



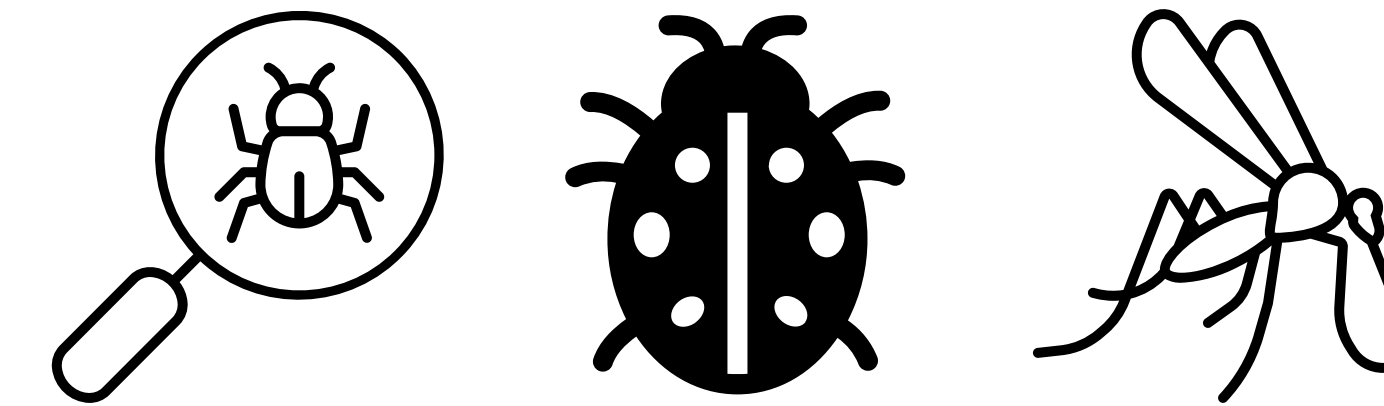
Performance and Debugging Tools

David Appelhans, NVIDIA Devtech Compute | SC25 / November 16th 2025

Goals for this session

Why you should use tools, and what they do

- All code has bugs. The more code, the more bugs.
- Different classes of „bugs“
 - Crashes, undefined behavior, deadlocks, correctness issues, ...
 - Time to solution, parallel efficiency, energy efficiency
- Treat performance issues as bugs, especially at scale



- Manual debugging: Mimic program execution, print state, time code regions
- Tool-assisted debugging: Automate „tedious“ part
 - More information, less effort
 - Otherwise unavailable information (hardware counters!)
- Fixing bugs not (yet 😊) automated: Tools simplify and enable analysis
- Introduce workflow and representative tools, focus on distributed GPU applications

Debugging Correctness: Best Practices

Before you start

- Crashes are "nice" – the stacktrace often points to the bug
- Prerequisite: Compile flags
 - While developing, always use `-g -lineinfo`
 - Use `-g -G` for manual debugging
 - Specific flags for compilers/languages (e.g. gfortran): `-fcheck=bounds`
- Memory corruption: Out-of-bounds accesses may or may not crash
 - *compute-sanitizer*: Automate finding these errors
- Other issues: Manual debugging
 - *cuda-gdb*: Command-line debugger, GPU extensions
 - `CUDA_LAUNCH_BLOCKING=1` forces synchronous kernel launches

NVCC compile flags for debugging

<code>-g</code>	Embed symbol info for host code
<code>-lineinfo</code>	Generate line correlation info for device code
<code>-G</code>	Device debug – slow

Focus on Performance

...without neglecting correctness

compute-sanitizer

Functional correctness checking suite for GPU
<https://docs.nvidia.com/compute-sanitizer/ComputeSanitizer/>

- compute-sanitizer is a collection of tools
- memcheck (default) tool comparable to [Valgrind's memcheck](#).
- Other tools include
 - racecheck: shared memory data access hazard detector
 - initcheck: uninitialized device/global memory access detector
 - synccheck: identify whether a CUDA application is correctly using synchronization primitives
- Example run:

```
srun -n 4 compute-sanitizer \  
--log-file jacobi.%q{SLURM_PROCID}.log \  
--save jacobi.%q{SLURM_PROCID}.compute-sanitizer \  
./jacobi -niter 10
```
- Stores (potentially very long) text output in *.log file, raw data separately, once per process
- One file per MPI rank - more on %q{} later

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Debugging MPI+CUDA applications

More environment variables for offline debugging

- With `CUDA_ENABLE_COREDUMP_ON_EXCEPTION=1` core dumps are generated in case of an exception
 - `CUDA_ENABLE_LIGHTWEIGHT_COREDUMP=1` does not dump application memory - faster
 - Can be used for post-mortem debugging
 - Helpful if live debugging is not possible
- Enable/Disable CPU part of core dump (enabled by default)
 - `CUDA_ENABLE_GPU_COREDUMP_ON_EXCEPTION`
- Specify name of core dump file with `CUDA_COREDUMP_FILE`
- Open GPU
 - (cuda-gdb) target **cuda**core core.cuda
- Open CPU+GPU
 - (cuda-gdb) target **core** core.cpu core.cuda

<https://doi.org/10.1016/j.sbsbs.2019.04.001>

Using cuda-qdb with MPI

- Launcher (mpirun/srun/...) complicates starting process inside debugger
- Workaround: Attach later

```
#include <unistd.h>
if (rank == 0) {
    char name[255]; gethostname(name, sizeof(name)); bool attached;
    printf("rank %d: pid %d on %s ready to attach\n", rank, getpid(), name);
    while (!attached) { sleep(5); }
}
```

- Launch process, sleep on particular rank


```
$ srun -n 4 ./jacobus -nter 18
rank 0: pid 28928 on jwb8801.juwels ready to attach
```
 - Then attach from another terminal (may need more flags)


```
[jwb@jin $] JOBDID=$(sequnce -ho %i -me) # obtain job ID of user's first job
[jwb@jin $] srun -n 1 -j$JOBDID $JOBDID -pty bash -l # launch interactive shell on job's node
[jwb@jin $] cuda-test -attach -j$JOBDID
```
 - Wake up sleeping process and continue debugging normally


```
(cuda-cg) set var attach=true
```
- JSC system shortcut:
sgoto -h -help

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Approaches for Multi-Process Tools

- Tools usually run on a single process - adapt for highly distributed applications?
 - Bugs in parallel programs are often serial bugs in disguise
 - Common MPI paradigm: Workload distributed, bug classes/performance similar for all processes
 - Not: Load imbalance, parallel race conditions, require parallel tools
 - Ergo: Run tool N times in parallel, have N output files, only look at 1 (or 2, ...)
 - “`iq(ENV_VAR)`” supported by all the NVIDIA tools discussed here, embed environment variable in file name
 - `ENV_VAR` should be set by the process launcher, unique ID
 - Evaluated only once tool starts running (on compute node) – not when launching job
 - Other tools: Use a launcher script, for late evaluation
- OpenMPI:**

```
OMPI_COMM_WORLD_RANK
OMPI_COMM_WORLD_LOCAL
```

```
OpenMPI:
OMPI_COMM_WORLD_RANK
OMPI_COMM_WORLD_LOCAL_RANK

MVAPICH2:
MV2_COMM_WORLD_RANK
MV2_COMM_WORLD_LOCAL_RANK

Slurm:
SLURM_PROCID
SLURM_LOCALID
```

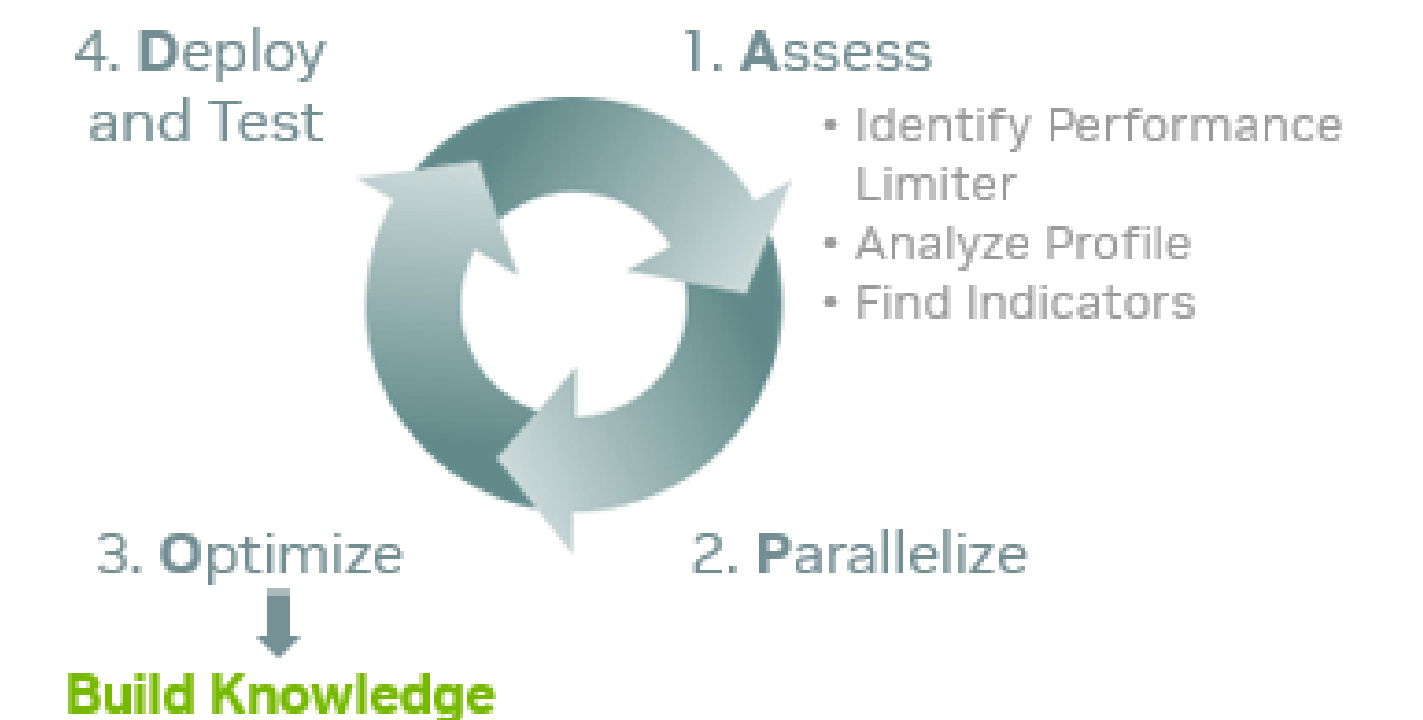
<https://www.majordna.org/category/news/ai/major-ai-environmental-variables>
<https://www.cba.edu.au/ai-environmental-variables>
<https://www.sciencedirect.com/science/article/pii/S0950080420300013>
 Might: Synthesize support: <https://doi.org/10.1016/j.sbspro.2014.03.001>

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Debugging Performance

Why you *must* use profilers

- Paraphrasing **Donald Knuth**:
 - Don't overoptimize - optimize your own time by using tools to focus on relevant parts
- Do not trust your gut instinct – very often *very* misleading
 - Easy to waste a lot of time chasing the "perceived" issue
- Getting the same information, you end up reimplementing your own profiler
- Iterative workflow
- Different kinds of measurement tools, different tradeoffs
 - Instrumenting/Sampling
 - Profiling/Tracing
 - multi-process, single-process, kernel-level
- Here: Focus on GPU and system-level: Nsight Systems



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compute-sanitizer

Functional correctness checking suite for GPU

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srun -n 4 compute-sanitizer \  
--log-file jacobi.%q{SLURM_PROCID}.log \  
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./jacobi -niter 10
```
- Stores (potentially very long) text output in *.log file, raw data separately, once per process.
- One file per MPI rank - more on %q{} later

compute-sanitizer

Anatomy of an error

- Look into log file, or use `compute-sanitizer --read <save file>`
- Actual output can be very long, if many GPU threads produce (similar) errors.

```
===== COMPUTE-SANITIZER
[....]
===== Invalid __global__ write of size 4 bytes
=====      at 0x6d0 in mpi/jacobi_kernels.cu:60:initialize_boundaries(float*, float*, float,
                                                                    int, int, int, int)
=====      by thread (1,0,0) in block (32,0,0)
=====      Address 0x14fb88020000 is out of bounds
=====      Saved host backtrace up to driver entry point at kernel launch time
=====      Host Frame: [0x20d6ea]
=====      in libcuda.so.1
=====      Host Frame: [0x115ab]
[....]
=====
===== ERROR SUMMARY: 10 errors
```

- We introduced an off-by-one error in line 60 ourselves:

```
a_new[iy * nx + (nx - 1) + 1] = y0;
```


Approaches for Multi-Process Tools

- Tools usually run on a single process – adapt for highly distributed applications?
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- Ergo: Run tool N times in parallel, have N output files, only look at 1 (or 2, ...)
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OpenMPI:

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OMPI_COMM_WORLD_LOCAL_RANK

MVAPICH2:

MV2_COMM_WORLD_RANK
MV2_COMM_WORLD_LOCAL_RANK

Slurm:

SLURM_PROCID
SLURM_LOCALID

<https://www.open-mpi.org/faq/?category=running#mpi-environmental-variables>

<http://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-userguide.html#x1-34600013>

https://slurm.schedmd.com/srun.html#SECTION_OUTPUT-ENVIRONMENT-VARIABLES

Nsight Systems support: <https://docs.nvidia.com/nsight-systems/UserGuide/index.html#multi-report-mpi-example>

Using cuda-gdb with MPI

- Launcher (mpirun/srun/...) complicates starting process inside debugger
- Workaround: Attach later

```
#include <unistd.h>
if (rank == 0) {
    char name[255]; gethostname(name, sizeof(name)); bool attached;
    printf("rank %d: pid %d on %s ready to attach\n", rank, getpid(), name);
    while (!attached) { sleep(5); }
}
```

- Launch process, sleep on particular rank

```
$ srun -n 4 ./jacobi -niter 10
rank 0: pid 28920 on jwb0001.juwels ready to attach
```

- Then attach from another terminal (may need more flags)

```
[jwlogin]$ JOBID=$(squeue -ho %i --me) # obtain job ID of user's first job
[jwlogin]$ srun -n 1 --jobid ${JOBID} --pty bash -i # launch interactive shell on job's node
[jwb0001]$ cuda-gdb --attach 28920
```

- Wake up sleeping process and continue debugging normally
(cuda-gdb) set var attached=true

JSC system shortcut:
sgoto --help

Using cuda-gdb with MPI

Environment variables for easier debugging

- Automatically wait for attach on exception without code changes:

```
$ CUDA_DEVICE_WAITS_ON_EXCEPTION=1 srun ./jacobi -niter 10
Single GPU jacobi relaxation: 10 iterations on 16384 x 16384 mesh with norm check every 1
iterations
jwb0129.juwels: The application encountered a device error and CUDA_DEVICE_WAITS_ON_EXCEPTION is
set. You can now attach a debugger to the application (PID 31562) for inspection.
```

- Same as before, go to node (see previous slide), then attach cuda-gdb:

```
$ cuda-gdb --pid 31562
CUDA Exception: Warp Illegal Address
The exception was triggered at PC 0x508ca70 (jacobi_kernels.cu:88)
```

```
Thread 1 "jacobi" received signal CUDA_EXCEPTION_14, Warp Illegal Address.
[Switching focus to CUDA kernel 0, grid 4, block (0,0,0), thread (0,20,0), device 0, sm 0, warp 21,
lane 0]
0x00000000508ca80 in jacobi_kernel<32, 32><<<(512,512,1),(32,32,1)>>> (/*...*/) at jacobi_kernels.c
u:88
88          real foo = *((real*)nullptr);
```

Debugging MPI+CUDA applications

More environment variables for offline debugging

- With `CUDA_ENABLE_COREDUMP_ON_EXCEPTION=1` core dumps are generated in case of an exception
 - `CUDA_ENABLE_LIGHTWEIGHT_COREDUMP=1` does not dump application memory - faster
 - Can be used for post-mortem debugging
 - Helpful if live debugging is not possible
- Enable/Disable CPU part of core dump (enabled by default)
 - `CUDA_ENABLE_CPU_COREDUMP_ON_EXCEPTION`
- Specify name of core dump file with `CUDA_COREDUMP_FILE`
- Open GPU
 - (cuda-gdb) target `cuda` core.cuda
- Open CPU+GPU
 - (cuda-gdb) target `core` core.cpu core.cuda

<https://docs.nvidia.com/cuda/cuda-gdb/index.html#gpu-core-dump-support>

Example: Opening a Core Dump

- Running and generating the core file

```
$ CUDA_ENABLE_COREDUMP_ON_EXCEPTION=1 CUDA_ENABLE_LIGHTWEIGHT_COREDUMP=1 srun ./jacobi -niter 10
Single GPU jacobi relaxation: 10 iterations on 16384 x 16384 mesh with norm check every 1 iterations
srun: error: jwb0021: tasks 0-3: Aborted (core dumped)

$ ls core*
core.jwb0021.juwels.23959  core_1633801834_jwb0021.juwels_23959.nvcudmp ...
```

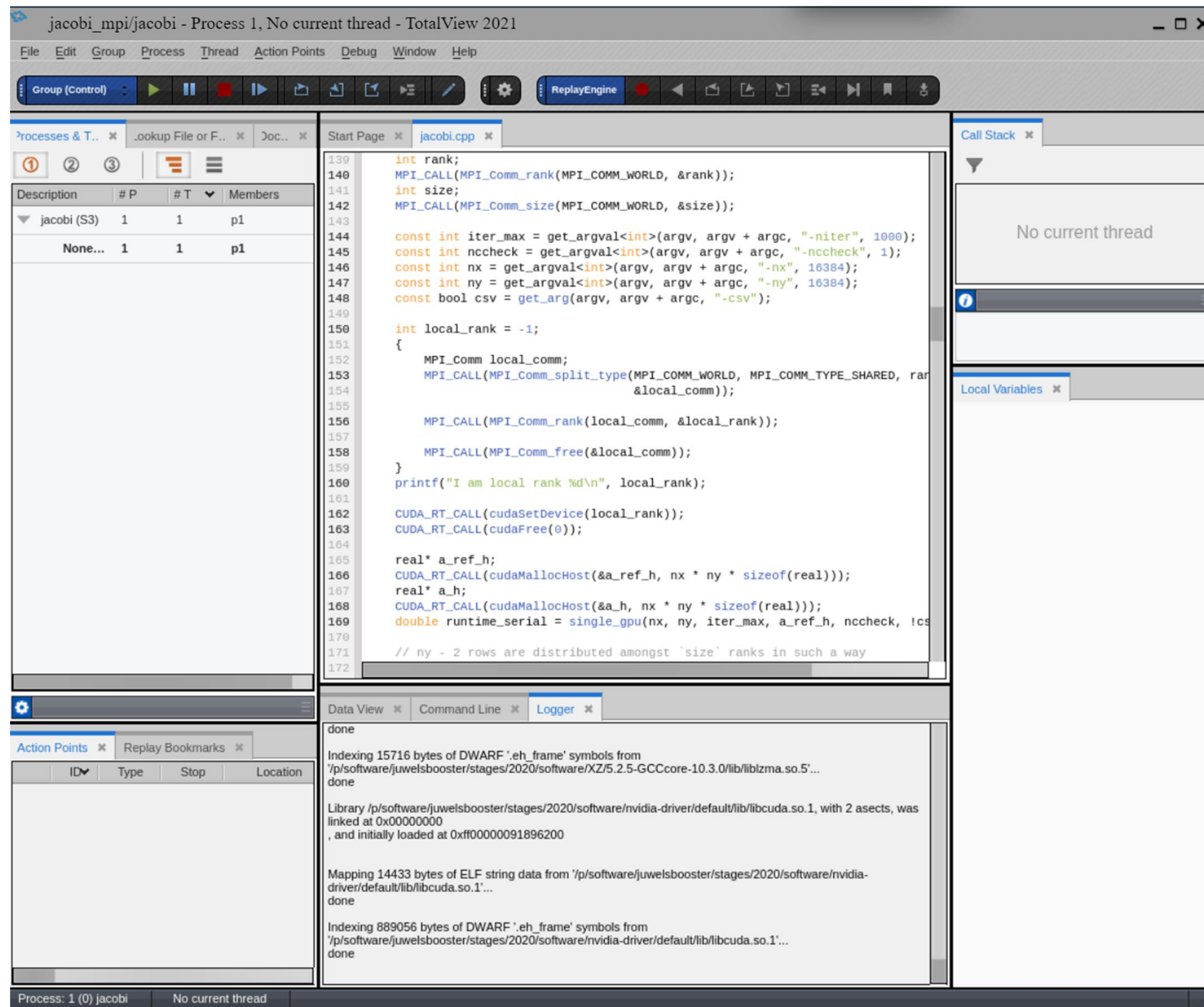
- And opening the core dump in `cuda-gdb`

```
(cuda-gdb) target cudacore core_1633801834_jwb0021.juwels_23959.nvcudmp
Opening GPU coredump: core_1633801834_jwb0021.juwels_23959.nvcudmp
[New Thread 23979]

warning: No exception was found on the device

[Current focus set to CUDA kernel 0, grid 4, block (0,0,0), thread (0,2,0), device 0, sm 0, warp 0, lane 0]
#0  0x0000000057e1ae0 in void jacobi_kernel<32, 32>(float*, float const*, float*, int, int, int, bool)
    <<<(512,512,1),(32,32,1)>>> ()
    at /p/project/cexalab/hrywniak1/code/multi-gpu-programming-models/mpi/jacobi_kernels.cu:87
87          real foo = *((real*)nullptr);
(cuda-gdb)
```

Specialized parallel debuggers



- `cuda-gdb` can debug multiple processes (`add-inferior`), although...
- For truly parallel bugs (e.g. multi-node, multi-process race conditions), third-party tools offer more convenience
 - Or enable „live“ analysis in the first place
- Linaro DDT (formerly ARM)
- Perforce TotalView (screenshot)
 - Available as module on JSC systems

Write Debuggable Software

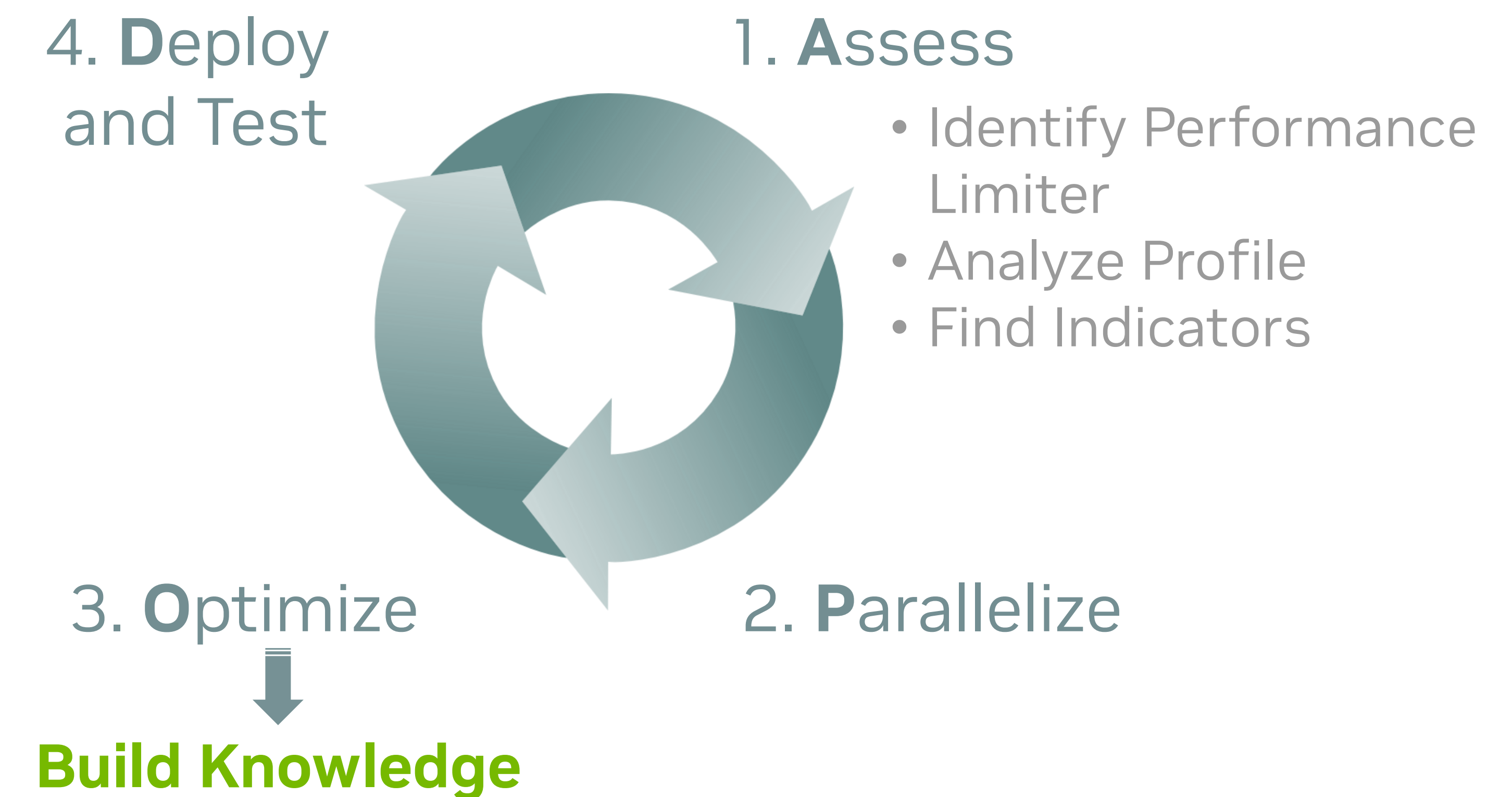
A case for modularity, and proper test cases

- Think about interfaces in your code: Which parts must depend on each other, etc.
 - Example: BLAS, linear algebra routines
- Think about structure and architecture („the big picture“)
- Don't go overboard: „I read this book, we need 100% test coverage“, etc.
 - For many research codes that would be overkill
- **“Everything should be made as simple as possible, but no simpler.”**
- Badly structured legacy code slows you down as well, as it resists change
 - Today's code is tomorrow's legacy
 - Strike a balance, avoid full rewrites. Code encapsulates hard-earned bug fixes and knowledge
- Representative test cases
 - Contain the correct science, walk the code paths
 - But run quickly, best on a single process, should run on a single node
 - Some (but not all) tests at full scale

Debugging Performance

Why you must use profilers

- Paraphrasing Donald Knuth:
 - Don't overoptimize - optimize your own time by using tools to focus on relevant parts
- Do not trust your gut instinct – very often very misleading
 - Easy to waste a lot of time chasing the "perceived" issue
- Getting the same information, you end up reimplementing your own profiler
- Iterative workflow
- Different kinds of measurement tools, different tradeoffs
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 - multi-process, single-process, kernel-level
- Here: Focus on GPU and system-level: Nsight Systems



The Nsight Suite Components

How the pieces fit together



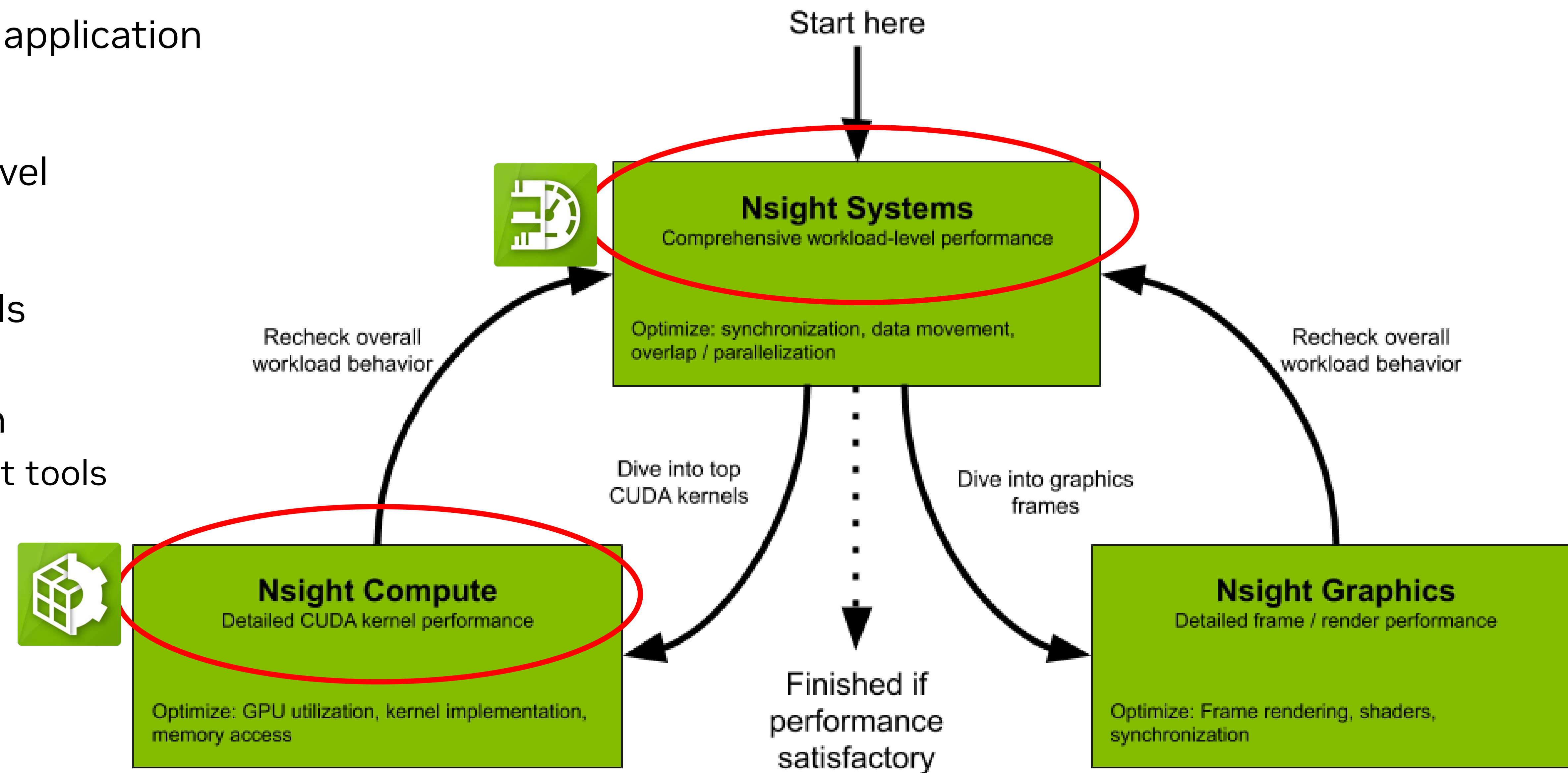
- Nsight **Systems**: Coarse-grained, whole-application



- Nsight **Compute**: Fine-grained, kernel-level

- NVTX: Support and structure across tools

- Main purpose: Performance optimization
 - But at their core, advanced measurement tools



A First (I)Nsight

Recording with the CLI

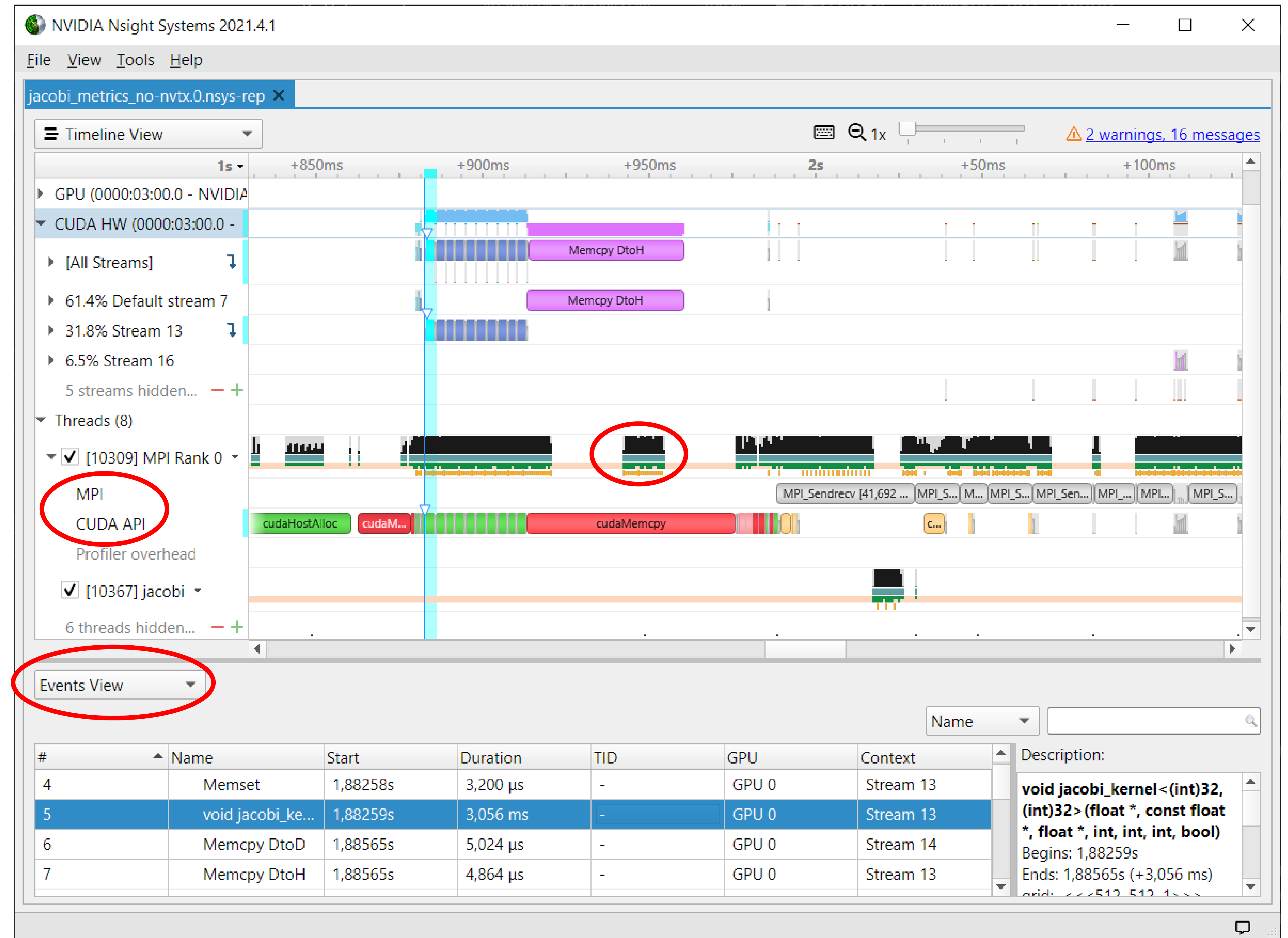
- Use the command line
 - `srun nsys profile --trace=cuda,nvtx,mpi --output=my_report.%q{SLURM_PROCID} ./jacobi -niter 10`
- Inspect results: Open the report file in the GUI
 - Also possible to get details on command line
 - Either add `--stats` to profile command line, or: `nsys stats --help`
- Runs set of reports on command line, customizable (**sqlite** + **Python**):
 - Useful to check validity of profile, identify important kernels

Running [.../reports/**gpukernsum.py** jacobi_metrics_more-nvtx.0.**sqlite**]

Time(%)	Total Time (ns)	Instances	Avg (ns)	Med (ns)	Min (ns)	Max (ns)	StdDev (ns)	Name
99.9	36750359	20	1837518.0	1838466.5	622945	3055044	1245121.7	void jacobi_kernel
0.1	22816	2	11408.0	11408.0	7520	15296	5498.5	initialize_boundaries

System-Level Profiling with Nsight Systems

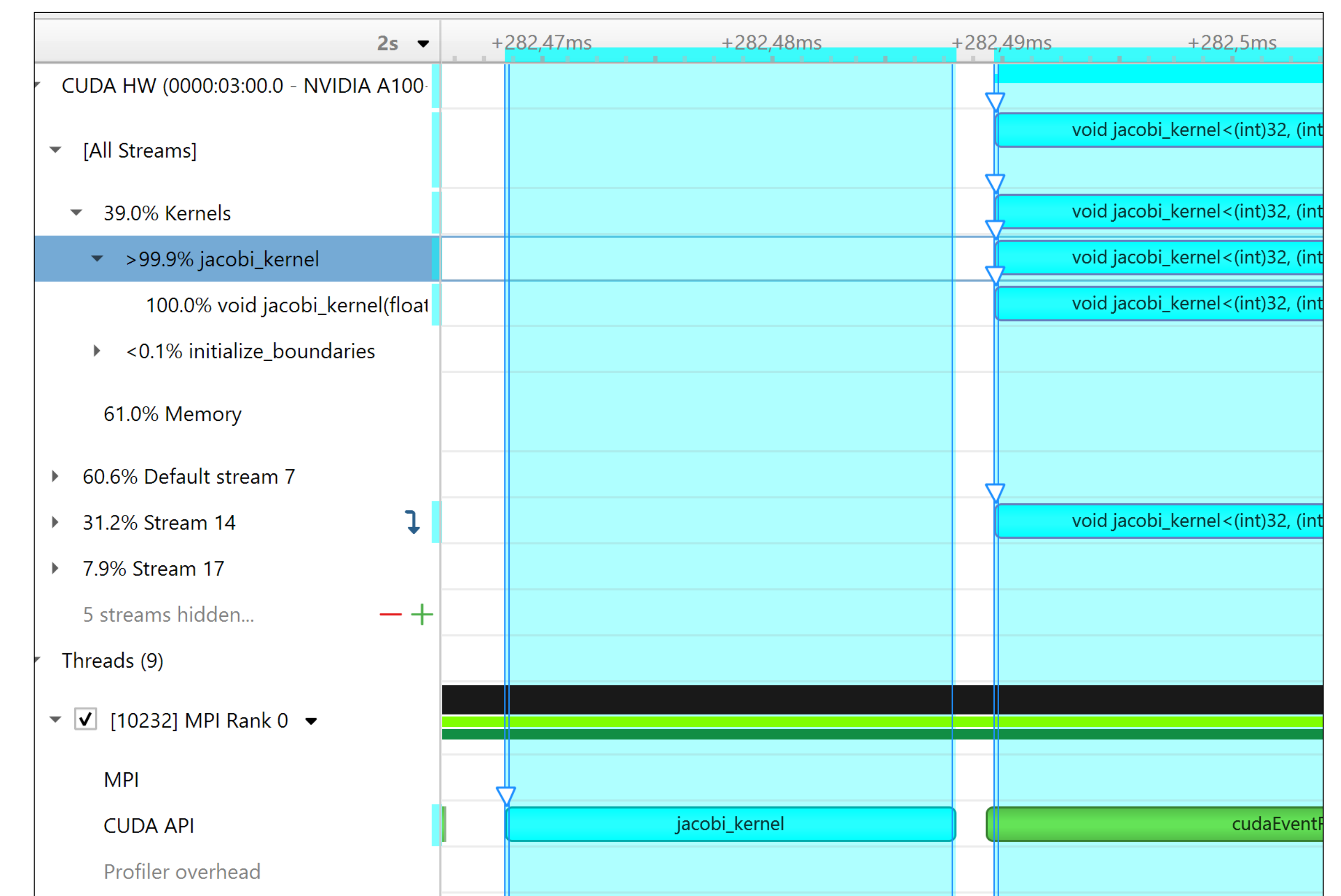
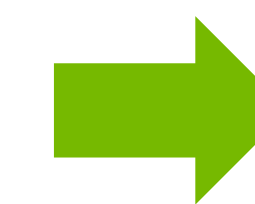
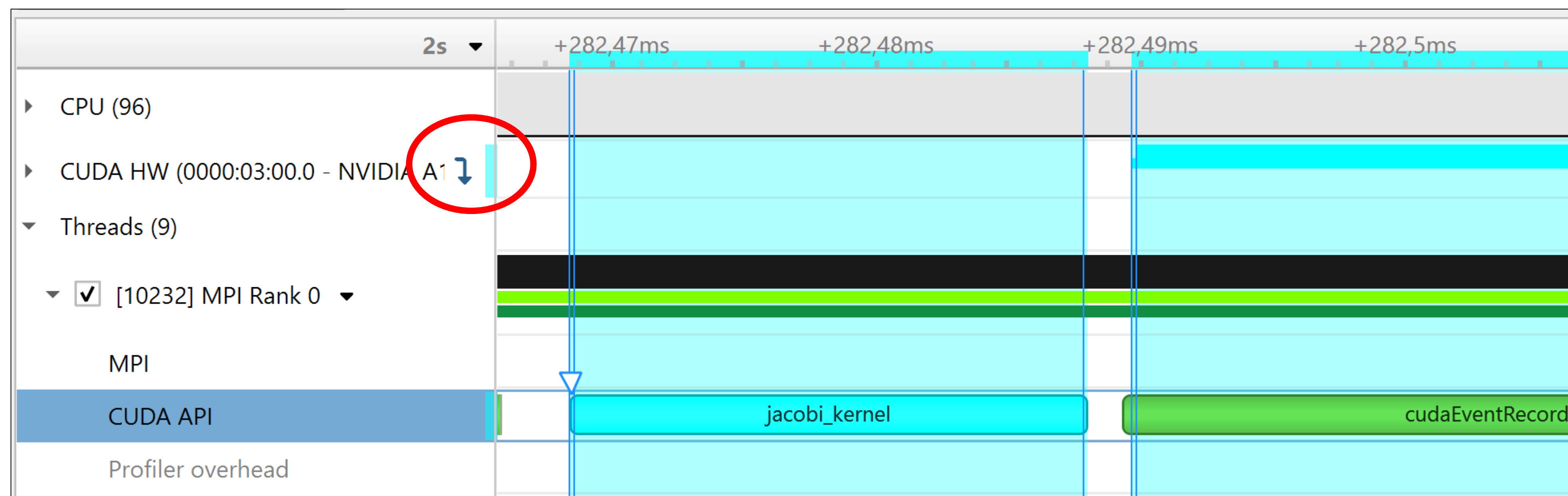
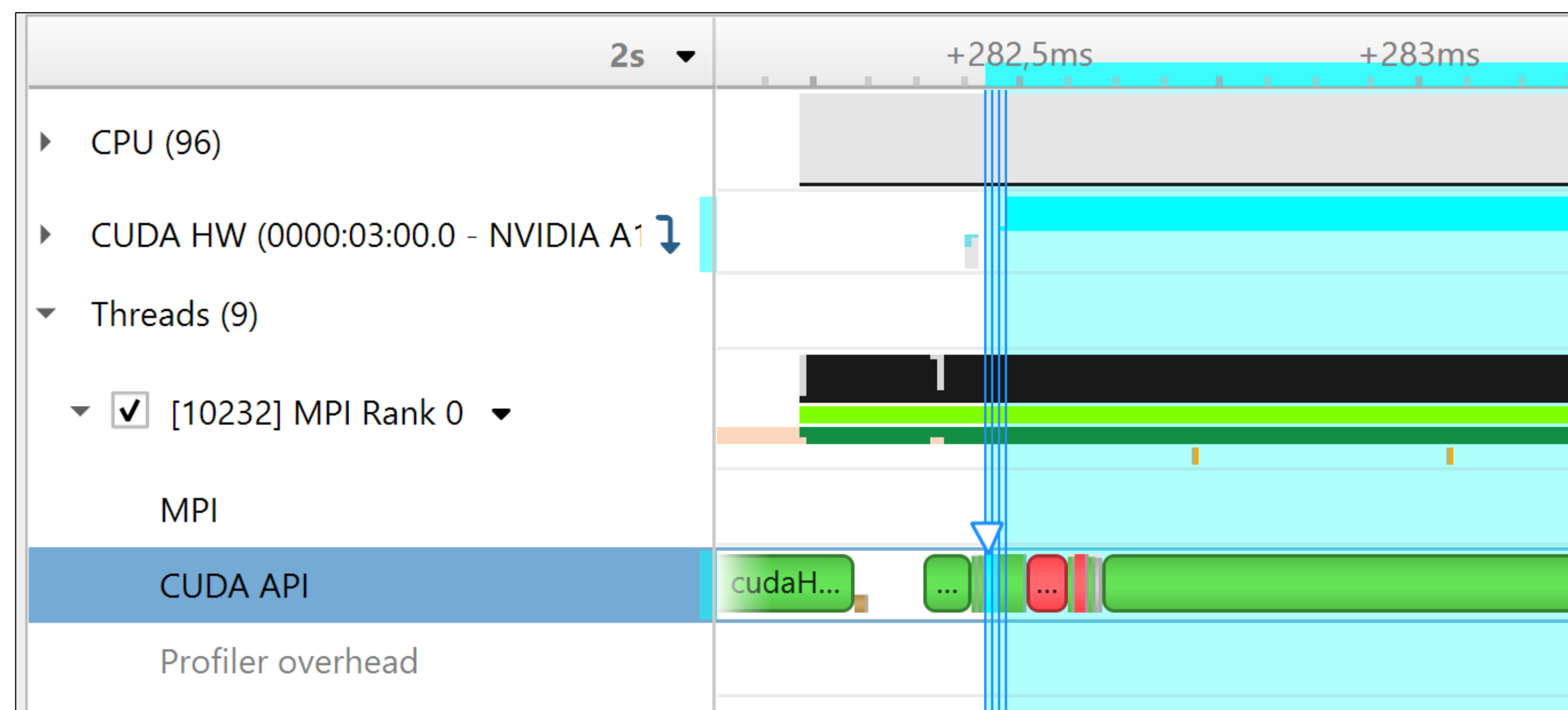
- Global timeline view
 - CUDA HW: streams, kernels, memory
- Different traces, e.g. CUDA, MPI
 - correlations API <-> HW
- Stack samples
 - bottom-up, top-down for CPU code
- GPU metrics
- Events View
 - Expert Systems
- looks at single process (tree)
 - correlate multi-process reports in single timeline



Correlating Events on the Timeline

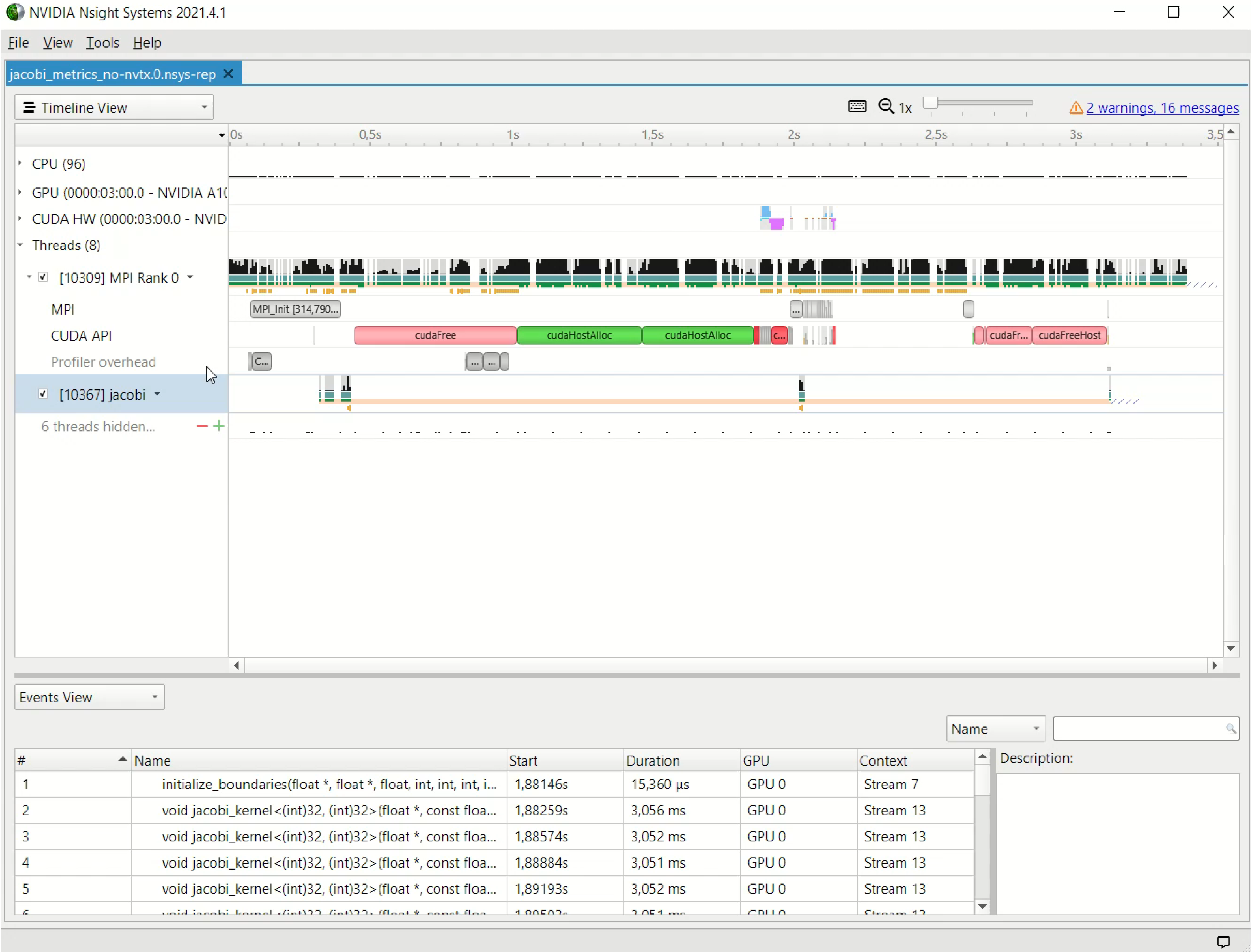
Selecting events in one row highlights related events

- CUDA's execution model is asynchronous
 - Kernel launch on host returns
 - Kernel runs on GPU
- Visualized in profiler



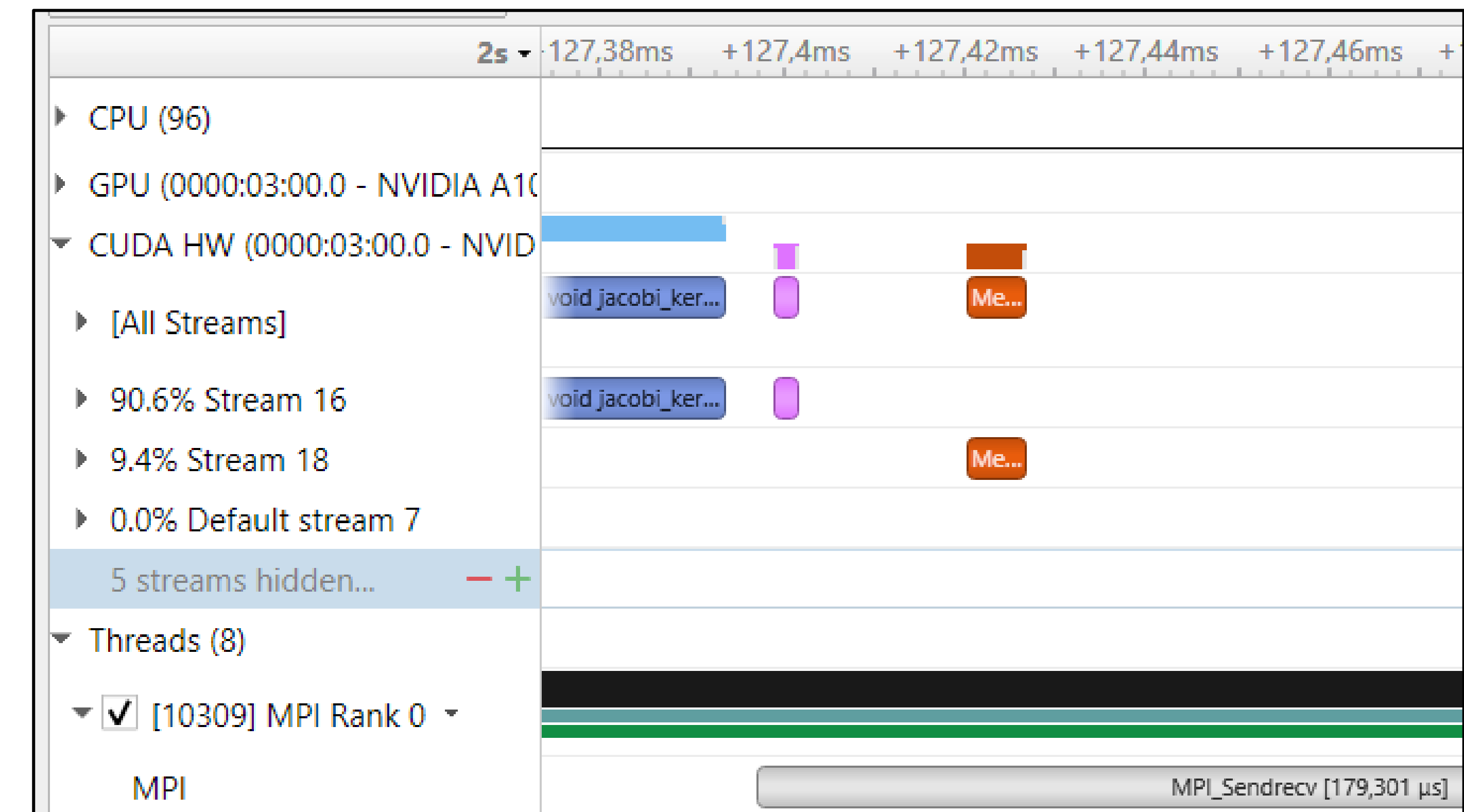
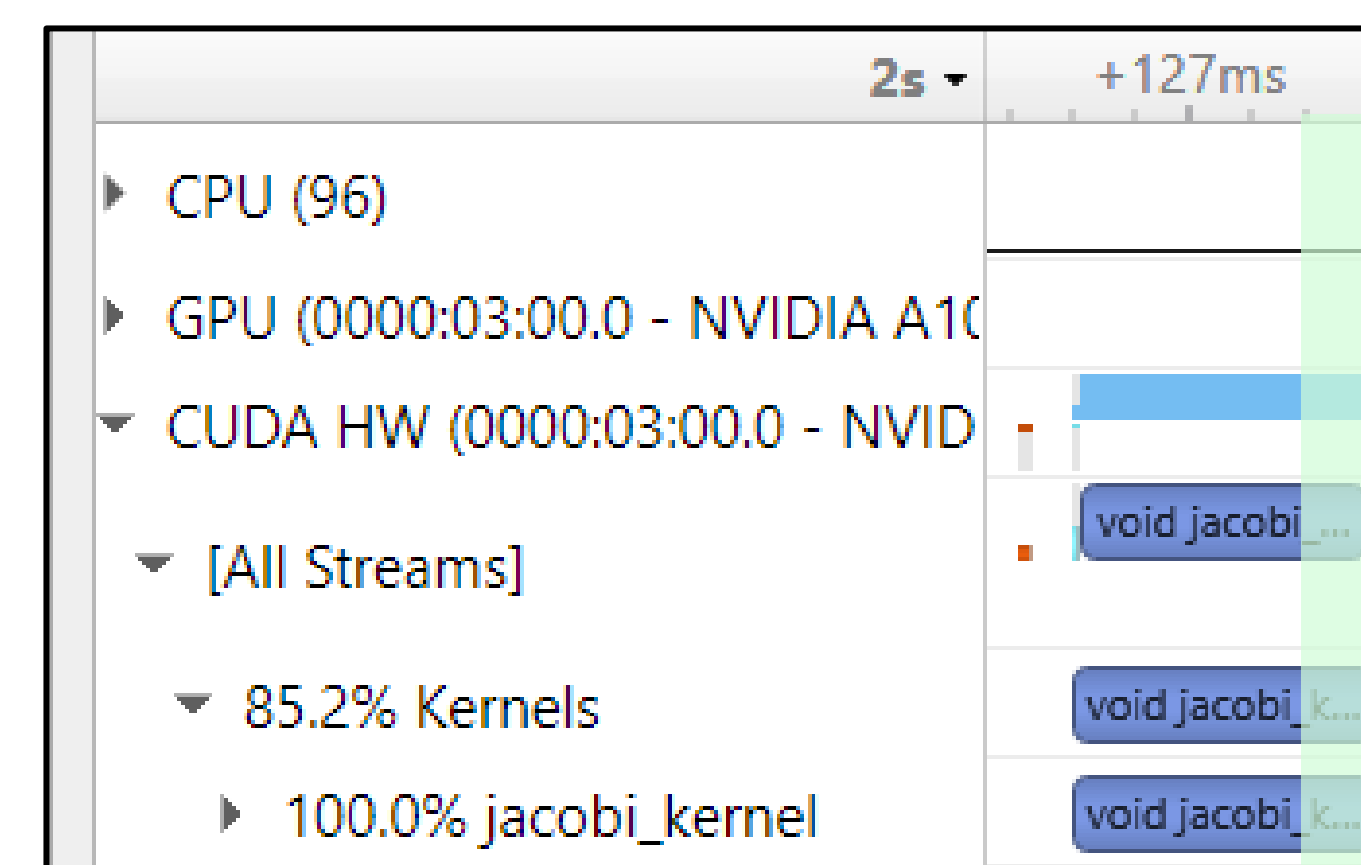
Nsight Systems Basic Workflow

Navigating the timeline and finding interesting areas



Discovering Optimization Potential

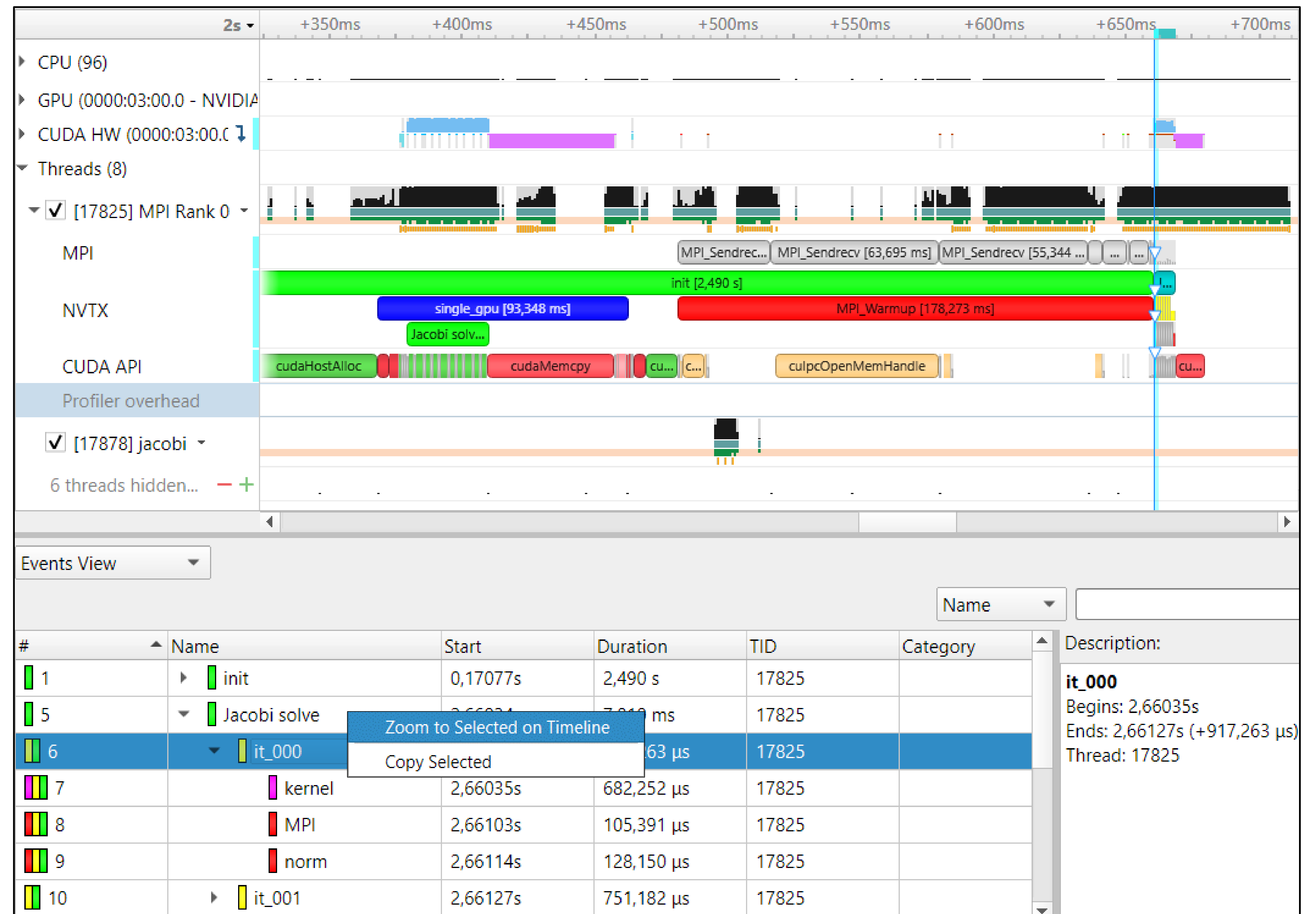
- Using our Jacobi example (see exercise)
- Spot kernels – lots of whitespace
 - Which part is „bad“?
 - Enhance!
- MPI calls
 - Memory copies
 - We know: This is CUDA-aware MPI
- Even without knowing source, insight
- Too complicated for repeated/reliable usage
 - How to simplify navigating and comparing reports?



Adding some Color

Code annotation with NVTX

- Same section of timeline as before
 - Events view: Quick navigation
- Like manual timing, only less work
- Nesting
- Correlation, filtering



Adding NVTX

Simple range-based API

- `#include "nvtx3/nvToolsExt.h"`
 - NVTX v3 is header-only, needs just `-ldl`
 - C++ and Python APIs
- Fortran: [NVHPC compilers include module](#)
 - Just use `nvtx` and `-cudalib=nvtx`
 - Other compilers: See blog posts linked below
- Definitely: Include PUSH/POP macros (see links below)
`PUSH_RANGE(name, color_idx)`
- Sprinkle them strategically through code
 - Use hierarchically: Nest ranges
- Not shown: Advanced usage (domains, ...)
- Similar range-based annotations exist for other tools
 - e.g. [SCOREP_USER_REGION_BEGIN](#)

```
int main(int argc, char** argv) {
    PUSH_RANGE("main", 0)
    PUSH_RANGE("init", 1)
    do_initialization();
    POP_RANGE
    /* ... */
    PUSH_RANGE("computation", 2)
    jacobi_kernel<<< /* ... */, compute_stream>>>(...);
    cudaStreamSynchronize(compute_stream);
    POP_RANGE
    /* ... */
    POP_RANGE
}
```

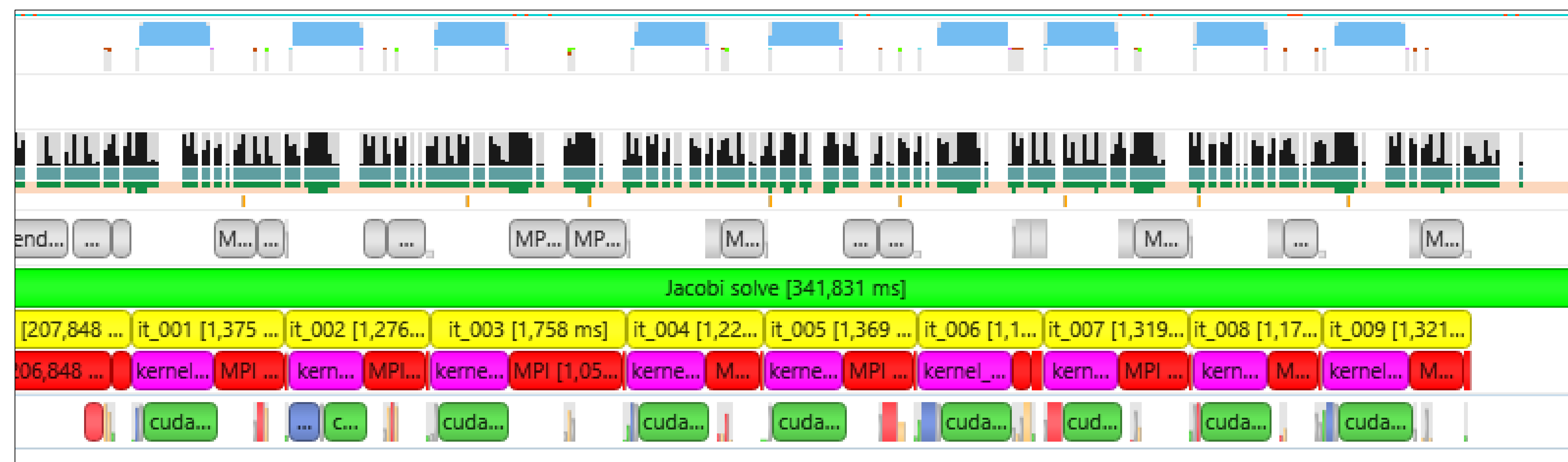
<https://github.com/NVIDIA/NVTX> and <https://nvidia.github.io/NVTX/#how-do-i-use-nvtx-in-my-code>

<https://developer.nvidia.com/blog/cuda-pro-tip-generate-custom-application-profile-timelines-nvtx/>
<https://developer.nvidia.com/blog/customize-cuda-fortran-profiling-nvtx/>

Minimizing Profile Size

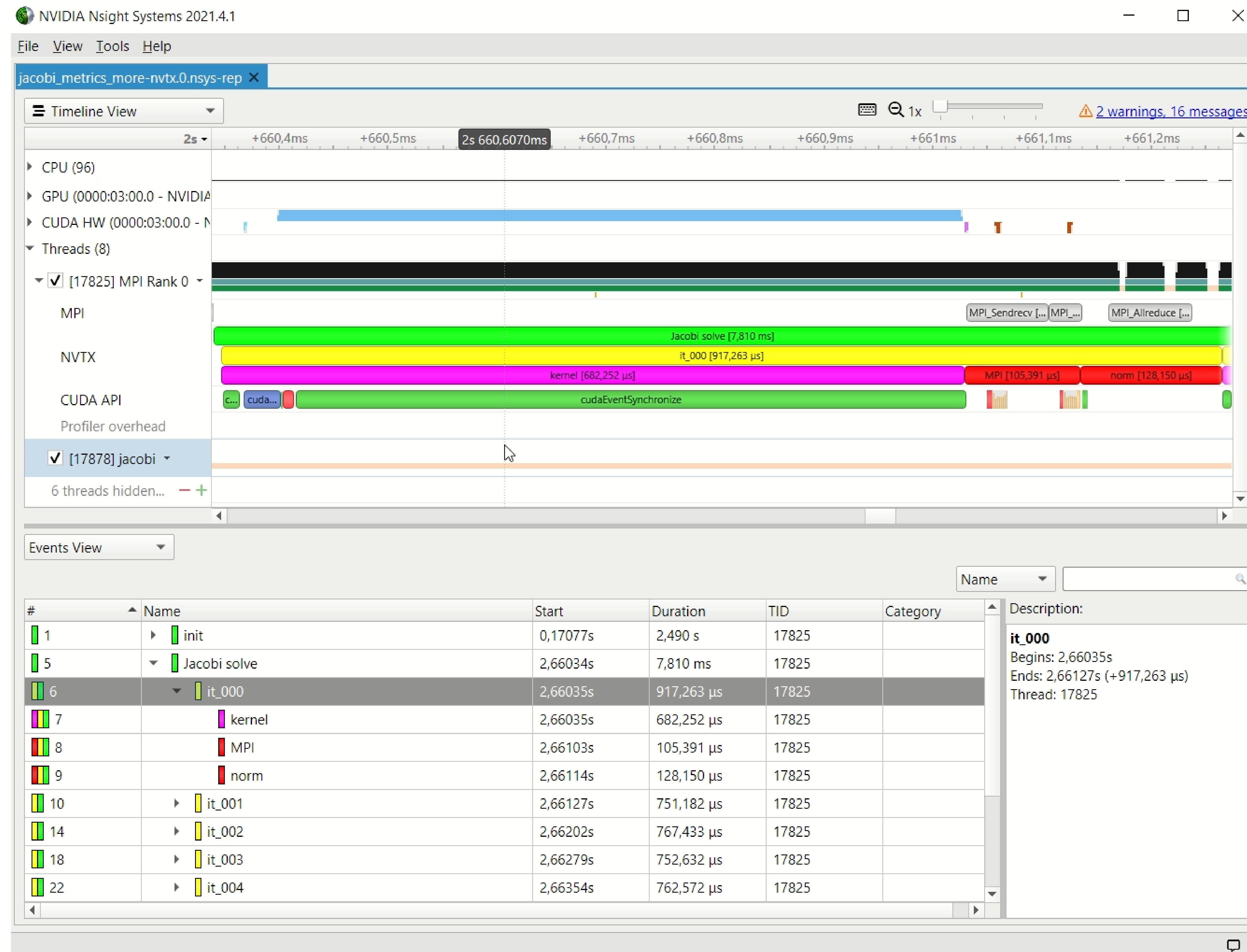
Shorter time, smaller files = quicker progress

- Only profile what you need – all profilers have some overhead
 - Example: Event that occurs after long-running setup phase
- Bonus: lower number of events leads to smaller file size
- Add to nsys command line:
 - `--capture-range=nvtx --nvtx-capture=any_nvtx_marker_name \`
`--env-var=NSYS_NVTX_PROFILER_REGISTER_ONLY=0 --kill none`
 - Use [NVTX registered strings](#) for best performance
- Alternatively: `cudaProfilerStart()` and `-Stop()`
 - `--capture-range=cudaProfilerApi`



Nsight Systems Workflow with NVTX

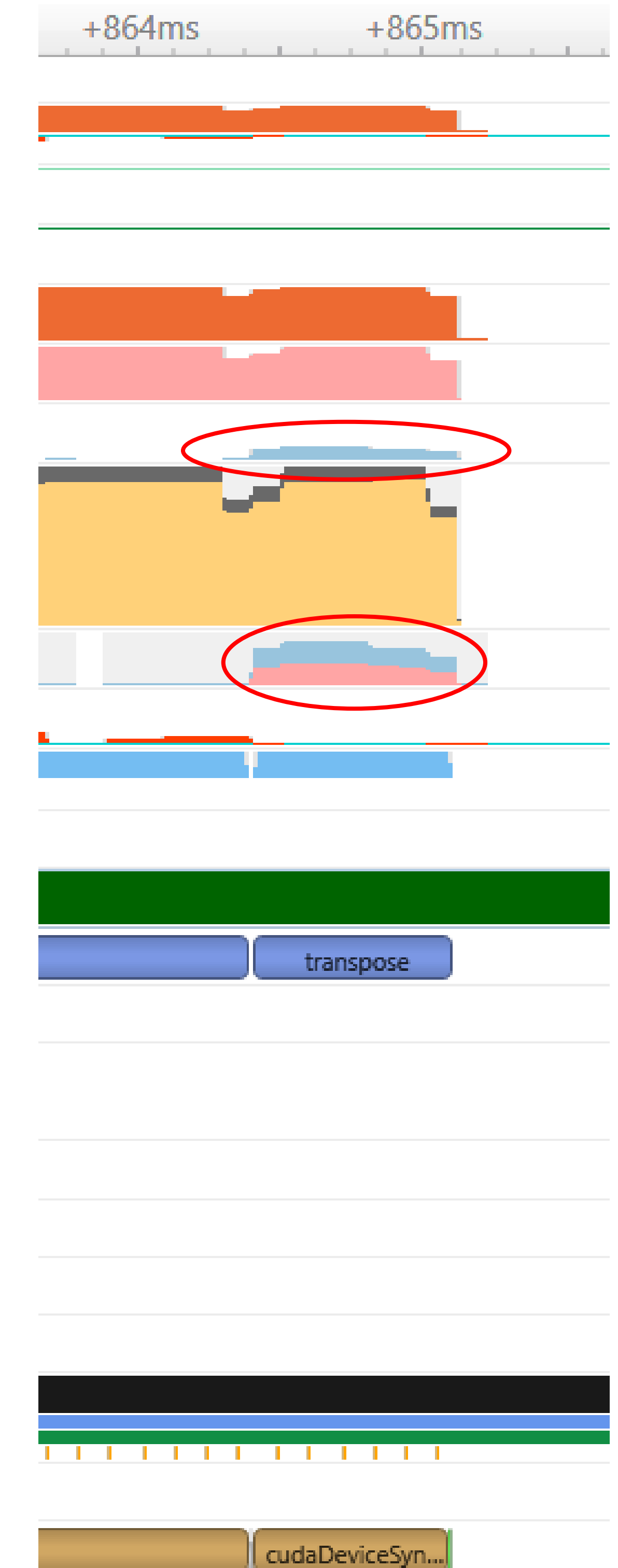
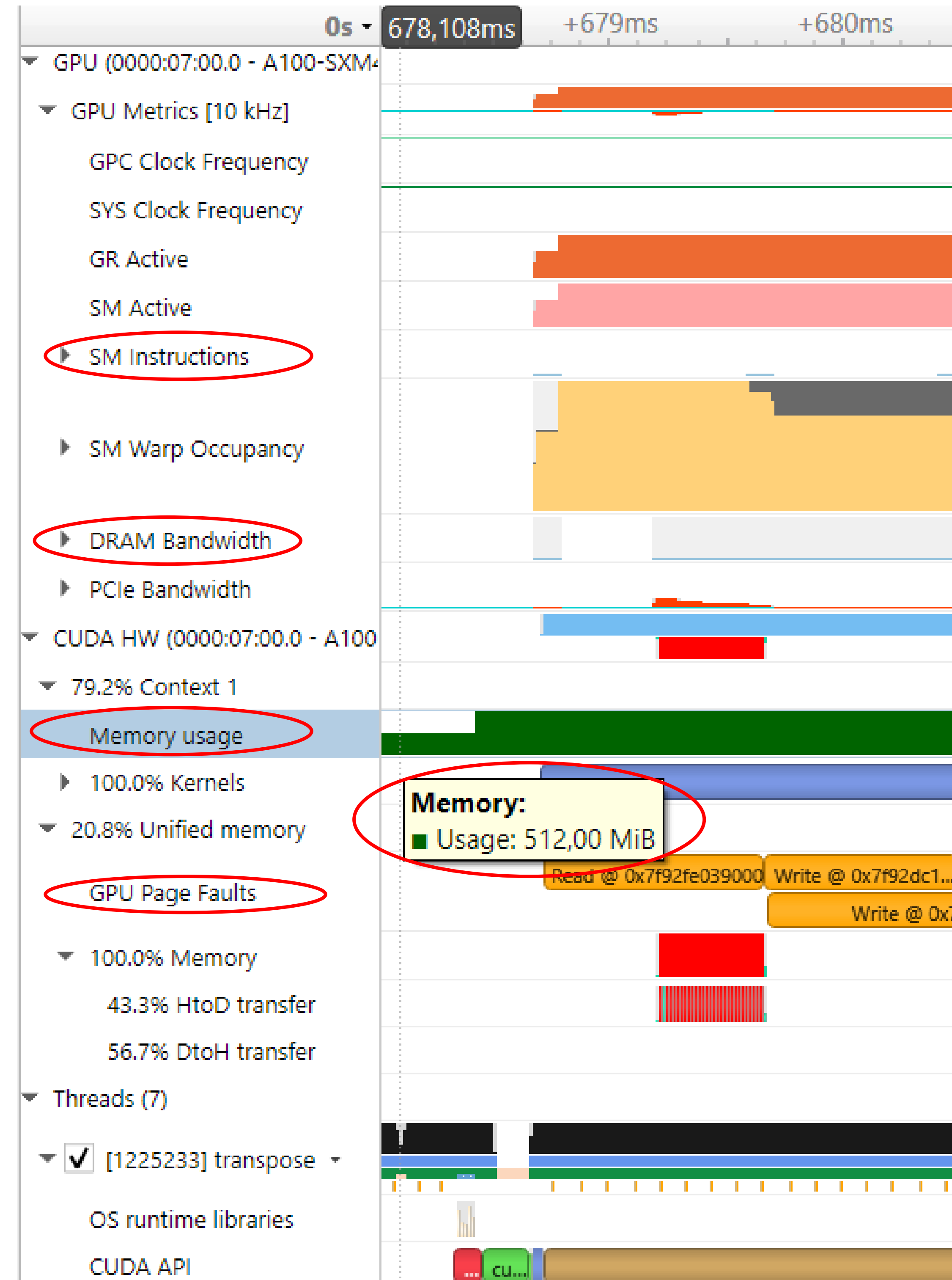
Repeating the analysis



GPU Metrics in Nsight Systems

...and other traces you can activate

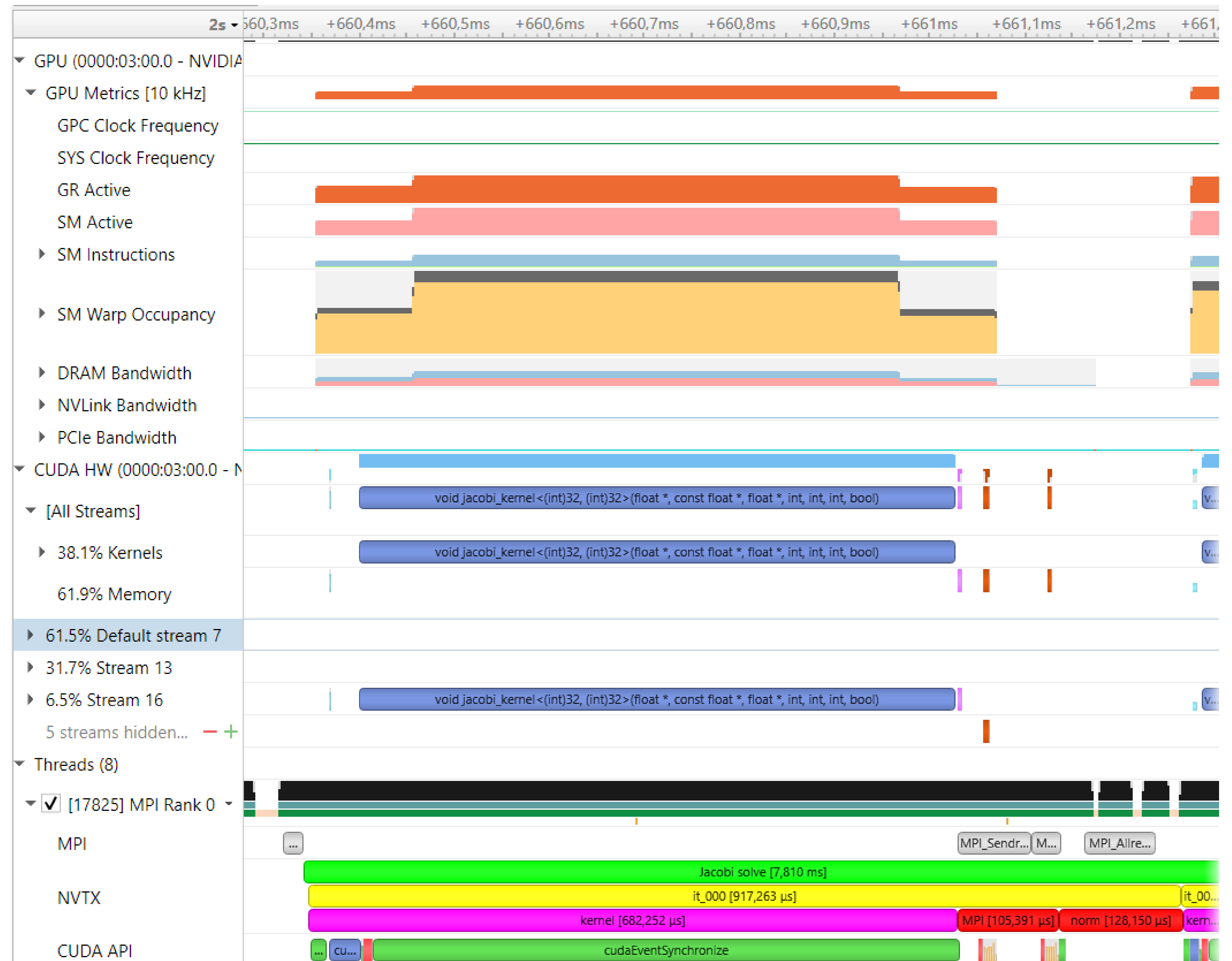
- Valuable low-overhead insight into HW usage:
 - SM instructions
 - DRAM Bandwidth, PCIe Bandwidth (GPUDirect)
- Also: Memory usage, Page Faults (higher overhead)
 - CUDA Programming guide: [Unified Memory Programming](#)
- Can save kernel-level profiling effort!
- nsys profile
 - gpu-metrics-device=0
 - cuda-memory-usage=true
 - cuda-um-cpu-page-faults=true
 - cuda-um-gpu-page-faults=true
 - ./app



Focusing the Analysis

Introducing GPU metrics sampling

- Discover the „unit cell“ of performance
 - in our case: single iteration
- Other blank spots during setup can be ignored (amortized, many more iterations)
- Maybe: Too small for proper comms profiling
- Kernel itself adequately using GPU
 - Remaning blank spots?
- Norm calculation
 - Can be turned off
- But still: Overlap potential? Can we run kernel during MPI?
 - later lectures



Using Multiple Reports in Nsight Systems

NVIDIA Nsight Systems 2022.4.1

File View Tools Help

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Timeline View

0s 0,5s 1s 1,5s 2s 2,5s 3s

CUDA HW (0000:03:00.0 - NVIDIA A100-SXM4-40GB)

39.0% Kernels

61.0% Memory

Threads (9)

[31252] MPI Rank 0

MPI

NVTX

CUDA API

Profiler overhead

[31329] async

7 threads hidden...

[31255] ./jacobi

Events View

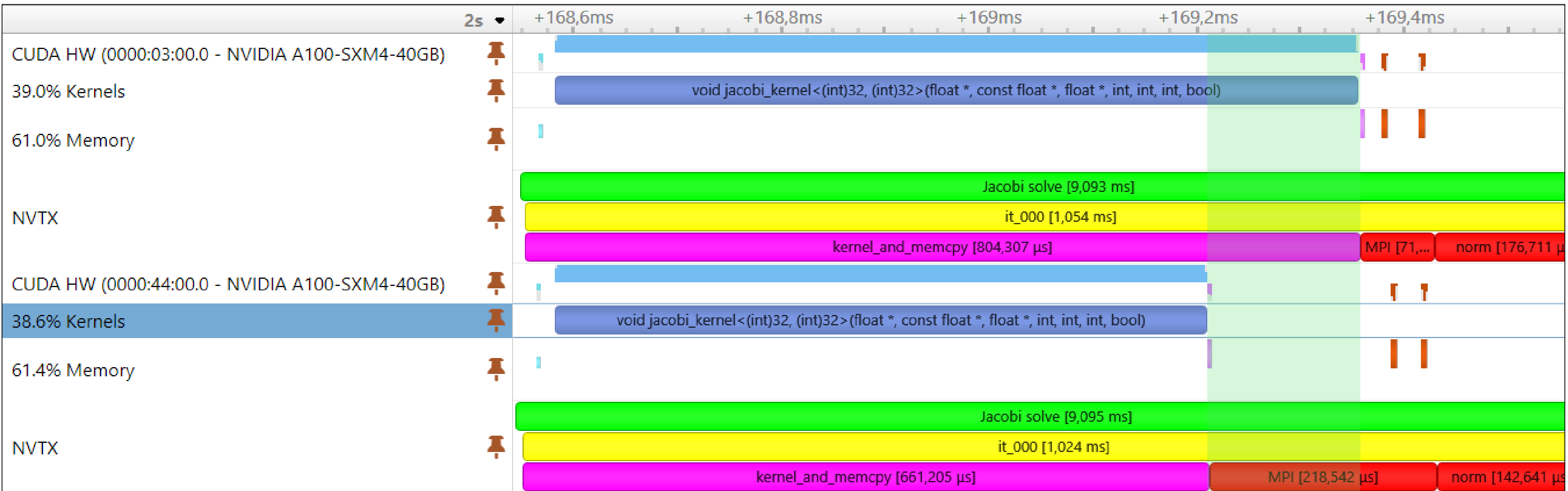
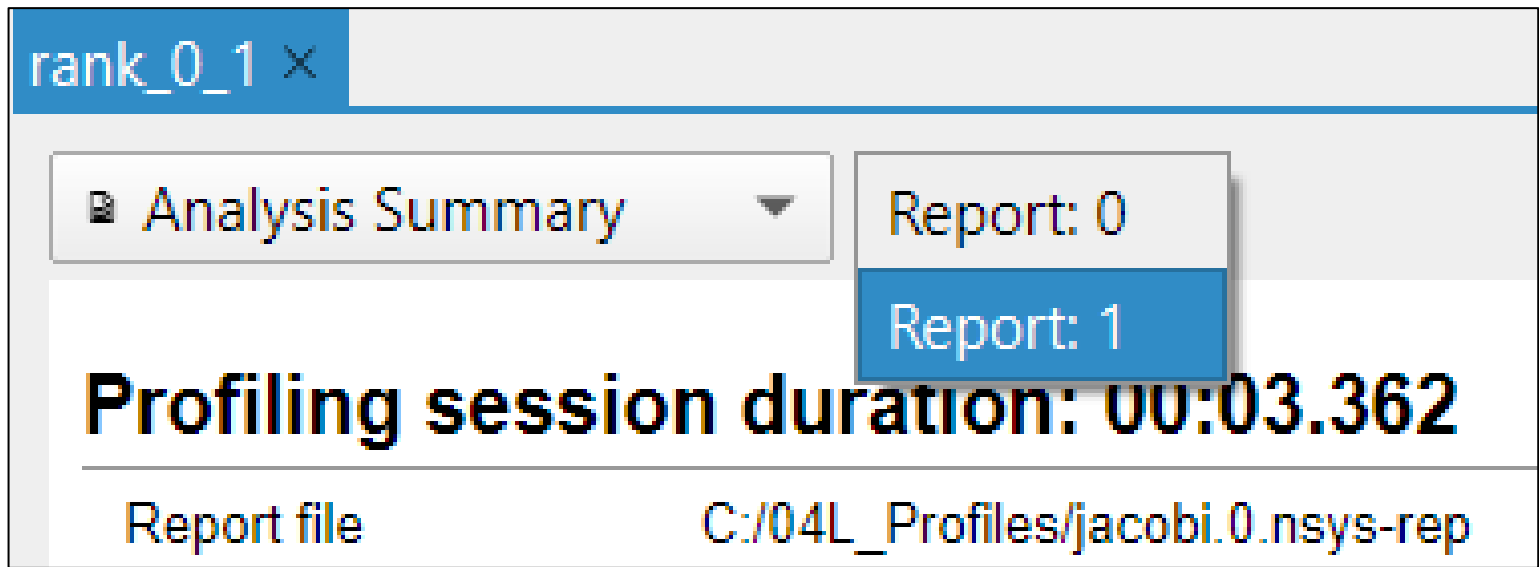
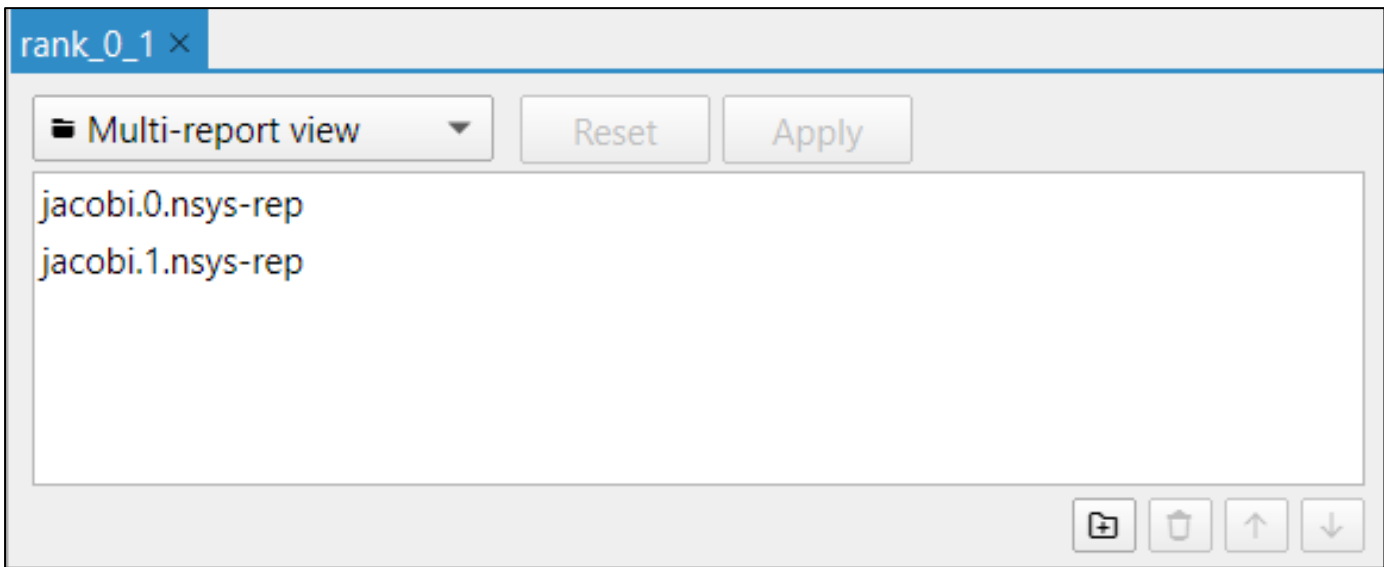
Name

Description:

Right-click a timeline row and select "Show in Events View" to see events here

Multi-Process GPU Analysis

- Load multiple reports into timeline
 - analyze differences in execution, GPU utilization
- Pin rows for comparison
- Example: End time of kernel execution



Community Profiling Tools

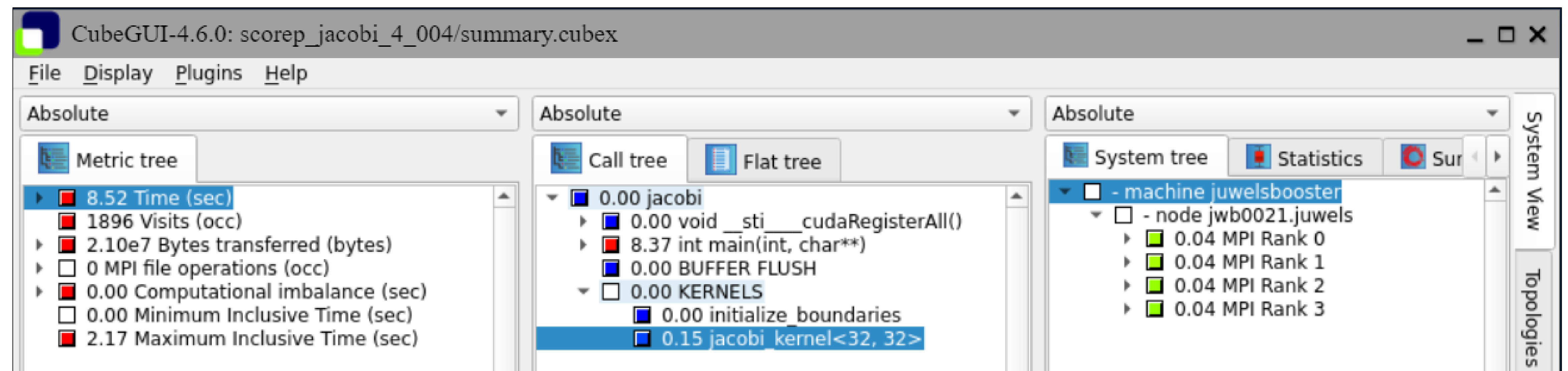
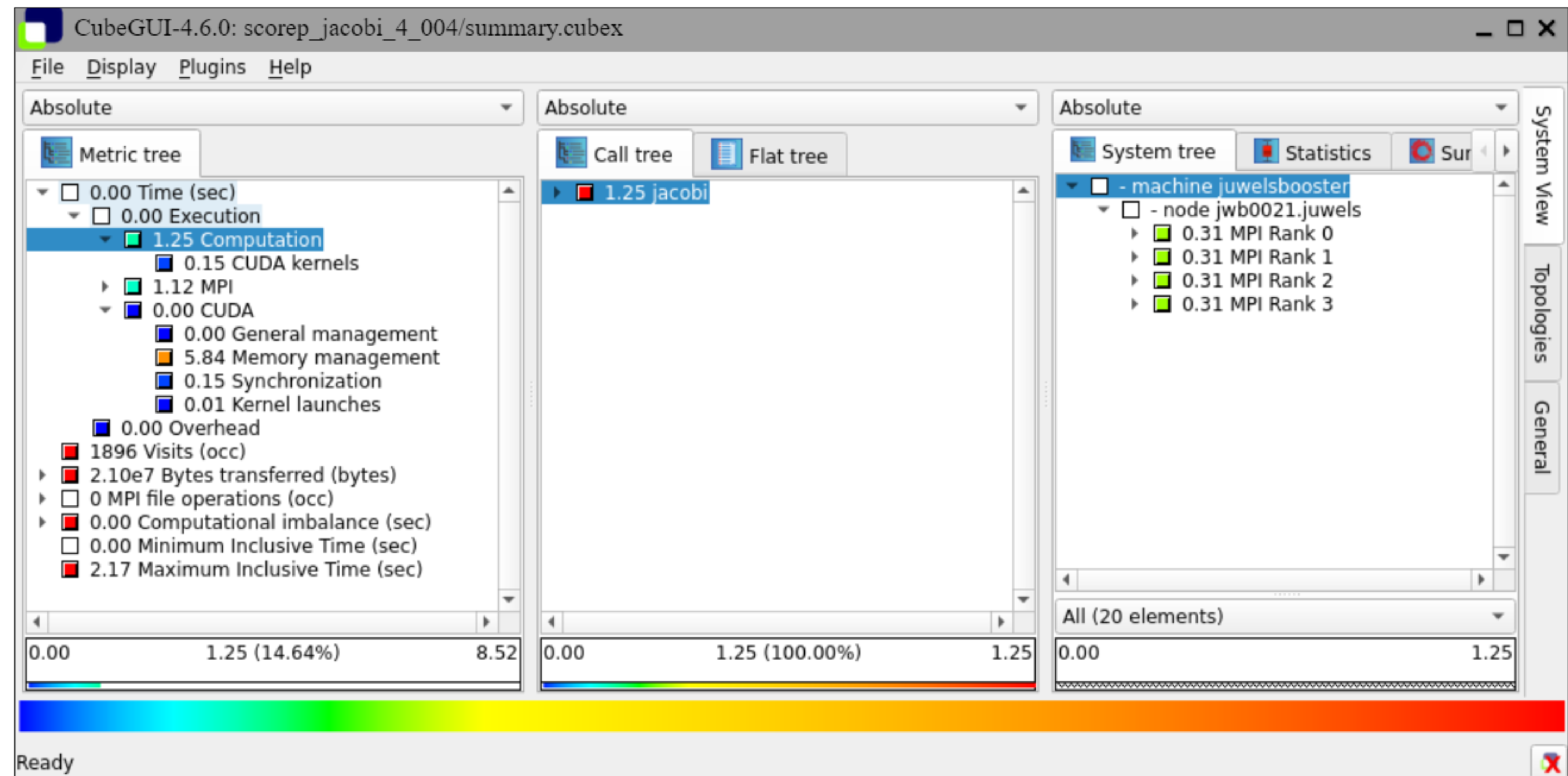
Specialized for large-scale distributed analysis

- Detecting issues at scale of thousands of GPUs (and processes)
 - Need to slice and dice data, too much to make sense of raw data
- Common measurement/instrumentation infrastructure: *Score-P*
 - Prefix all compilation/linker commands with `scorep -cuda`
- GPU data integration
 - CUDA profiling tools interface (CUPTI)
- Run the application to collect...
 - profiling data, for Scalasca
 - tracing data, for Vampir
 - (selection of tools not exhaustive)
- Tracing in particular: Careful tuning to keep overhead low (filtering)



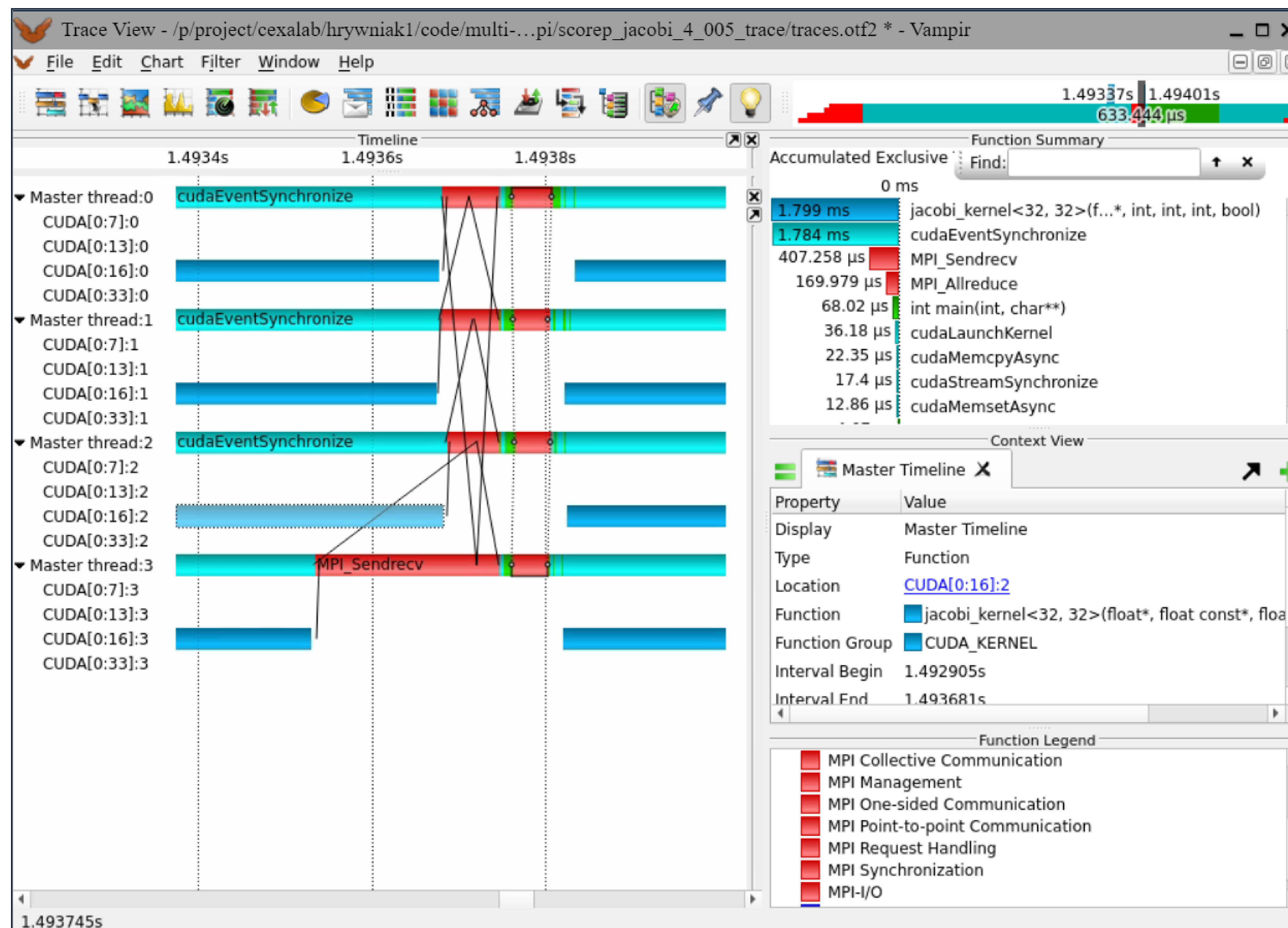
Scalasca / CUBE

- Breakdown of different metrics across functions and processes
- Left-to-right: Selection influences breakdown
- Expanding changes inclusive/exclusive
- Example analysis:
 - Detect computational imbalance
- <https://scalasca.org/>



Vampir trace

- Analyze multi-process patterns
- What you can see in screenshot
 - Main timeline
 - Function summary
- Example analysis: Pinpoint MPI message relationships
 - e.g. late sender issues
- <https://vampir.eu/>



Summary

- Looked at a wide selection of different tools
 - compute-sanitizer
 - cuda-gdb
 - Nsight-Systems
 - Score-P: Scalasca, Vampir, ...
 - and don't forget compiler flags and checks
- Correctness is paramount, but so is optimal resource usage
- Pick right tool for the job – and take the time to learn it thoroughly
 - Do not trust your gut when analyzing performance, easy to be misled
 - How to adapt serial (or small-scale) tooling to highly distributed applications
- Meant as guideline, not gospel
 - Especially performance issues often require creativity to solve
- Workflow is equally important

Further Material

- GTC on-demand talks
 - [What, Where, and Why? Use CUDA Developer Tools to Detect, Locate, and Explain Bugs and Bottlenecks \(s41493, GTC 2022\)](#)
 - [Tuning GPU Network and Memory Usage in Apache Spark \(s31566, GTC 2022\)](#)
- Documentation for [cuda-gdb](#), [compute-sanitizer](#) and [Nsight Systems](#) and blog posts:
 - [Efficient CUDA Debugging: Memory Initialization and Thread Synchronization with NVIDIA Compute Sanitizer](#)
 - [Optimizing CUDA Memory Transfers with NVIDIA Nsight Systems](#)
 - ...and other posts: <https://developer.nvidia.com/blog/tag/nsight/>
- GTC labs from Nsight teams: <https://github.com/NVIDIA/nsight-training>
- GPU bootcamp material, e.g., https://github.com/openhackathons-org/nways_accelerated_programming

