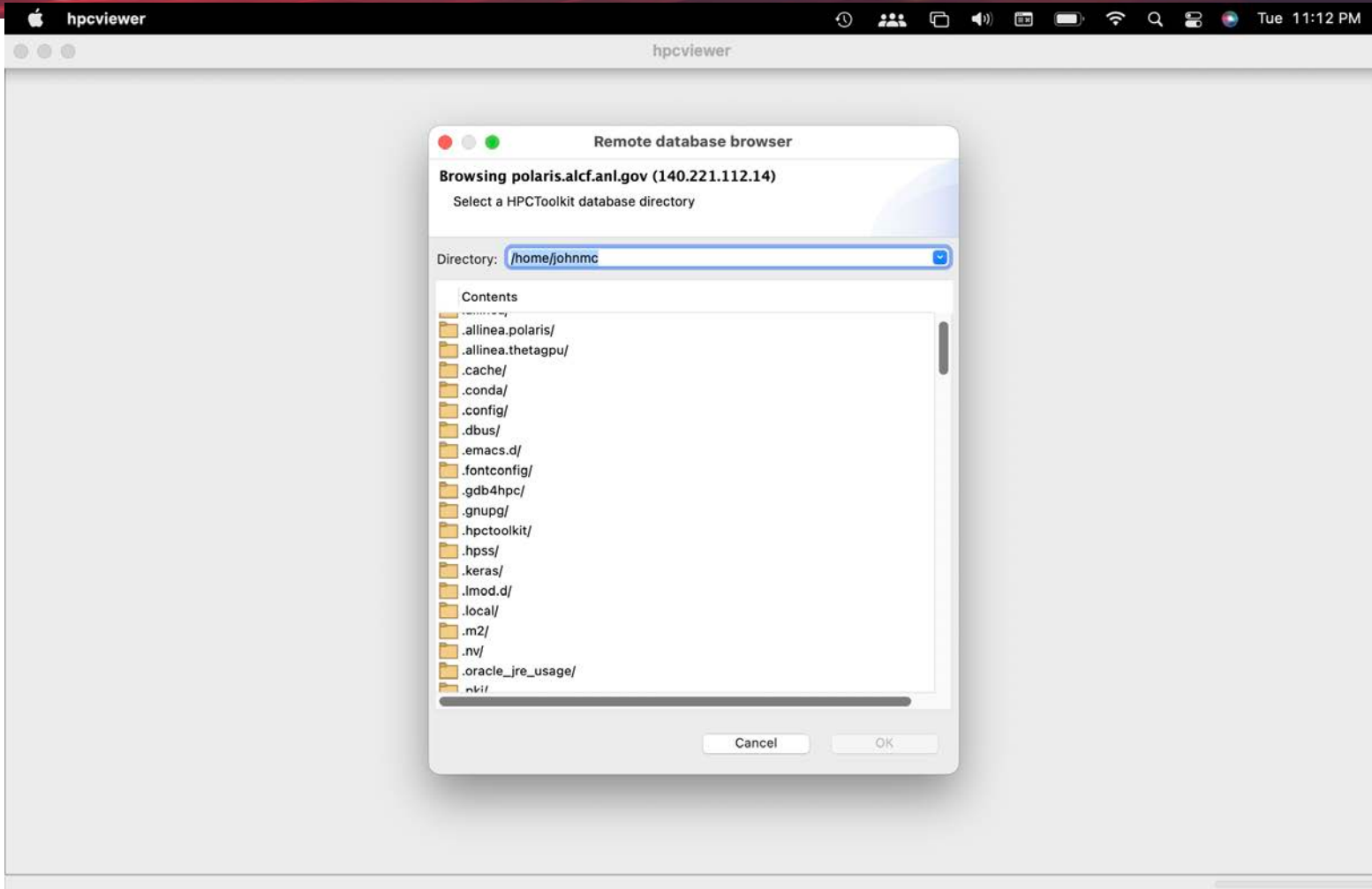
# Opening a Remote Database



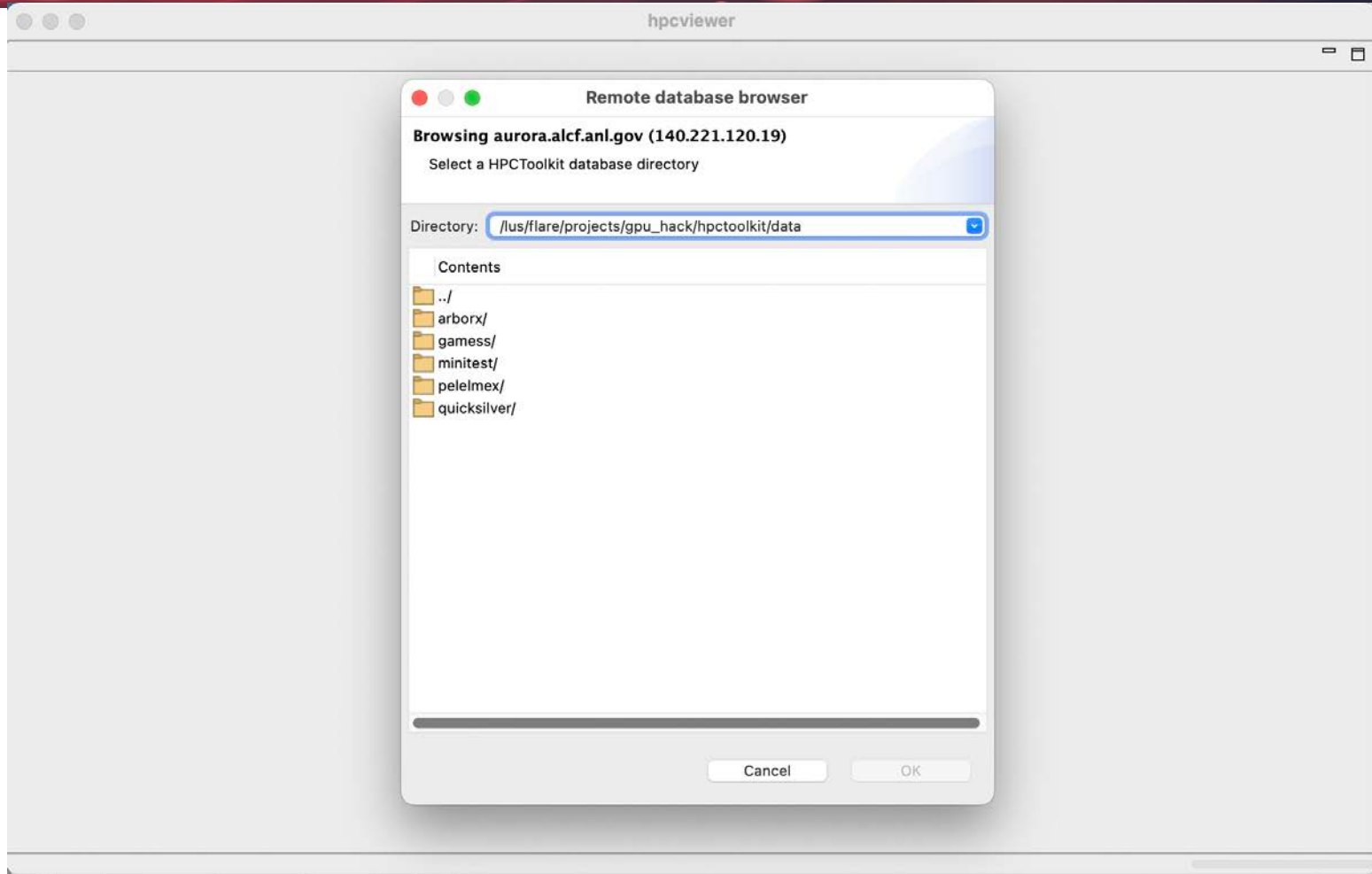
# Configuring for remote access to Aurora using hpcserver



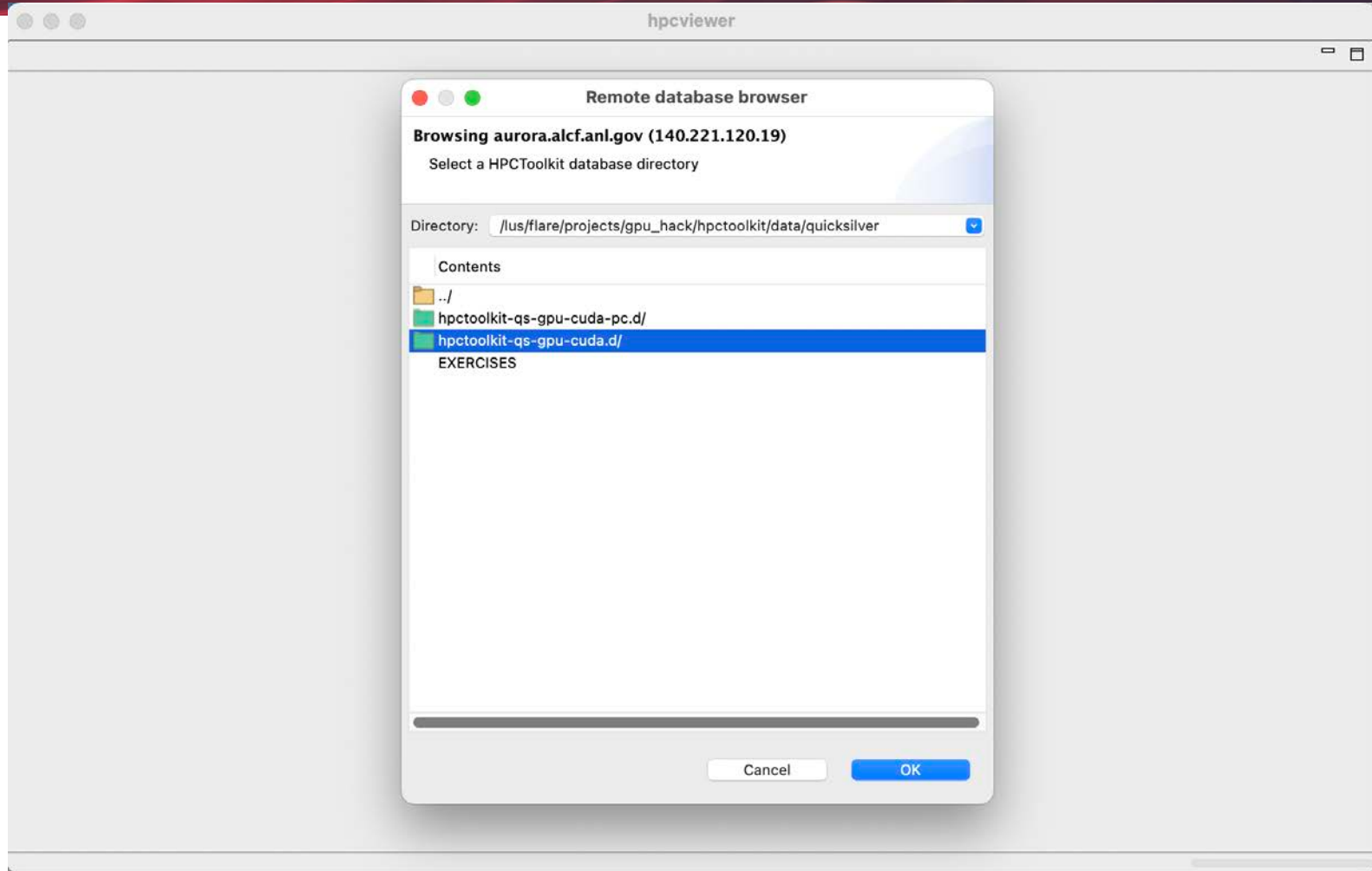
# First View of Aurora: Your Home Directory



# Navigate to Example Databases



# Select a Quicksilver Database with Traces



## The screenshot shows the 'hpcviewer' application window. At the top, there are three colored window control buttons (red, yellow, green) and the title 'hpcviewer'. Below the title bar, there's a tabbed interface with two tabs: 'Profile: qs' (active) and 'Trace: qs'. The main area of the window is mostly blank, suggesting a large visualization or plot that isn't clearly visible. At the bottom, there's a toolbar with various icons for navigation and analysis, including arrows, a flame icon, a function icon, a CSV icon, a zoom icon, a pan icon, a reset icon, and a search icon. Below the toolbar is a table displaying performance metrics. The table has five columns: 'Scope', 'REALTIME (sec): Sum (I)', 'REALTIME (sec): Sum (E)', 'GPUOP (sec): Sum (I)', 'GPUOP (sec): Sum (E)', and 'GKER (sec): Sum'. The first row is highlighted in yellow and contains the text 'Experiment Aggregate Metrics'. The second row is highlighted in blue and contains the text '&lt;program root&gt;'. Both rows show numerical values in scientific notation (e.g., 1.58e+01, 2.23e+00) followed by '100.0%'. There are several empty rows below these, indicating more data points or a scrollable list.

# Troubleshooting Tips

# Why can't I see my Source Code?

- To relate performance measurements to your application source code, the code must be compiled with a “-g” option in addition to your optimization flags. Otherwise, there is no information for any tool to map performance to anything finer grain than at the procedure level
  - For instance, if you are building with make, you will want to build **RelWithDebInfo** rather than **Release** for the best experience



# ARGONNE ATPESC2026 EXTREME - SCALE COMPUTING

## ARGONNE TRAINING PROGRAM ON EXTREME-SCALE COMPUTING

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