



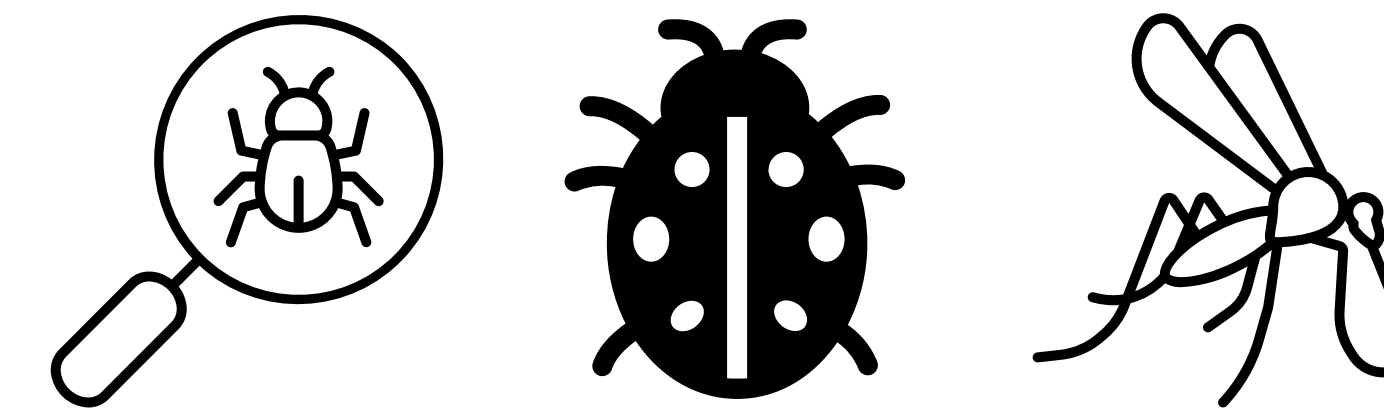
Performance and Debugging Tools

Markus Hrywniak, Senior Devtech Compute | SC24 / November 17th 2024

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 <i>host</i> code
<code>-lineinfo</code>	Generate line correlation info for <i>device</i> 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:

```
srunk -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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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, ...)
- %q{ENV_VAR} supported by all the NVIDIA tools discussed here, embed environment variable in file name
 - ENV_VAR should be one 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_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/mpi2/mpi2ch/mpi2ch32-userguide.html#x134600013>
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>

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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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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>

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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=$(squeue -h %i --me)
[jwlogin]$ 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

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# compute-sanitizer

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

[https://slurm.schedmd.com/srun.html#SECTION\\_OUTPUT-ENVIRONMENT-VARIABLES](https://slurm.schedmd.com/srun.html#SECTION_OUTPUT-ENVIRONMENT-VARIABLES)

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# Using cuda-gdb with MPI

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- Launch process, sleep on particular rank

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$ 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 cudacore 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 ...
```

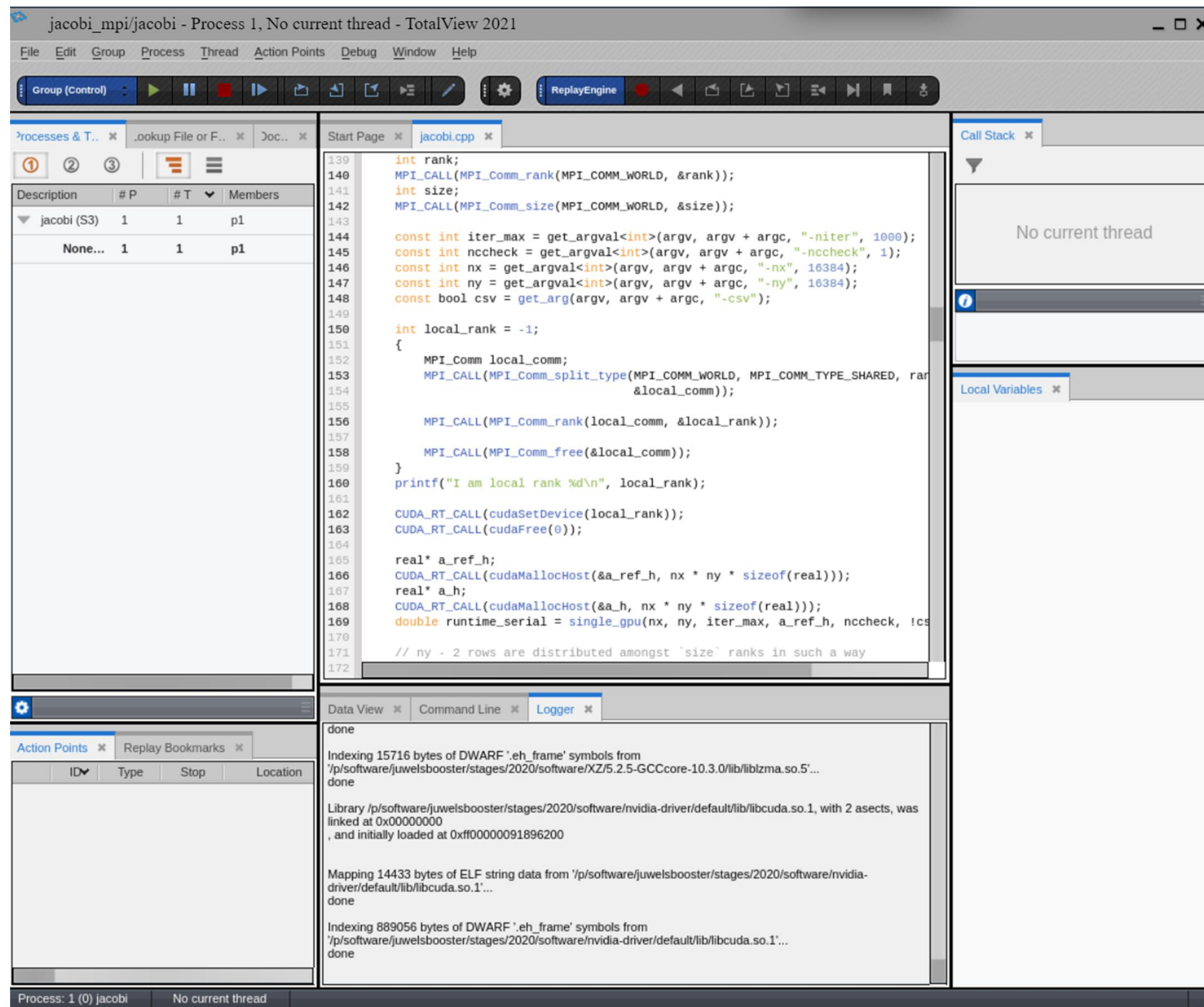
- And opening the core dump in `cuda-gdb`

```
(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

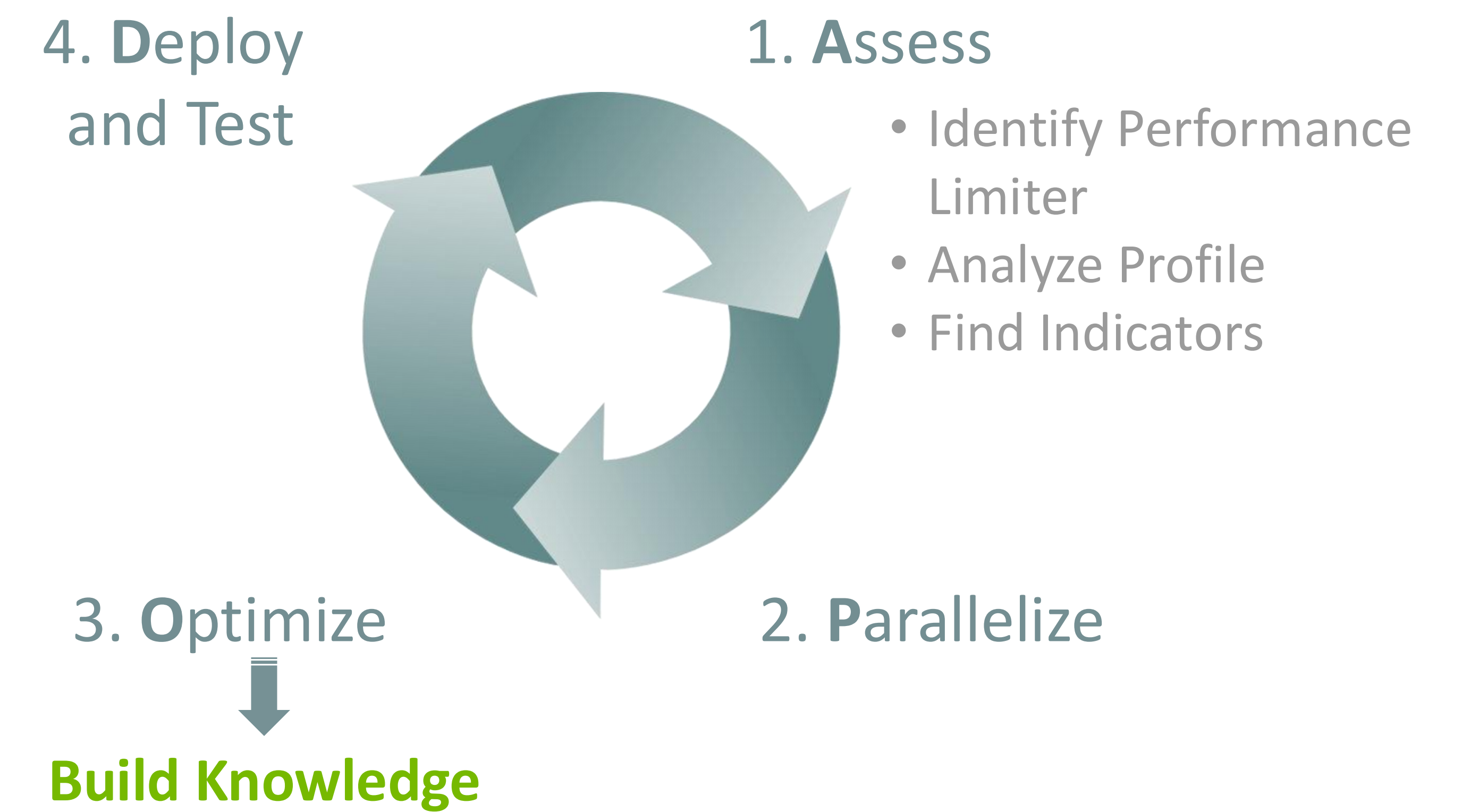
A case for modularity, and proper test cases

- 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
  - Instrumenting/Sampling
  - Profiling/Tracing
  - multi-process, single-process, kernel-level
- Here: Focus on GPU and system-level: Nsight Systems





# The Nsight Suite Components

How the pieces fit together



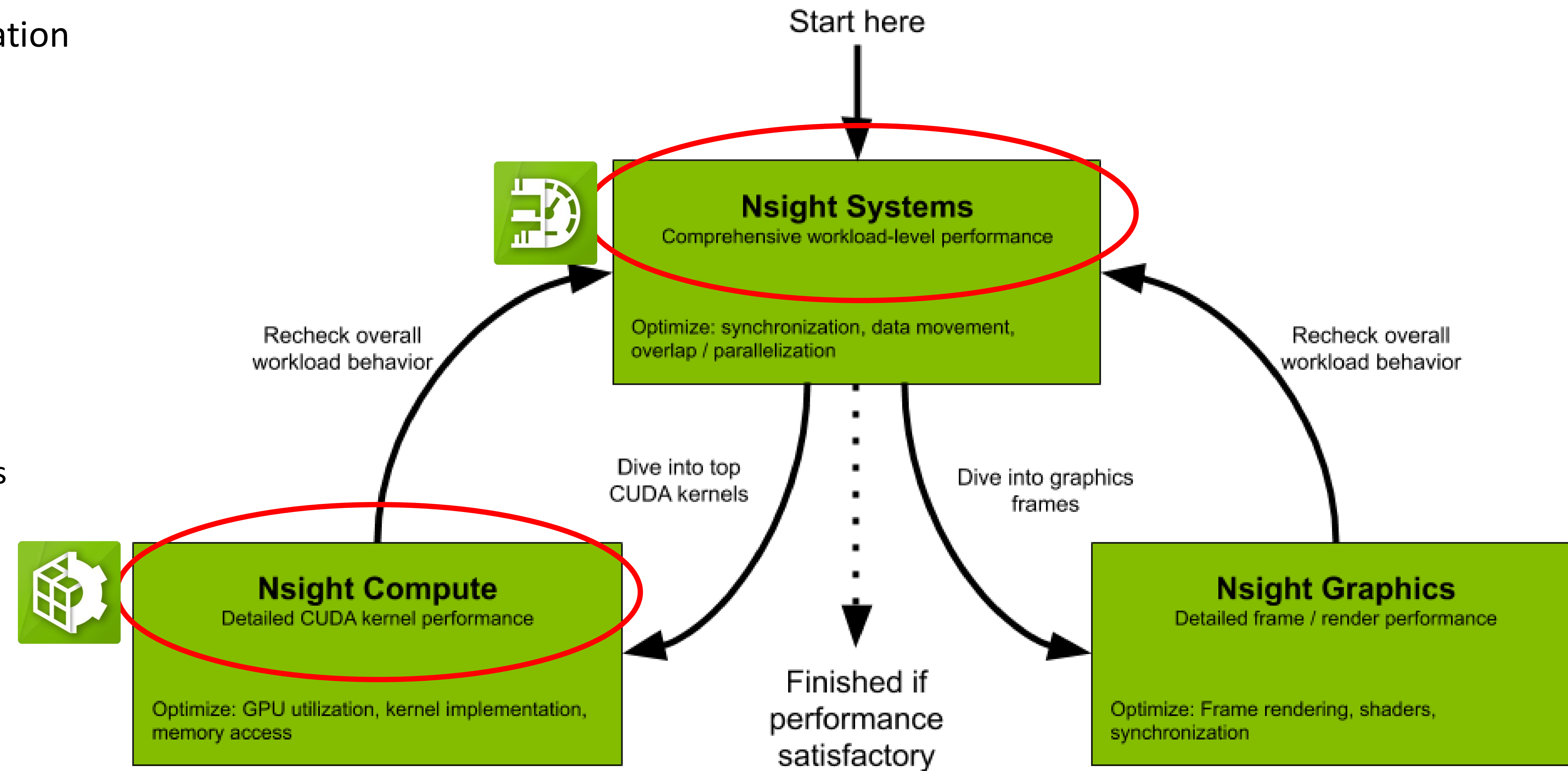
- Nsight **Systems**: Coarse-grained, whole-application



- 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

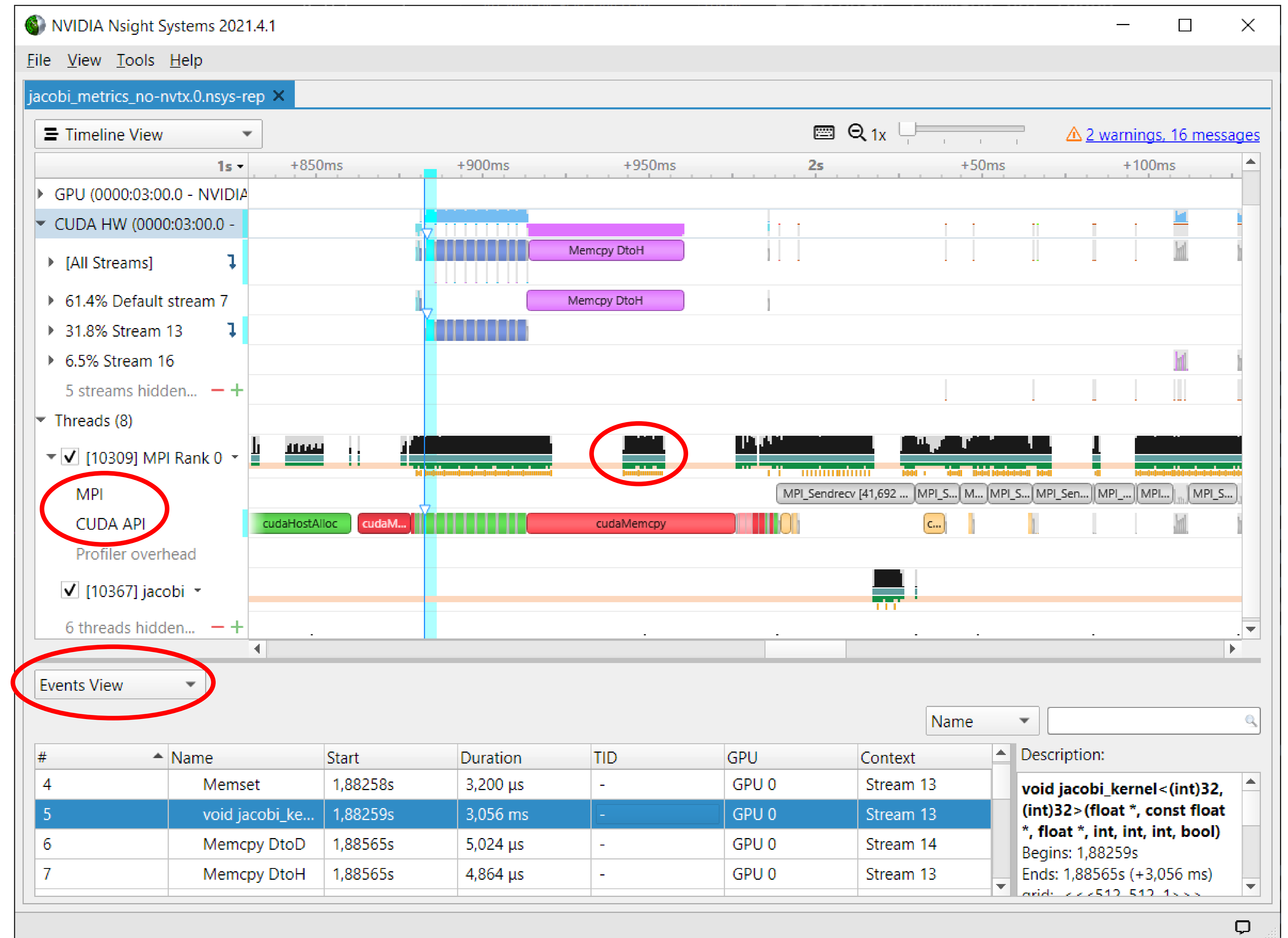
Running [.../reports/**gpukernsum.py** jacobi\_metrics\_more-nvtx.0.**sqlite**]

| 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

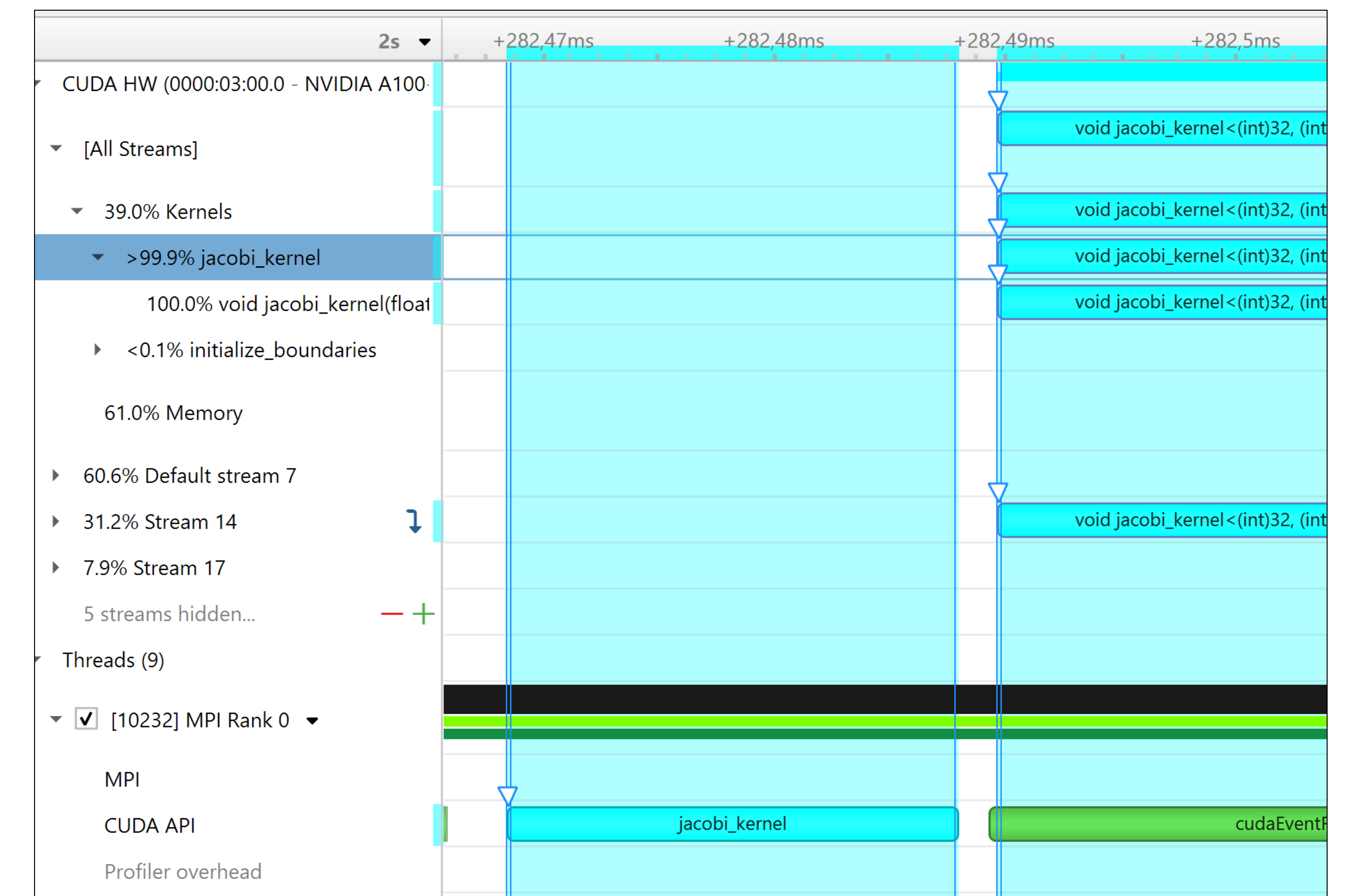
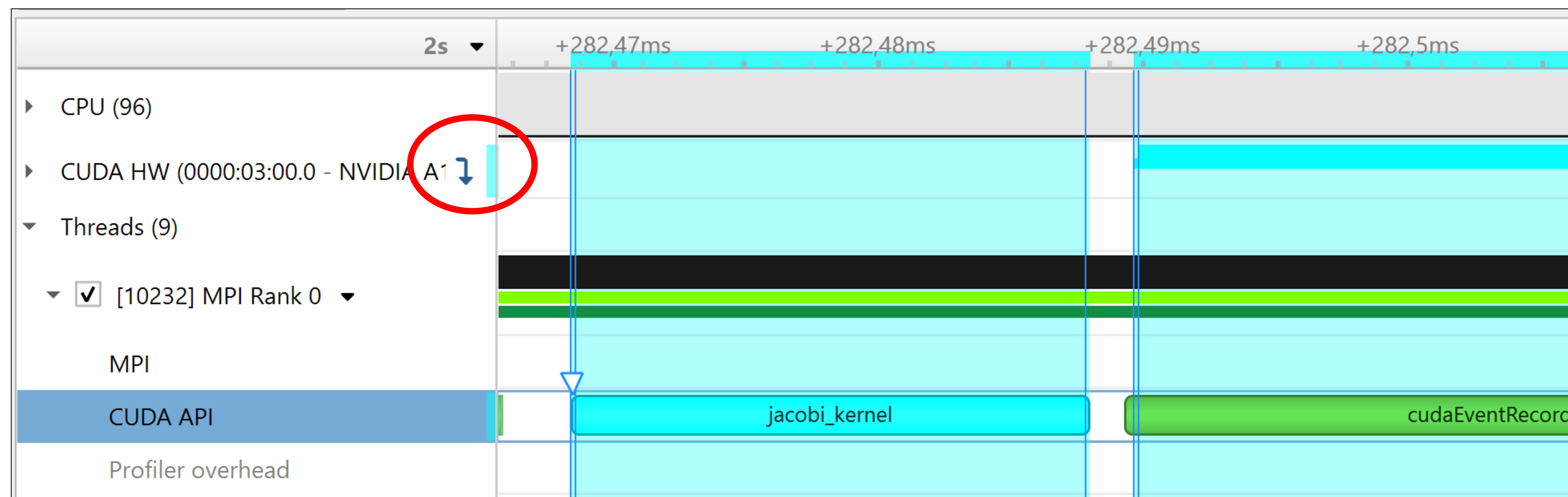
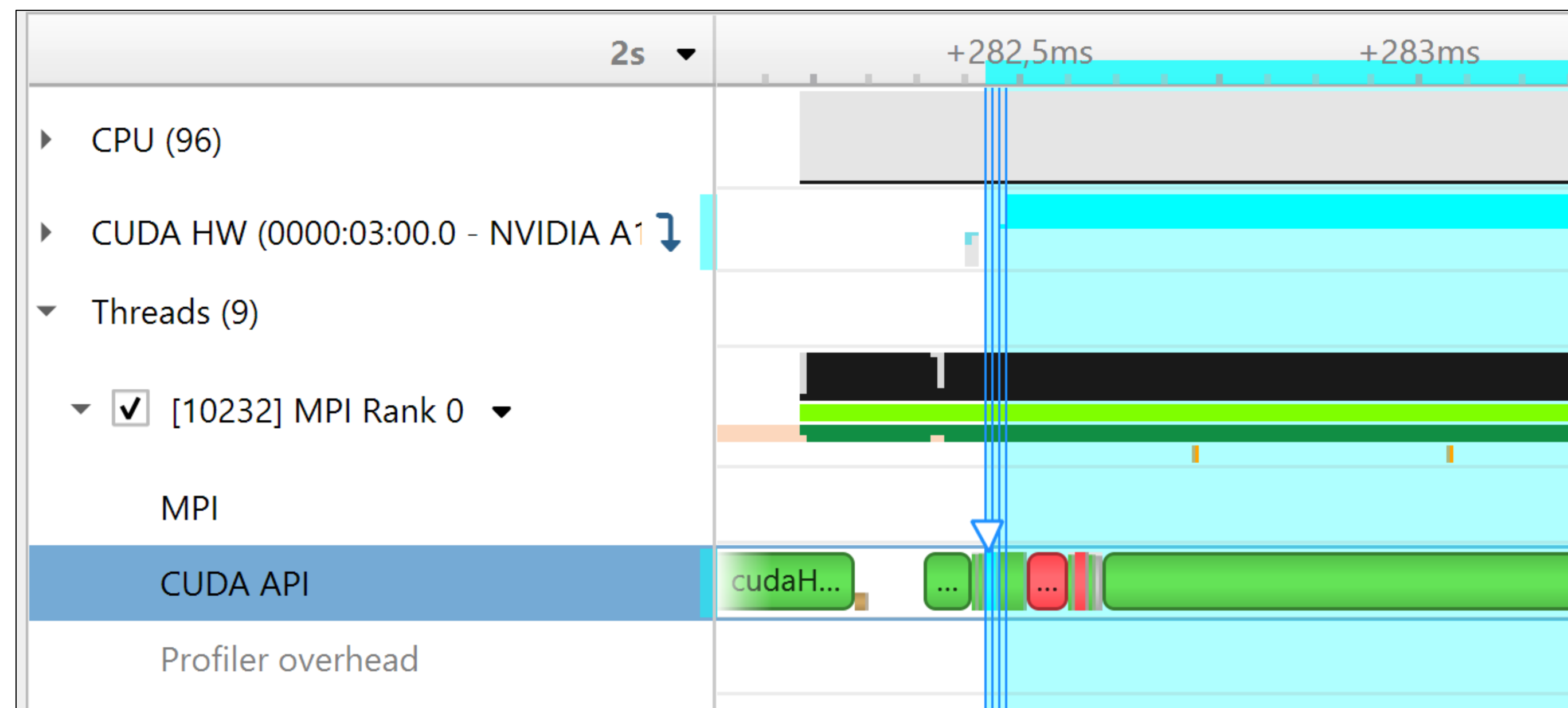
- Global timeline view
  - CUDA HW: streams, kernels, memory
- Different traces, e.g. CUDA, MPI
  - correlations API <-> HW
- Stack samples
  - bottom-up, top-down for CPU code
- GPU metrics
- Events View
  - Expert Systems
- looks at single process (tree)
  - correlate multi-process reports in single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



# Correlating Events on the Timeline

Selecting events in one row highlights related events

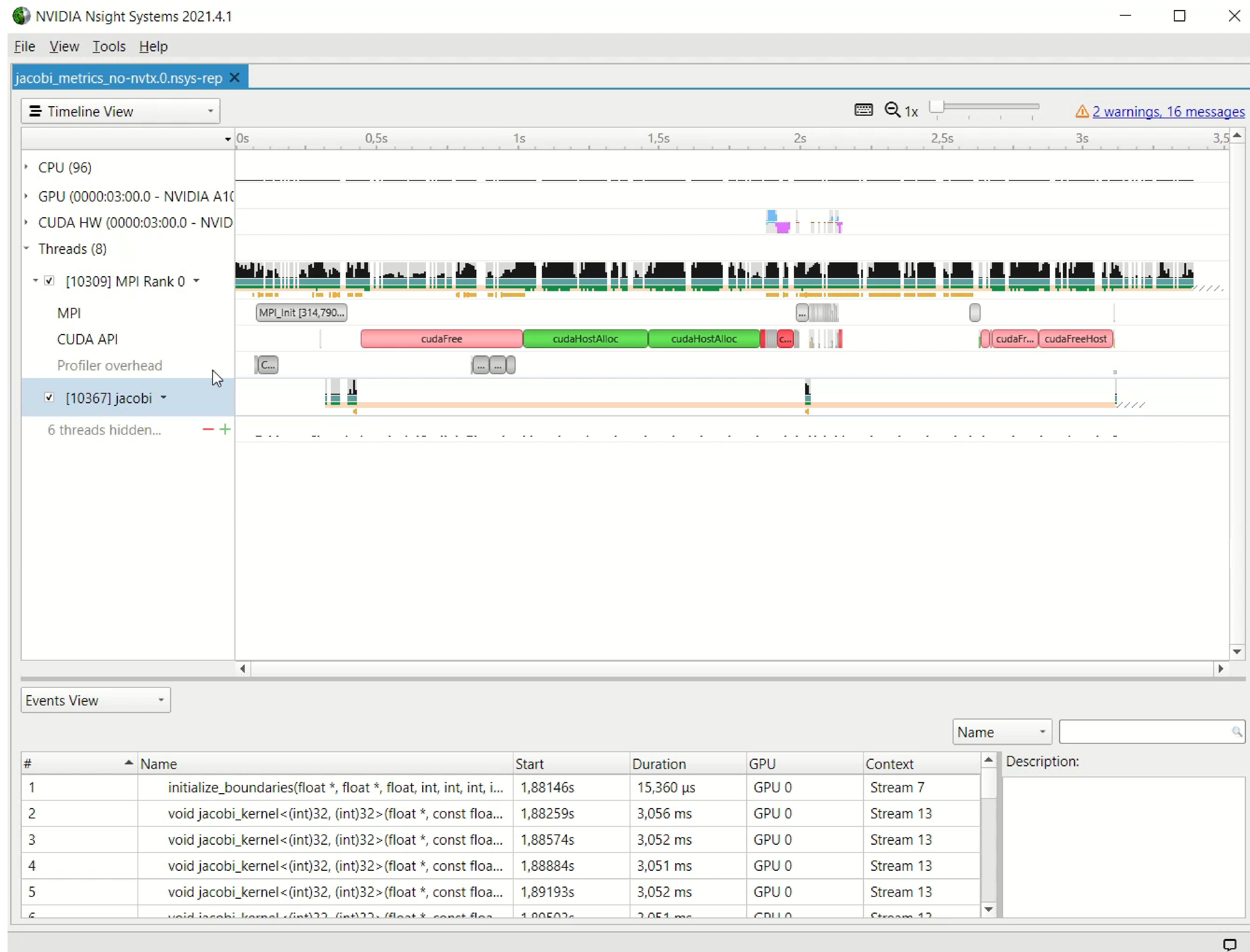
- CUDA's execution model is asynchronous
  - Kernel launch on host returns
  - Kernel runs on GPU
- Visualized in profiler





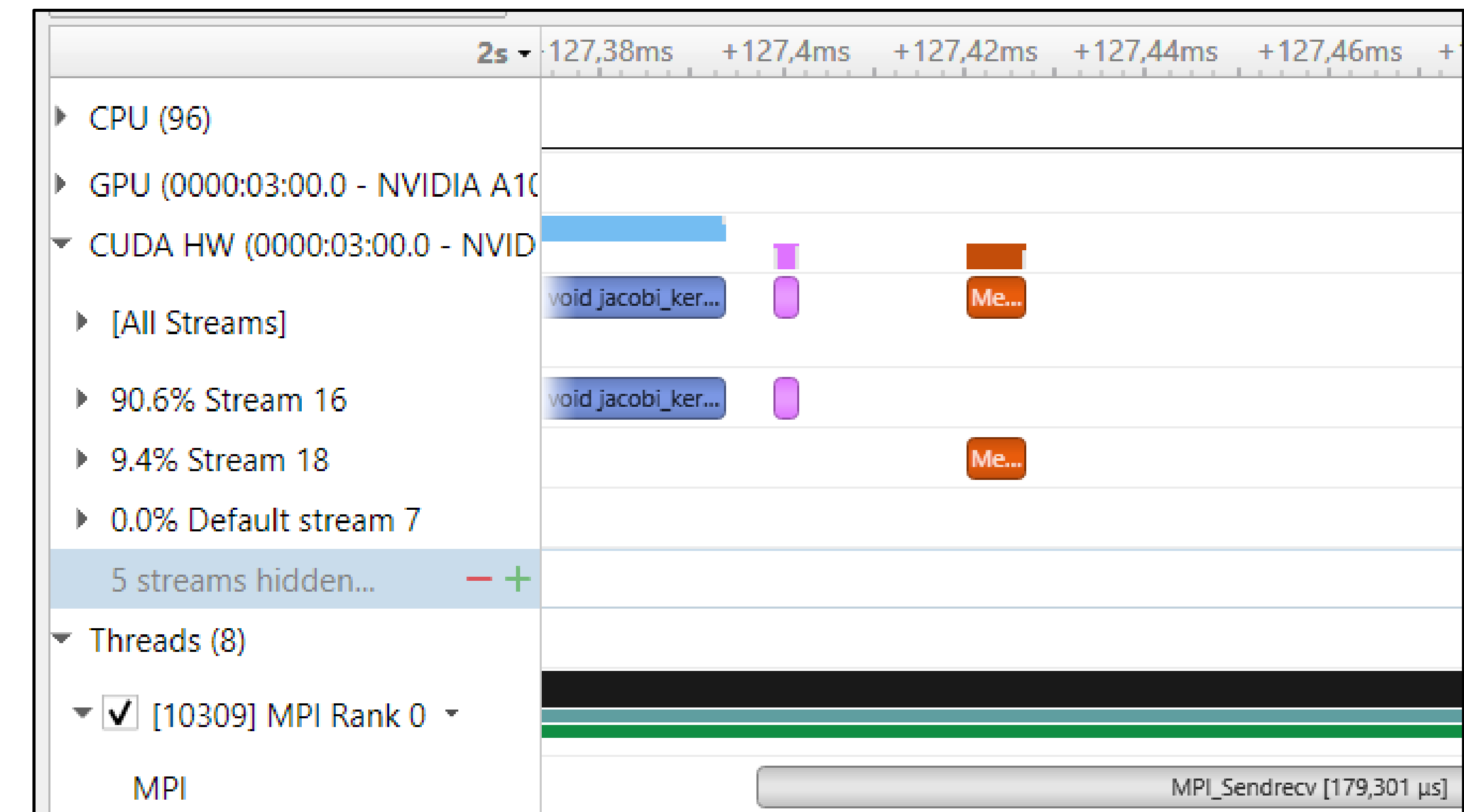
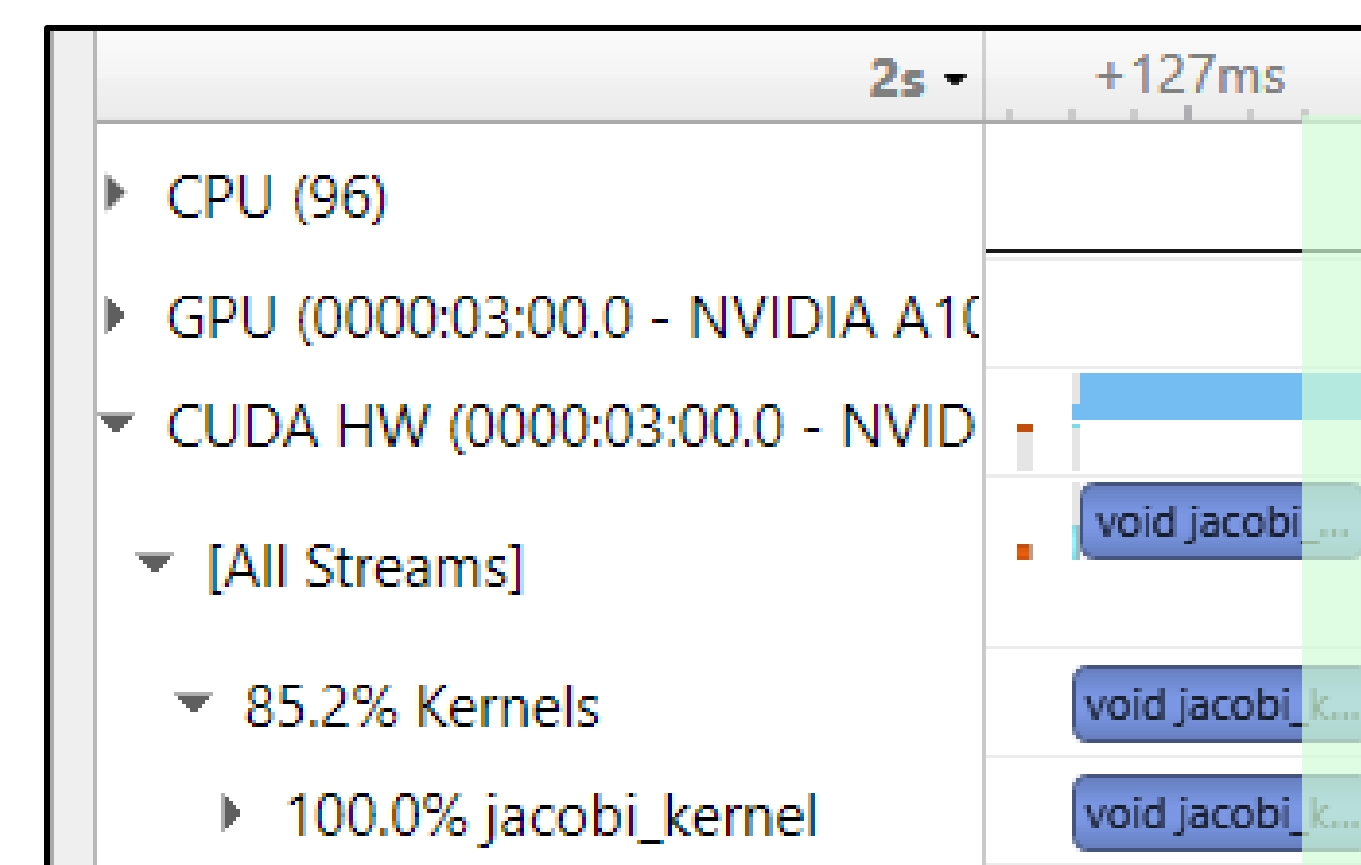
# Nsight Systems Basic Workflow

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?

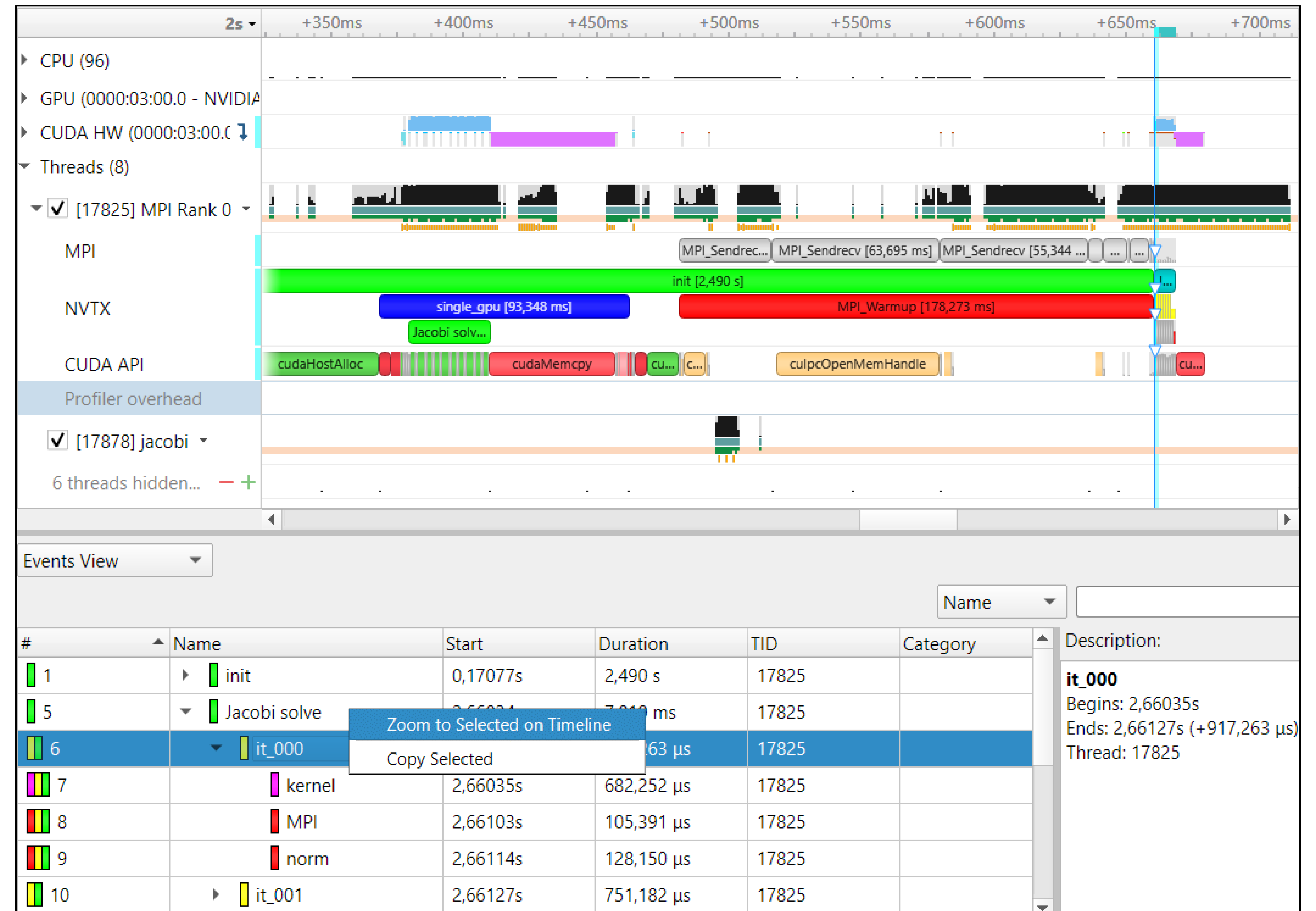




# Adding some Color

## 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>

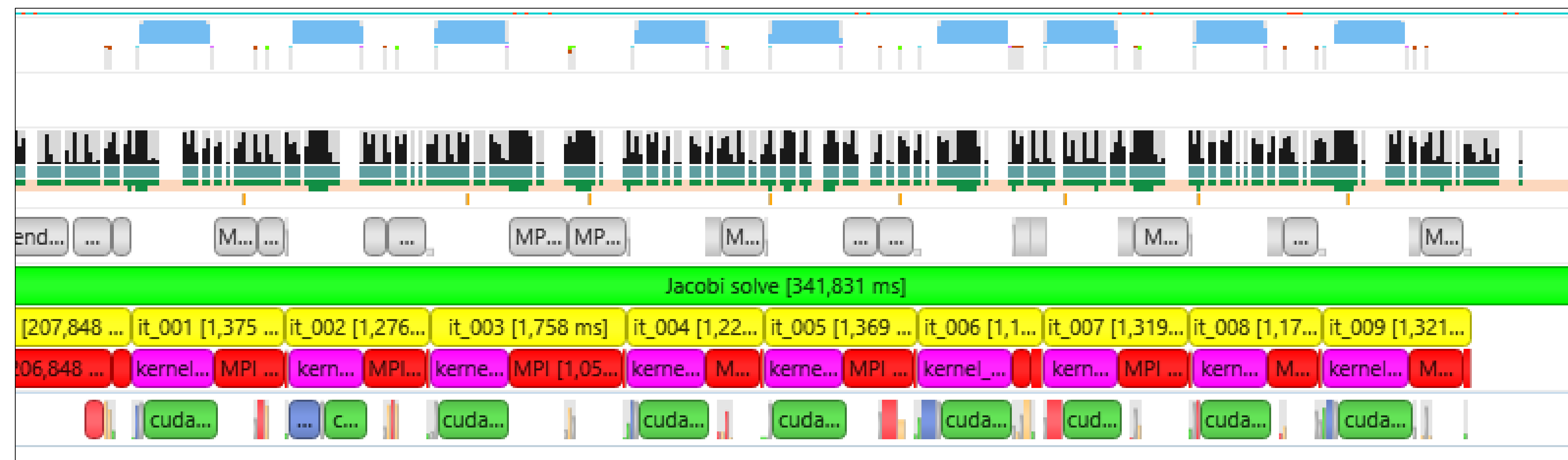
<https://developer.nvidia.com/blog/cuda-pro-tip-generate-custom-application-profile-timelines-nvtx/>  
<https://developer.nvidia.com/blog/customize-cuda-fortran-profiling-nvtx/>



# Minimizing Profile Size

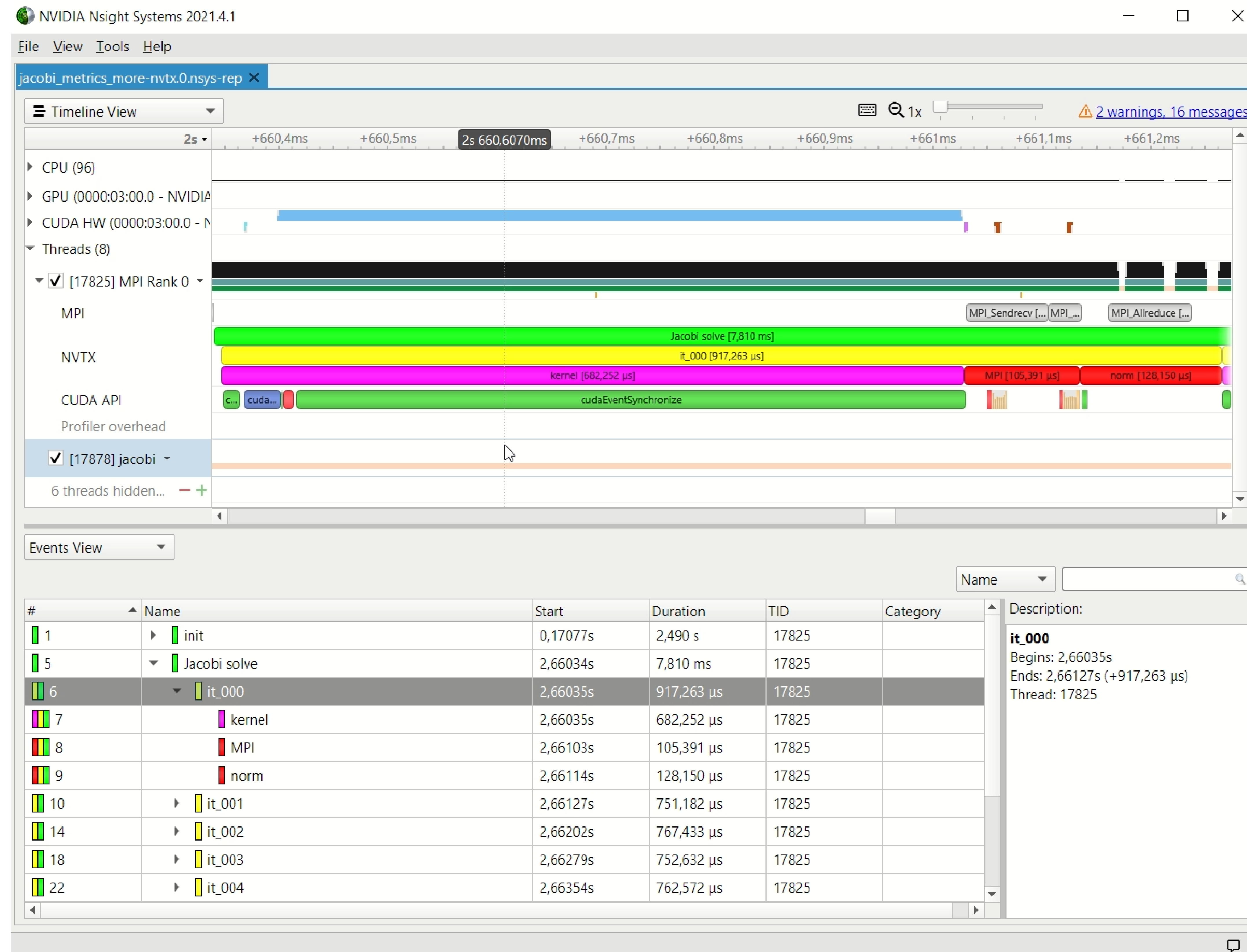
Shorter time, smaller files = quicker progress

- 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

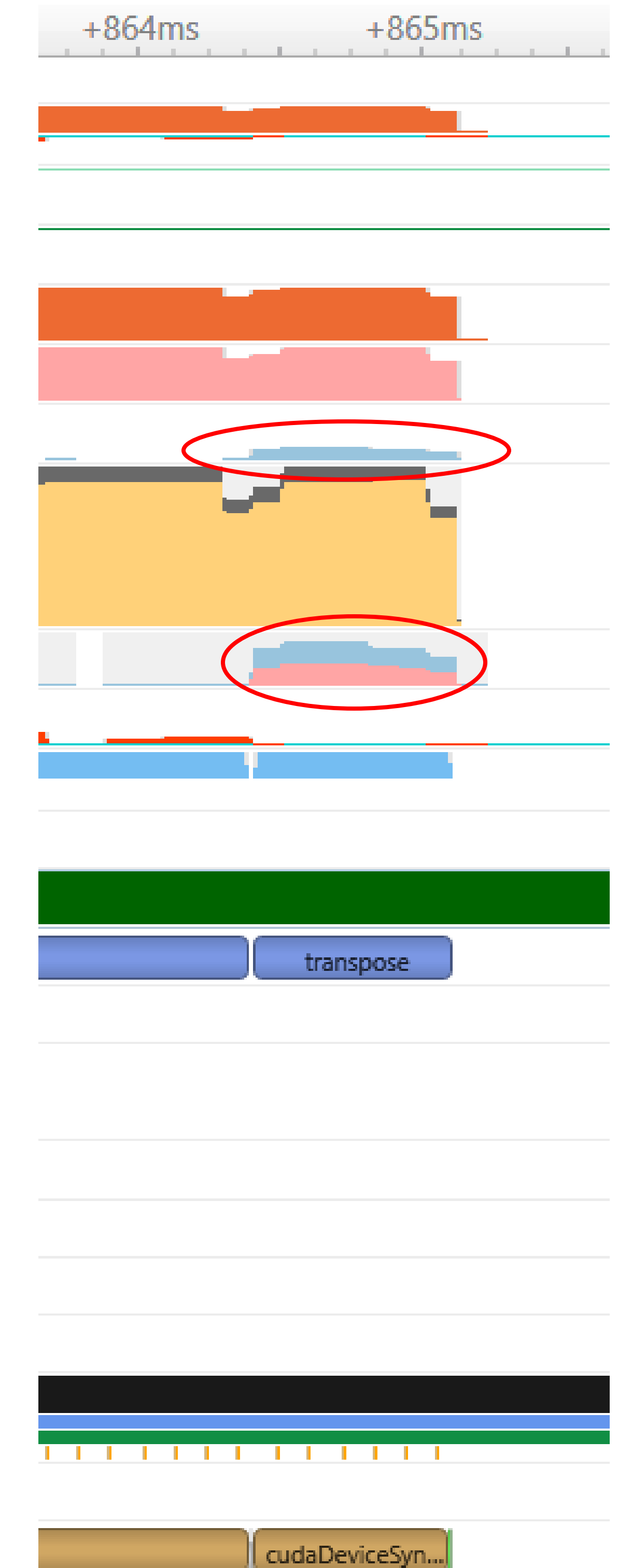
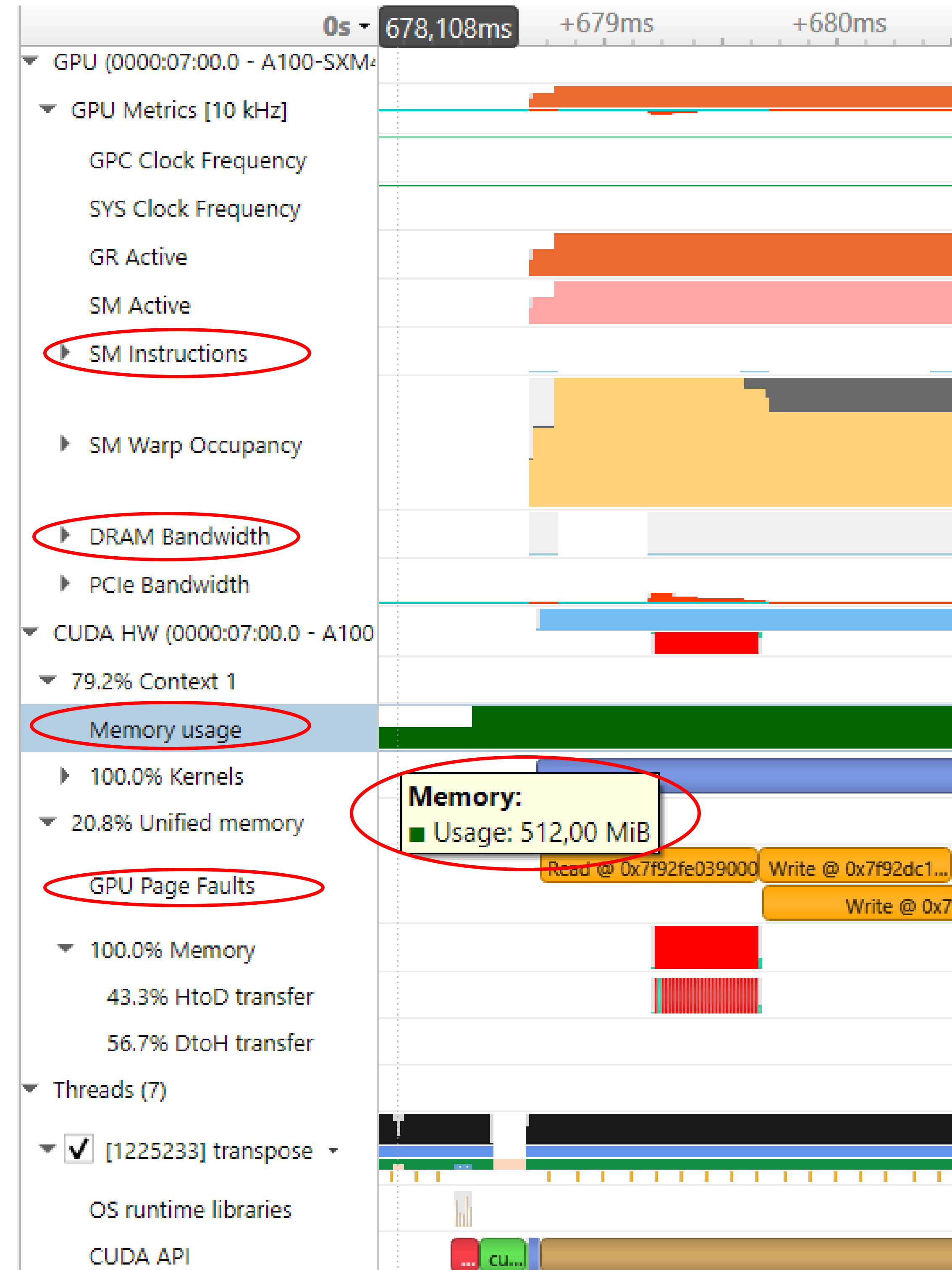




# GPU Metrics in Nsight Systems

...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

Untitled 8 \* x

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

init [2,008 s]

cudaStreamCreateWithFlags

cudaHostAlloc

cudaHostAlloc

cudaF...

cudaF...

sin...

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

Events View

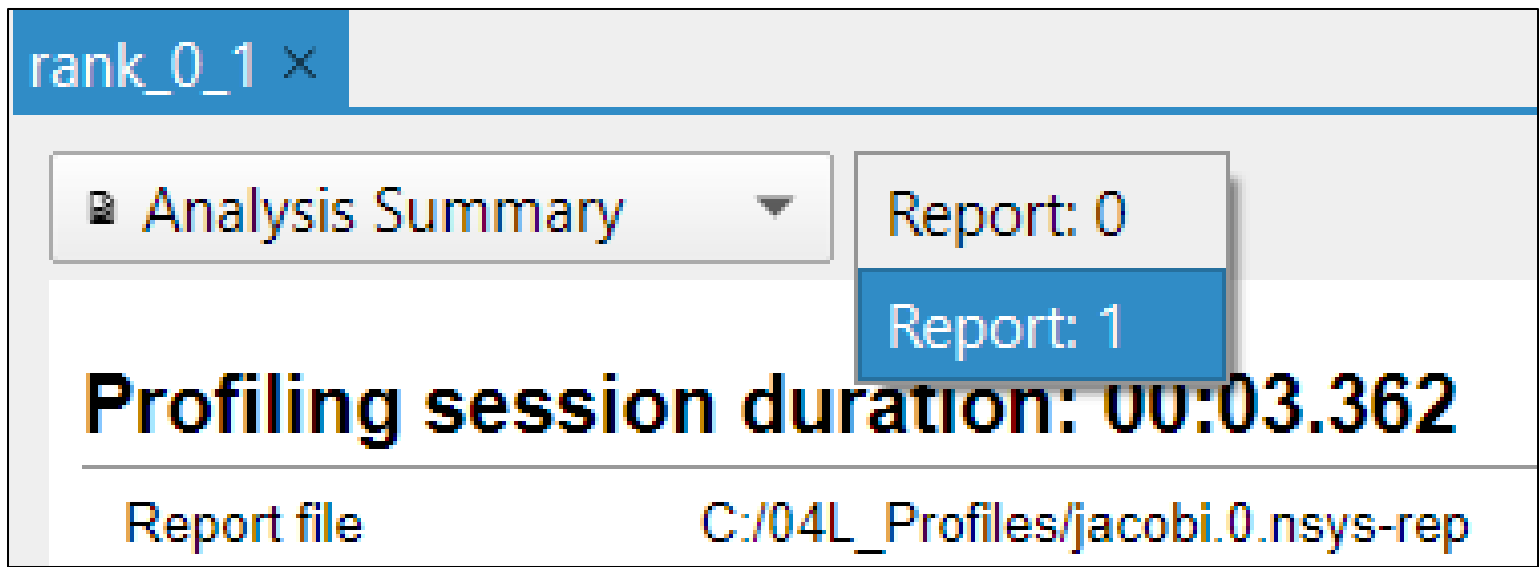
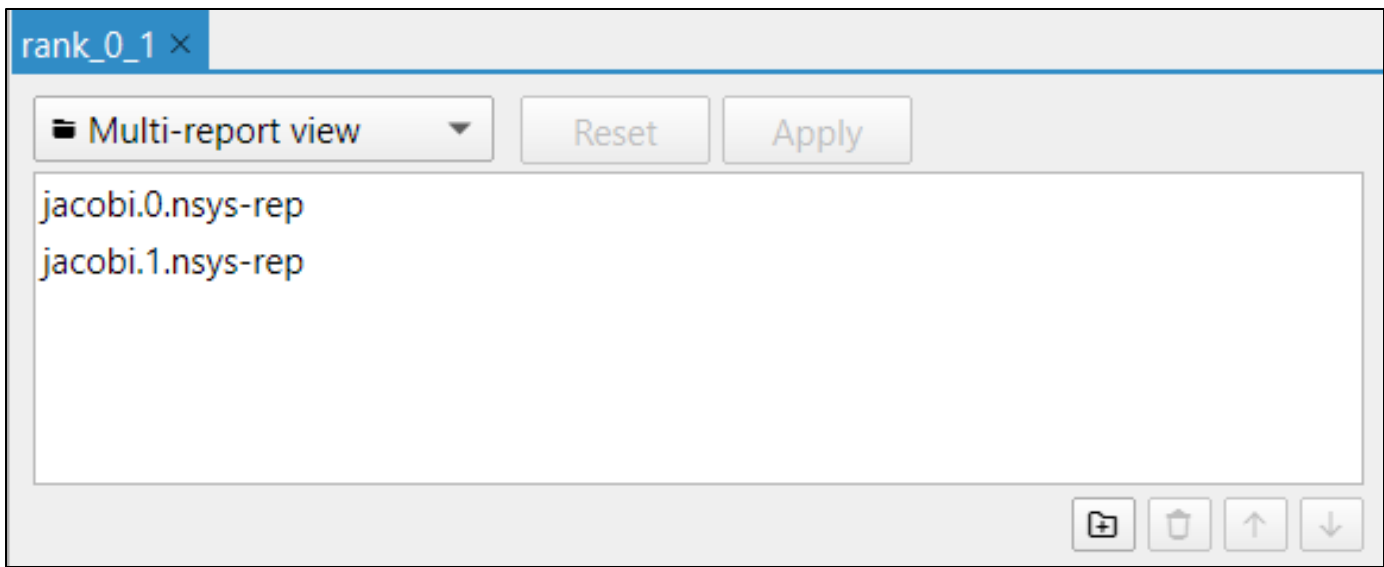
Name

Description:



# 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

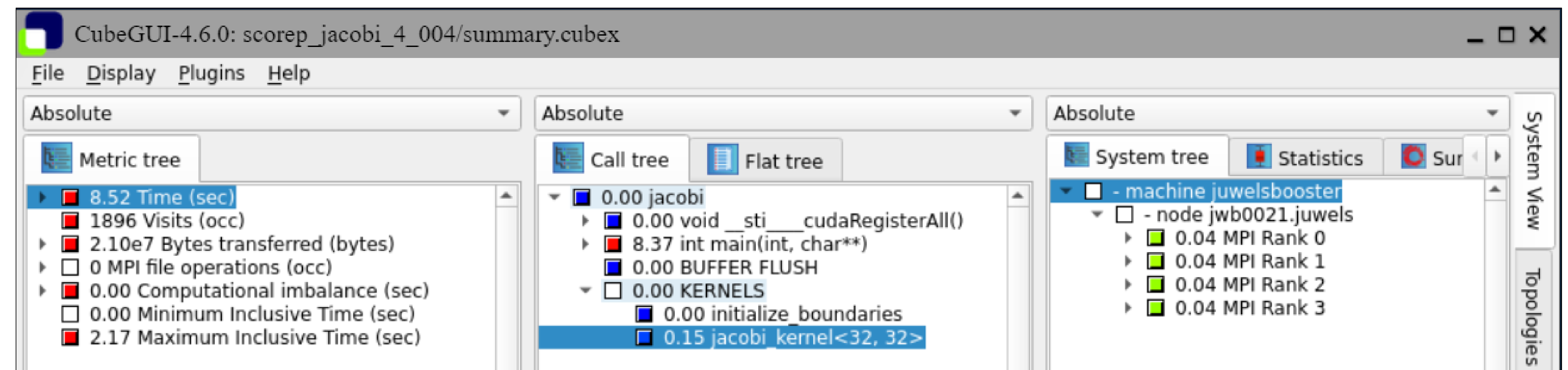
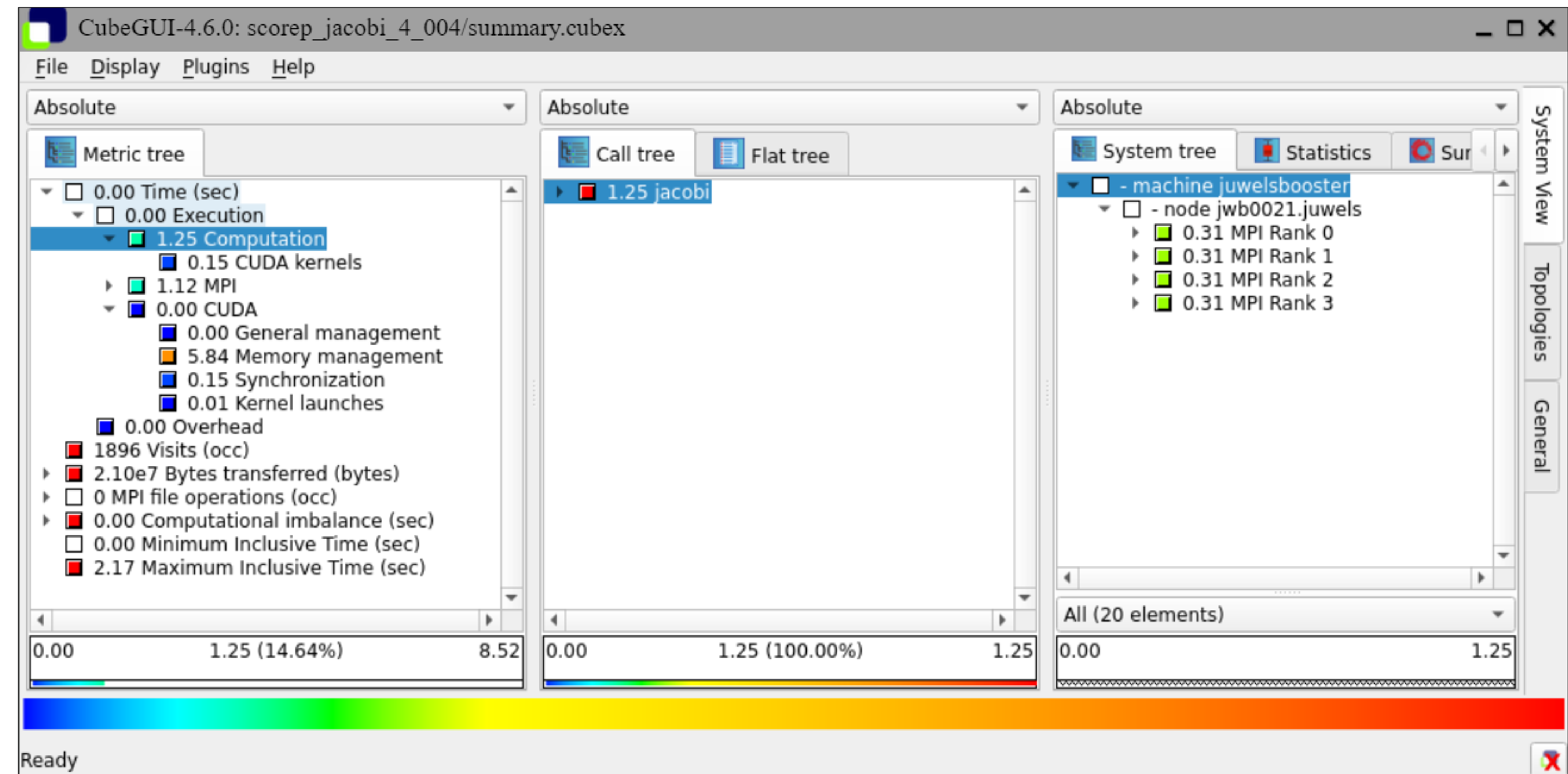
Specialized for large-scale distributed analysis

- 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

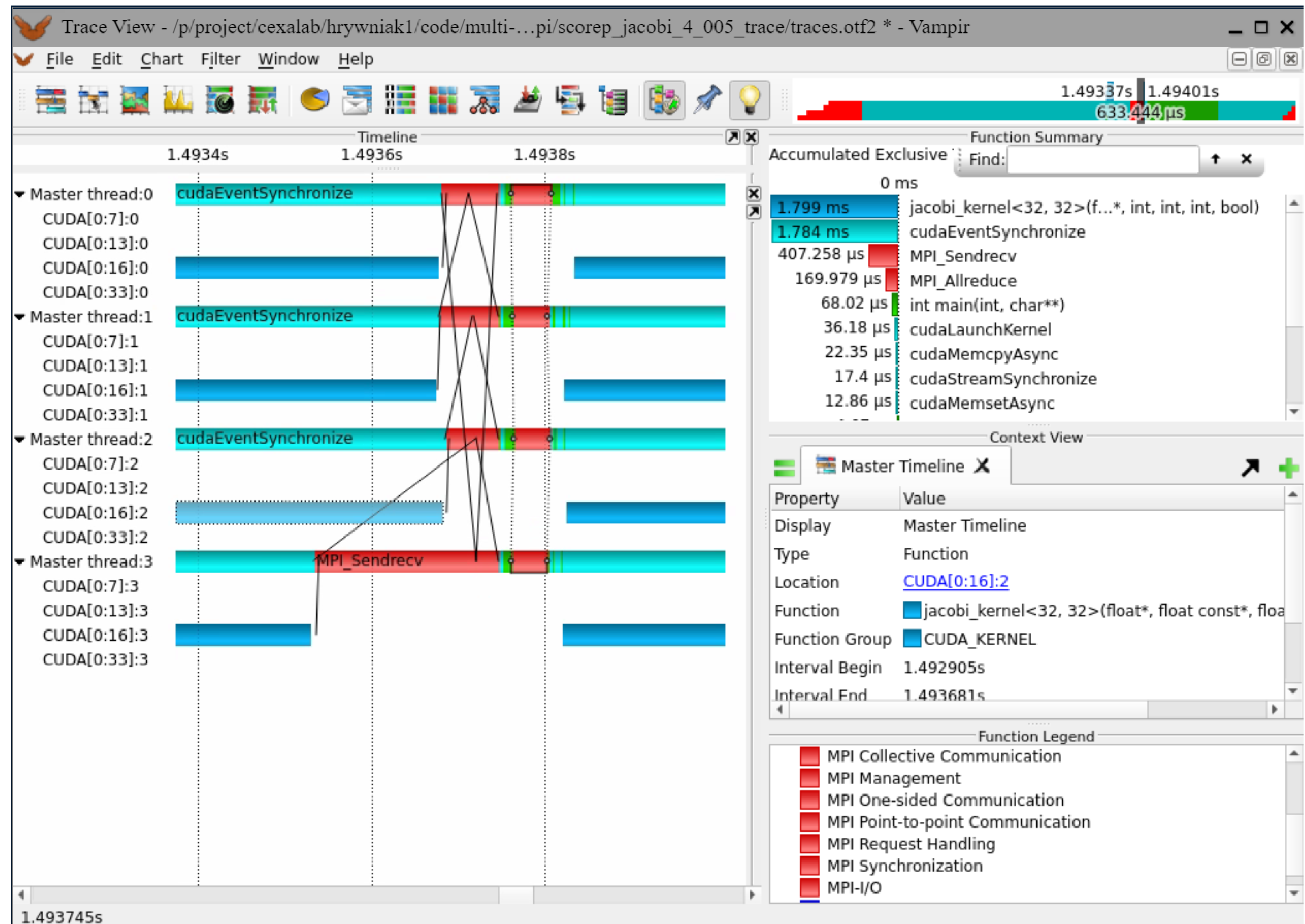
- Breakdown of different metrics across functions and processes
- Left-to-right: Selection influences breakdown
- Expanding changes inclusive/exclusive
- Example analysis:
  - Detect computational imbalance
- <https://scalasca.org/>





# 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](https://github.com/openhackathons-org/nways_accelerated_programming)



