PERFORMANCE AND DEBUGGING TOOLS

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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 errrors
- Other issues: Manual debugging
  - *cuda-gdb*: Command-line debugger, GPU extensions

NVCC compile flags for debugging	
`-g`	Embed symbol info for ***host*** code
`-lineinfo`	Generate line correlation info for ***device*** code
`-G`	Device debug – slow

COMPUTE-SANITIZER

Functional correctness checking suite for GPU

- `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

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, ...)
- `%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/static/media/mvapich/mvapich2-2.2-userguide.html#x1-32100013
https://slurm.schedmd.com/srun.html#SECTION_OUTPUT-ENVIRONMENT-VARIABLES

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]
0x000000000508ca80 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-coredump

EXAMPLE: OPENING A CORE DUMP

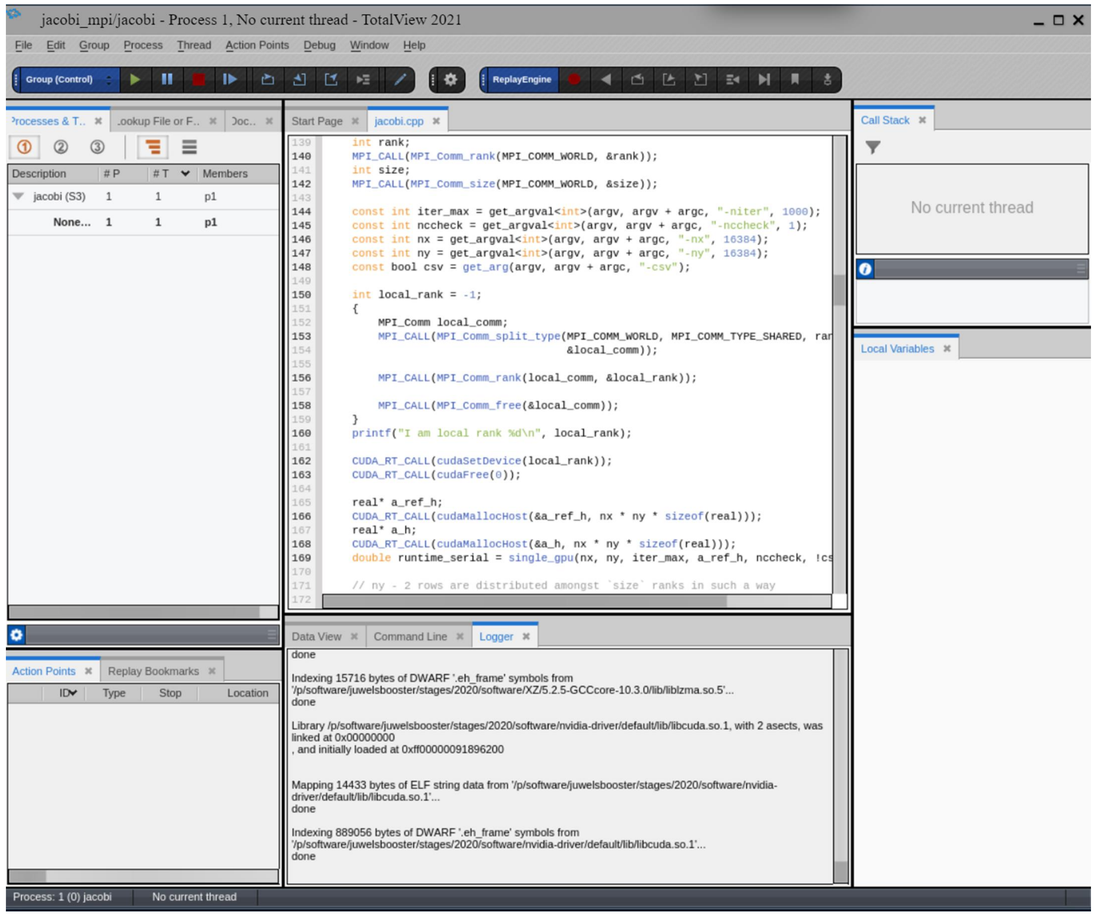
- Running and generating the core file

```
$ 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  0x00000000057e1ae0 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
- ARM DDT
- Perforce TotalView (screenshot)
  - Available as module on JSC systems

WRITE DEBUGGABLE SOFTWARE

A case for modularity, and proper test cases

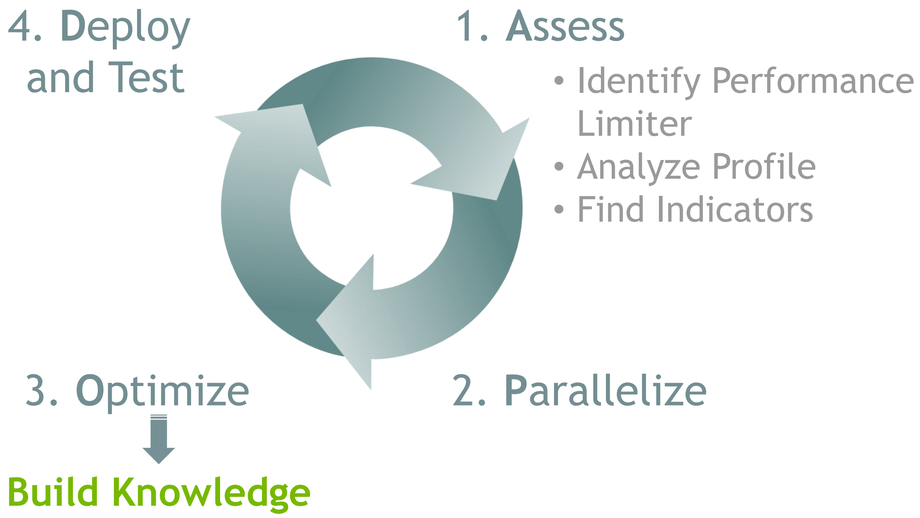
- Think about interfaces in your code: Which parts must depend on each other, etc.
  - Example: BLAS, linear algebra routines
- Think about structure and architecture („the big picture“)
- Don‘t go overboard: „I read this book, we need 100% test coverage“, etc.
  - For many research codes that would 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, but meta-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

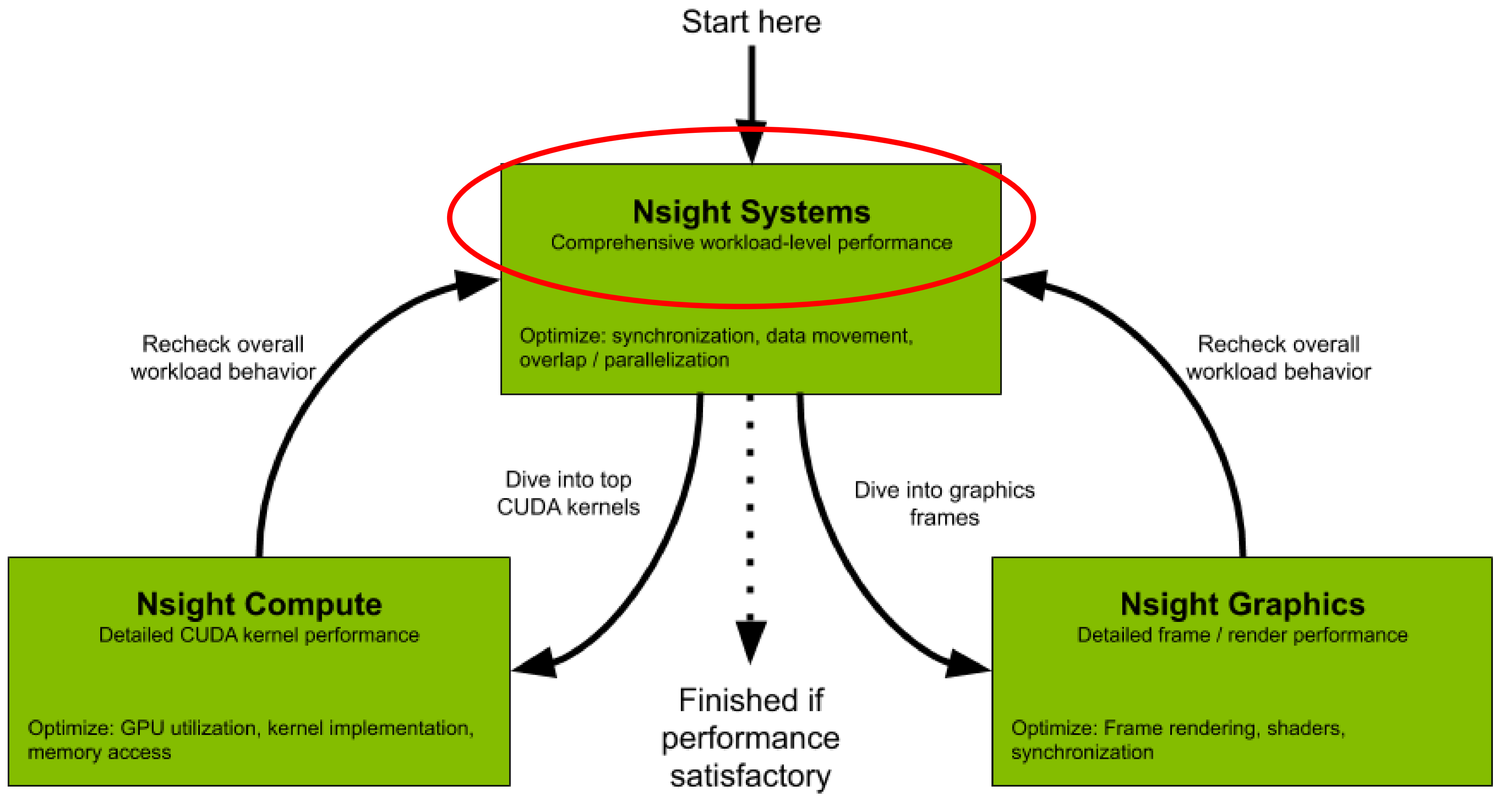
How the pieces fit together

- 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

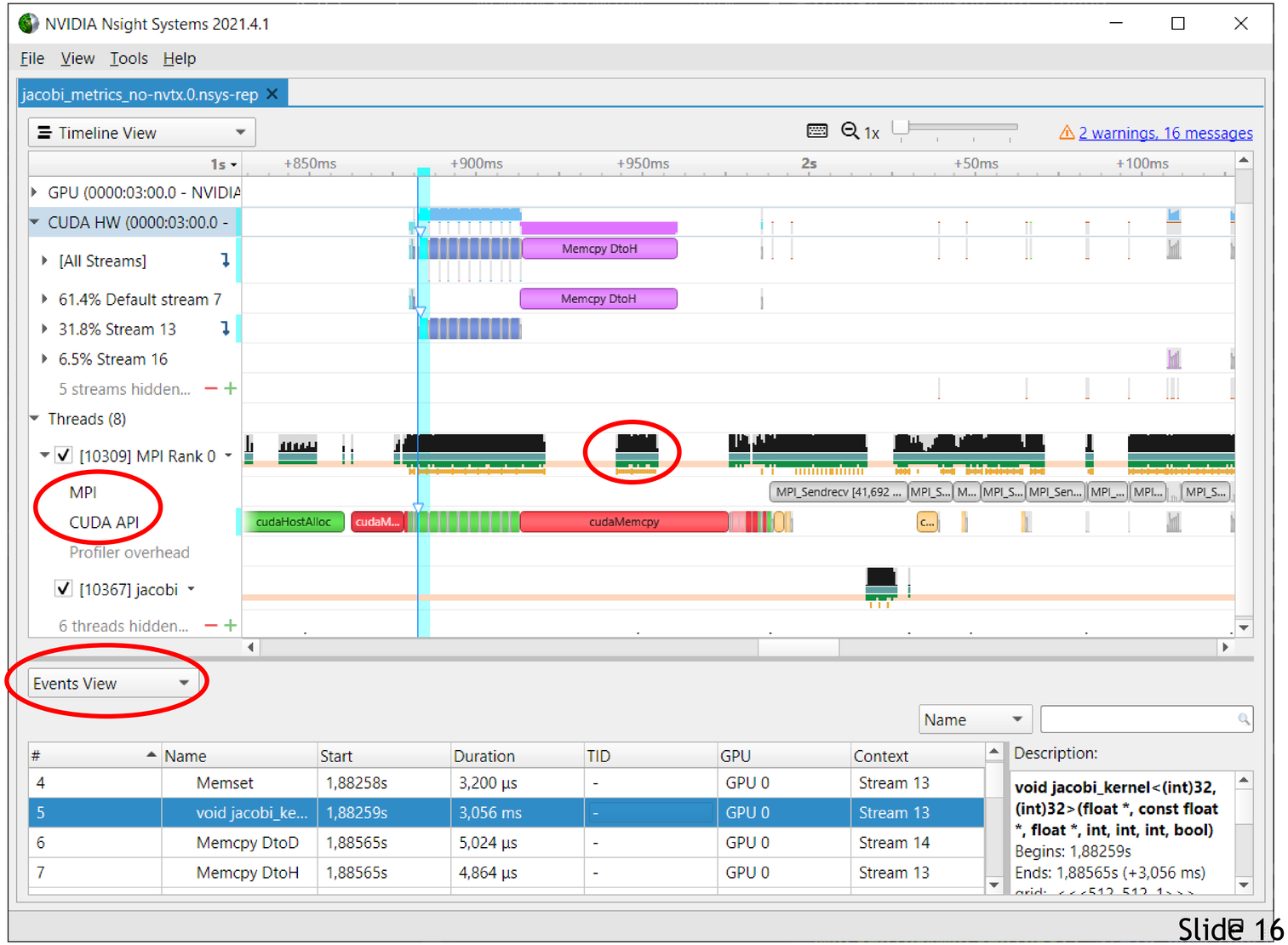
- Use the command line
  - `srun nsys profile --trace=cuda,nvtx,mpi --output=my_report.%q{SLURM_PROCID} ./jacobi -niter 10`
- Inspect results: Open the report file in the GUI
  - Also possible to get details on command line
  - Either add `--stats` to profile command line, or: `nsys stats --help`

- 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
```

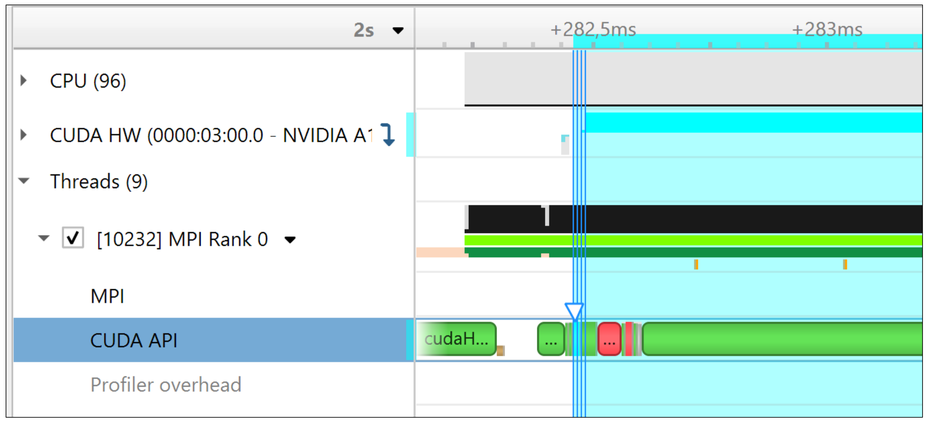
SYSTEM-LEVEL PROFILING WITH NSIGHT SYSTEMS

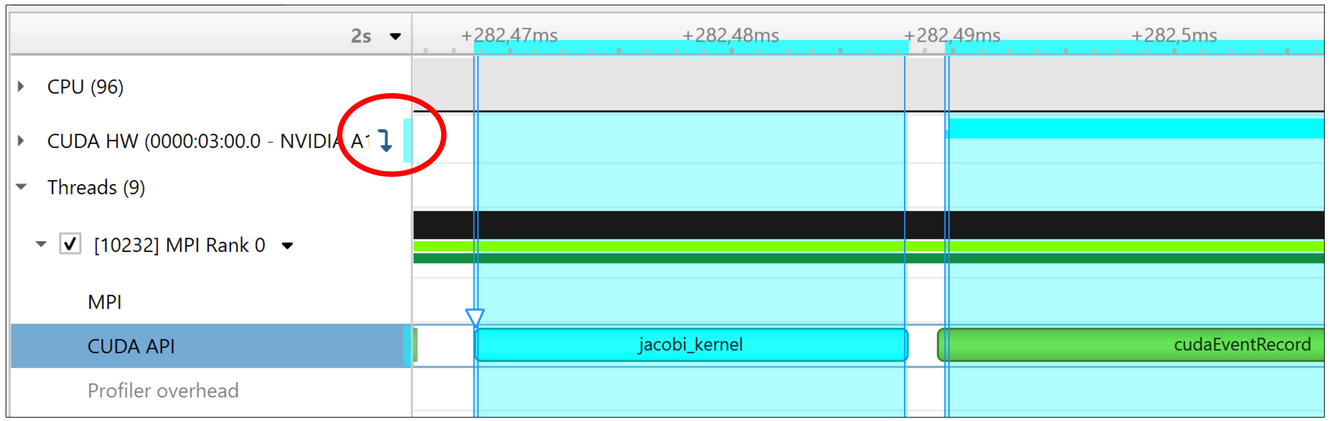
- Global timeline view
  - CUDA HW: streams, kernels, memory
- Different traces, e.g. CUDA, MPI
  - correlations API <-> HW
- Stack samples
  - bottom-up, top-down for CPU code
- GPU metrics
- Events View
  - Expert Systems
- looks at single process (tree)
  - correlate multi-process reports in single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

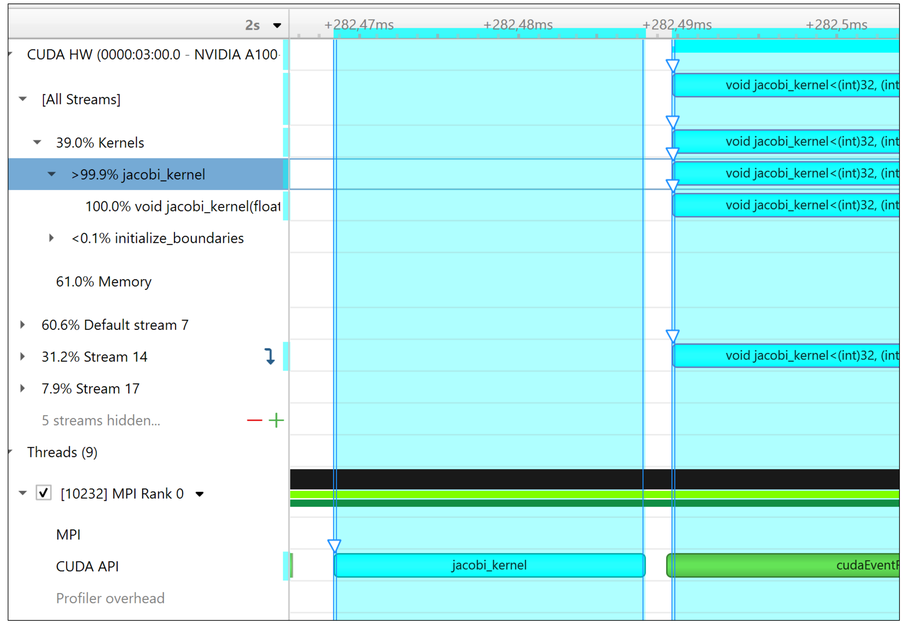


CORRELATING EVENTS ON THE TIMELINE

Selecting events in one row highlights related events

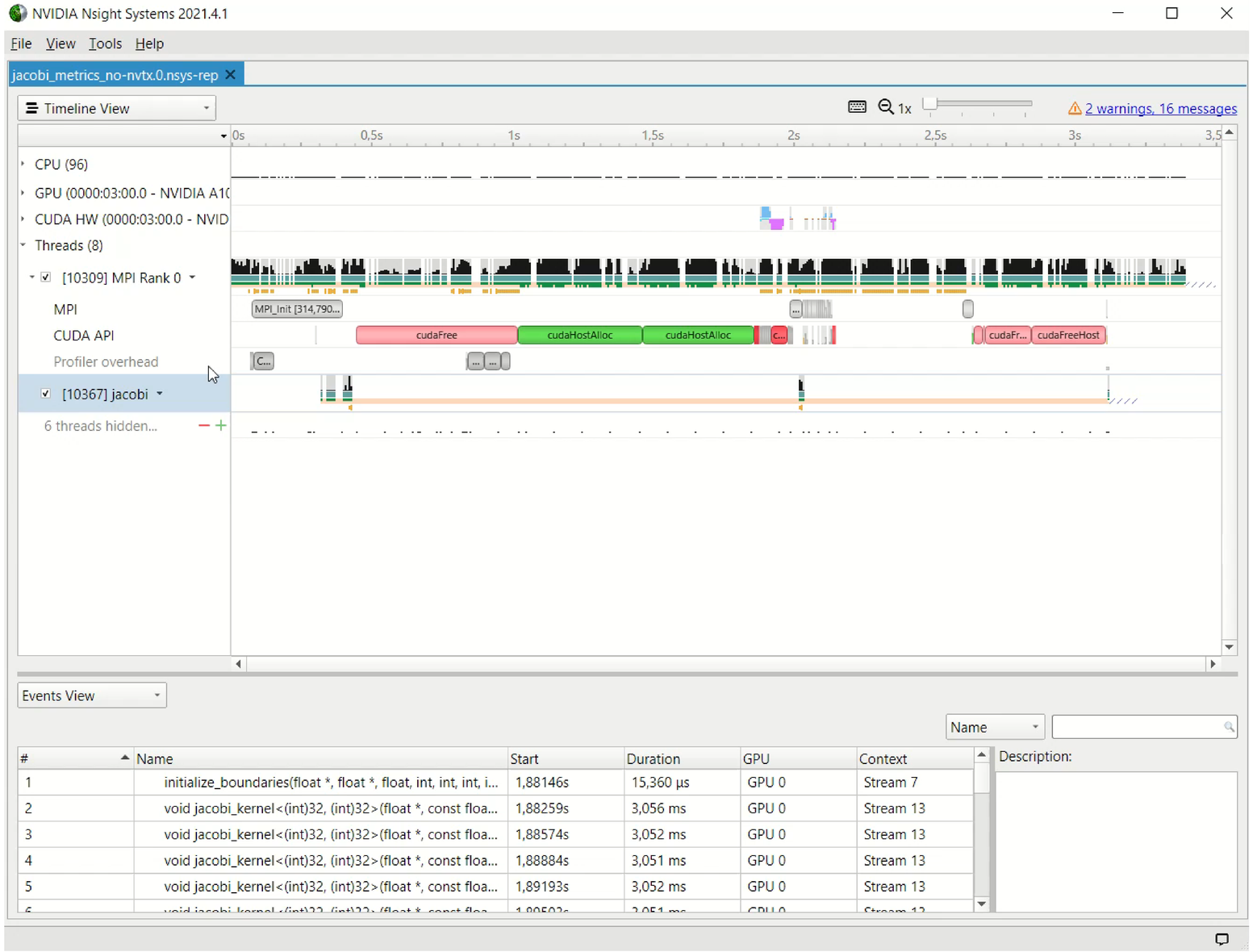






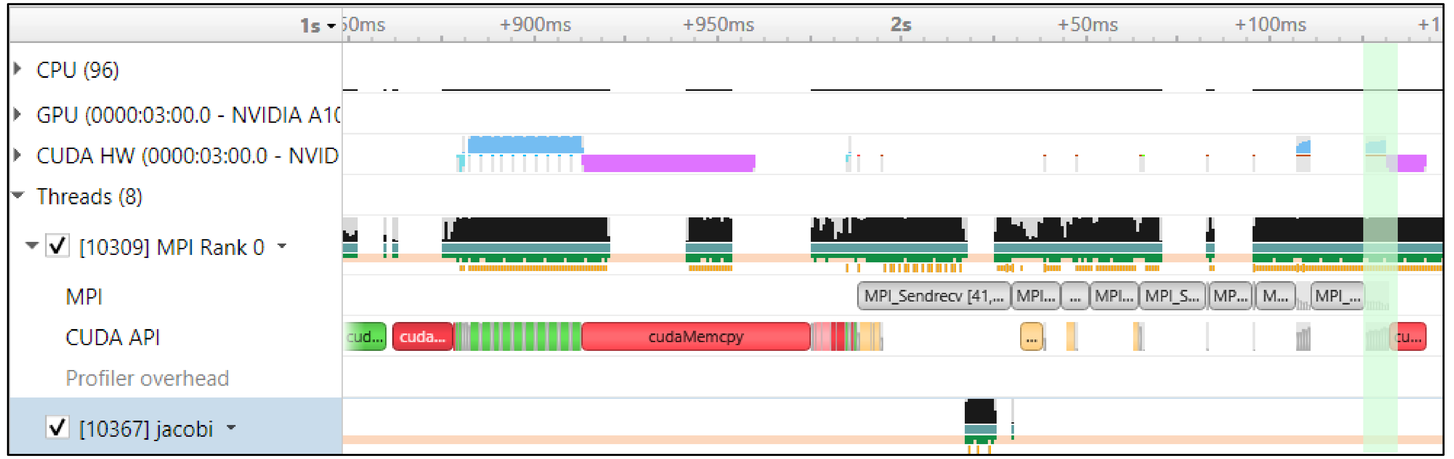
NSIGHT SYSTEMS BASIC WORKFLOW

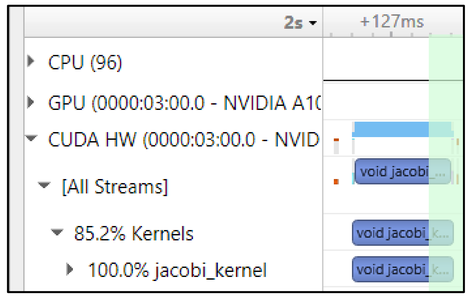
Navigating the timeline and finding interesting areas

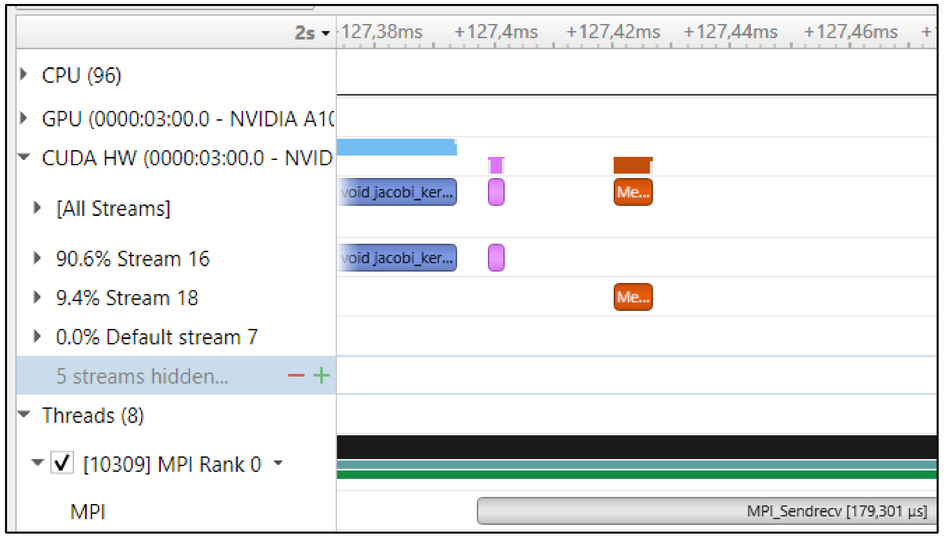


DISCOVERING OPTIMIZATION POTENTIAL

- 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?



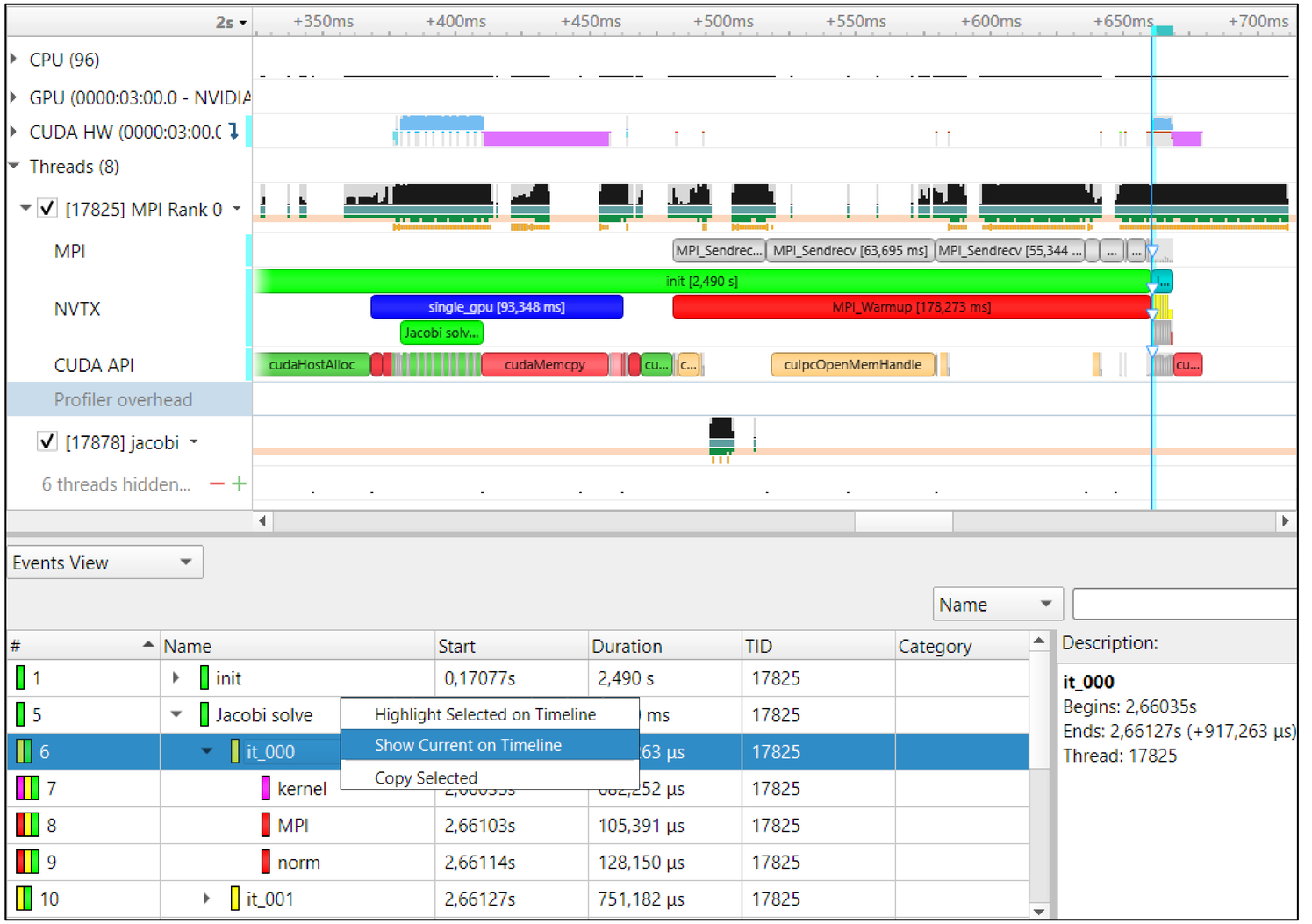




ADDING SOME COLOR

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 `-lnvhpcwrapnvtx`
  - 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
}
```

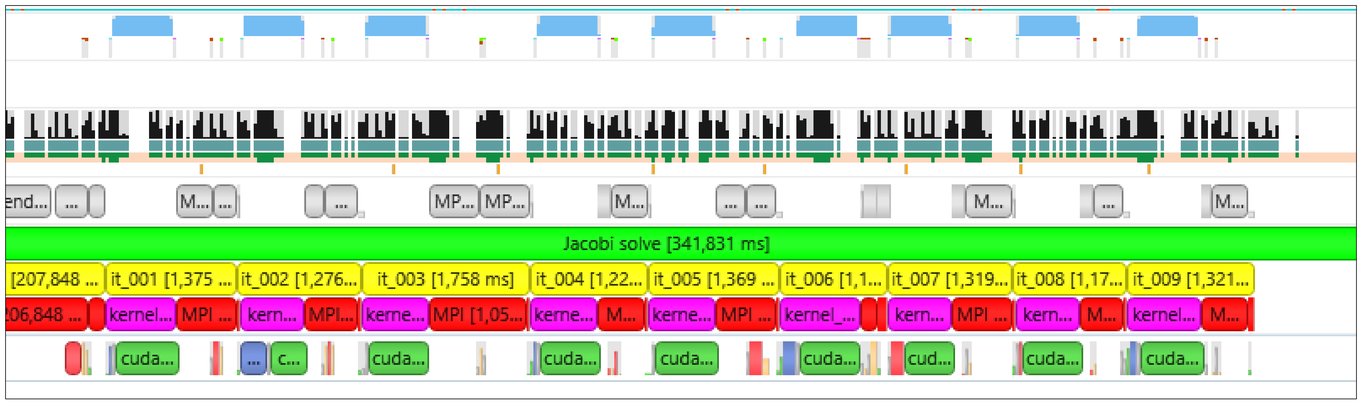
https://github.com/NVIDIA/NVTX and https://nvidia.github.io/NVTX/#how-do-i-use-nvtx-in-my-code

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

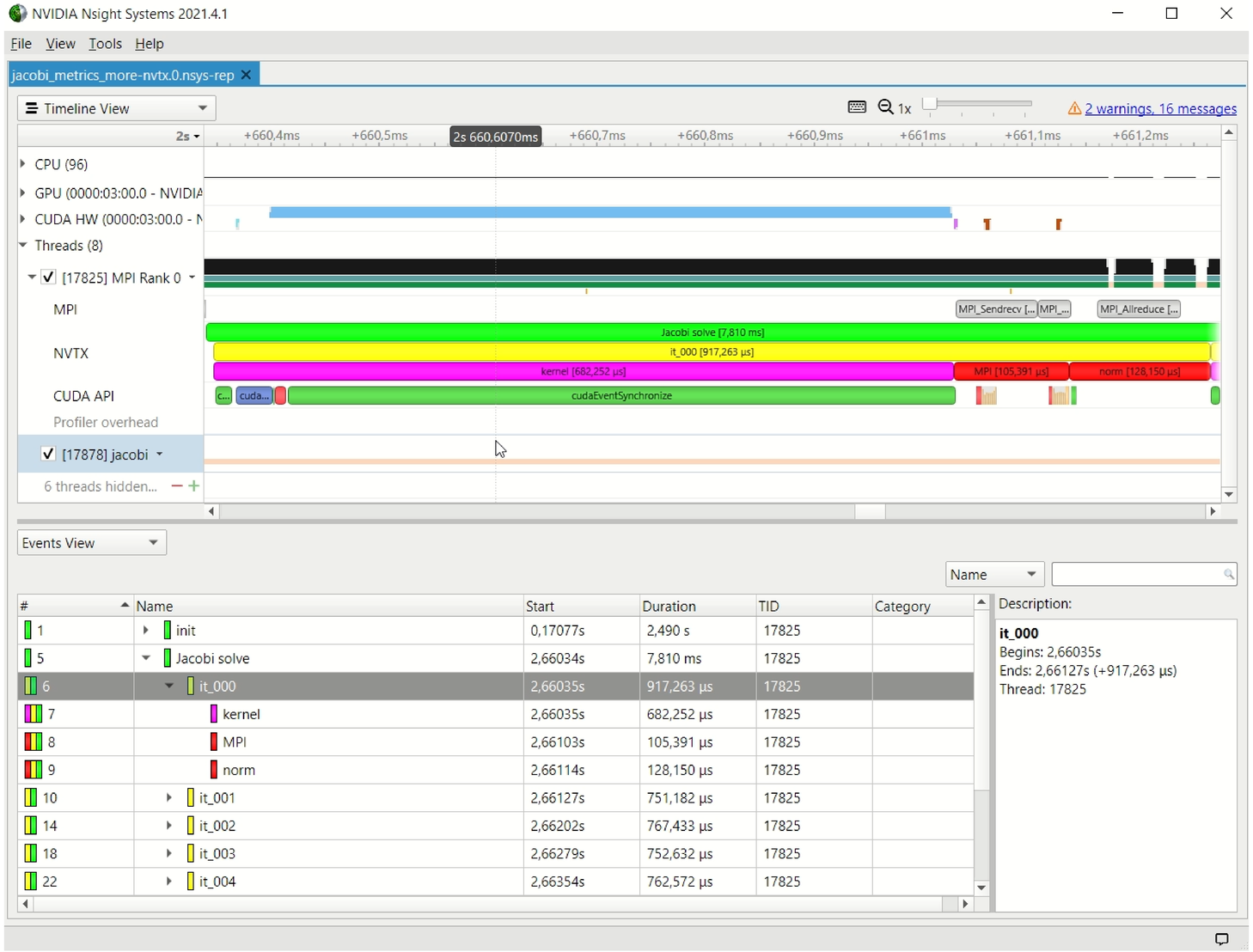
Shorter time, smaller files = quicker progress

- 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



#	Name	Start	Duration	TID	Category
1	init	0,17077s	2,490 s	17825	
5	Jacobi solve	2,66034s	7,810 ms	17825	
6	it_000	2,66035s	917,263 µs	17825	
7	kernel	2,66035s	682,252 µs	17825	
8	MPI	2,66103s	105,391 µs	17825	
9	norm	2,66114s	128,150 µs	17825	
10	it_001	2,66127s	751,182 µs	17825	
14	it_002	2,66202s	767,433 µs	17825	
18	it_003	2,66279s	752,632 µs	17825	
22	it_004	2,66354s	762,572 µs	17825	

GPU METRICS IN NSIGHT SYSTEMS

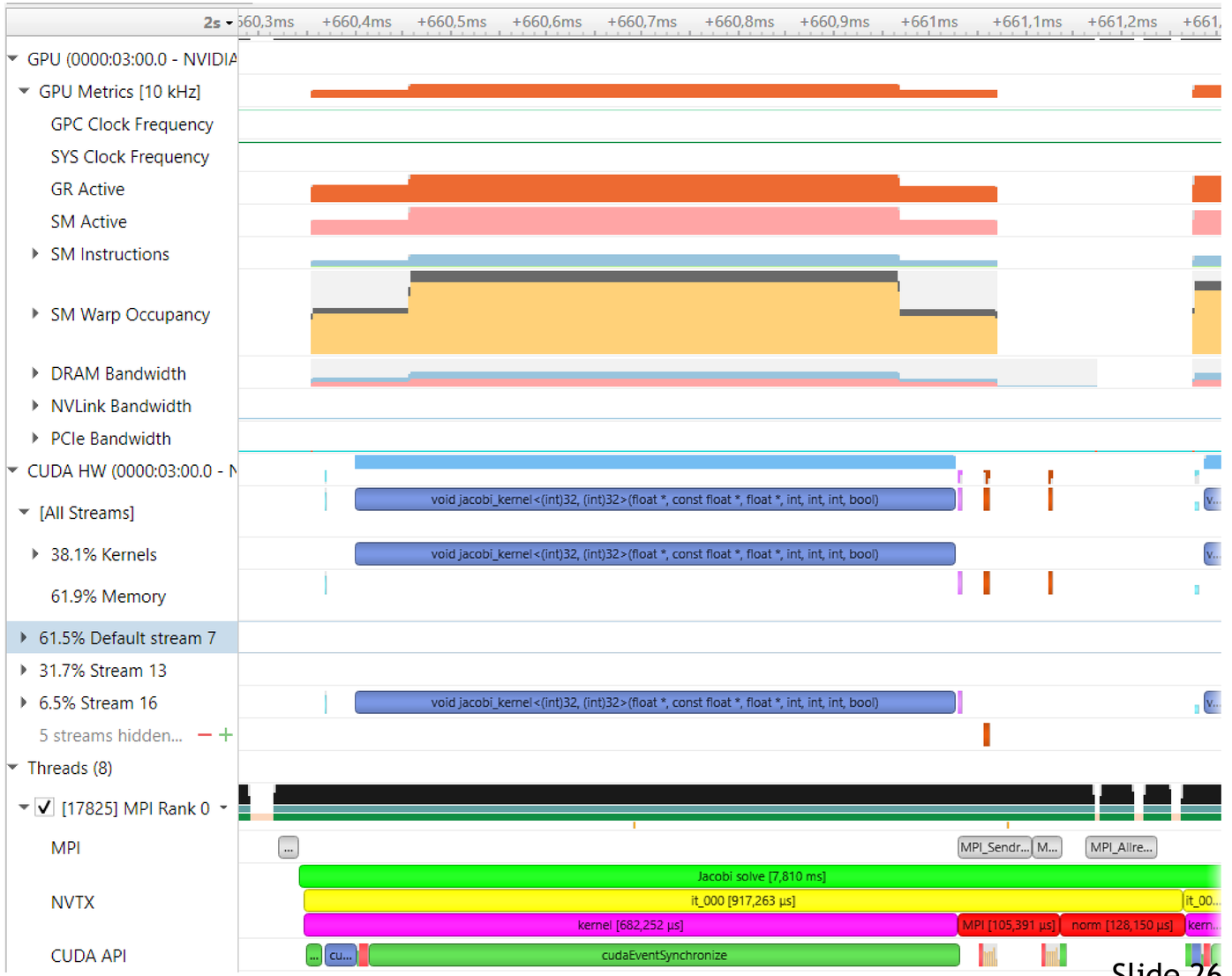
...and other traces you can activate

- Valuable low-overhead insight into HW usage:
  - SM instructions
  - DRAM Bandwidth, PCIe Bandwith (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`

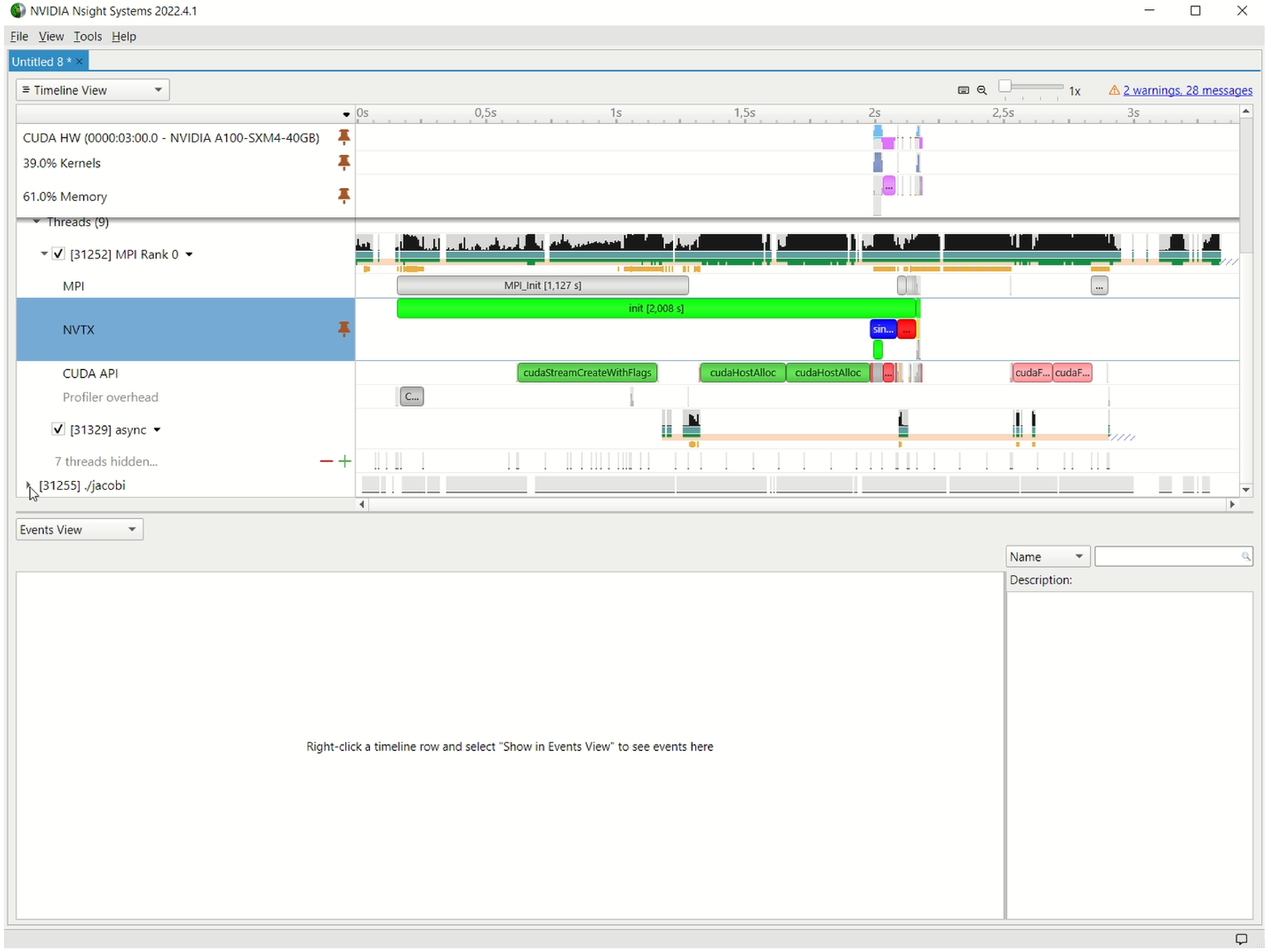
FOCUSING THE ANALYSIS

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

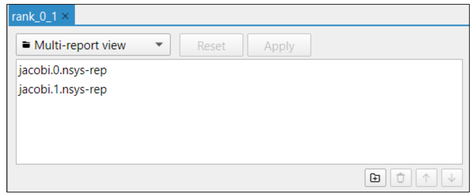


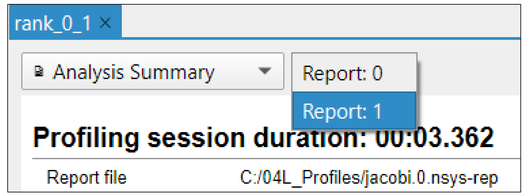
USING MULTIPLE REPORTS IN NSIGHT SYSTEMS

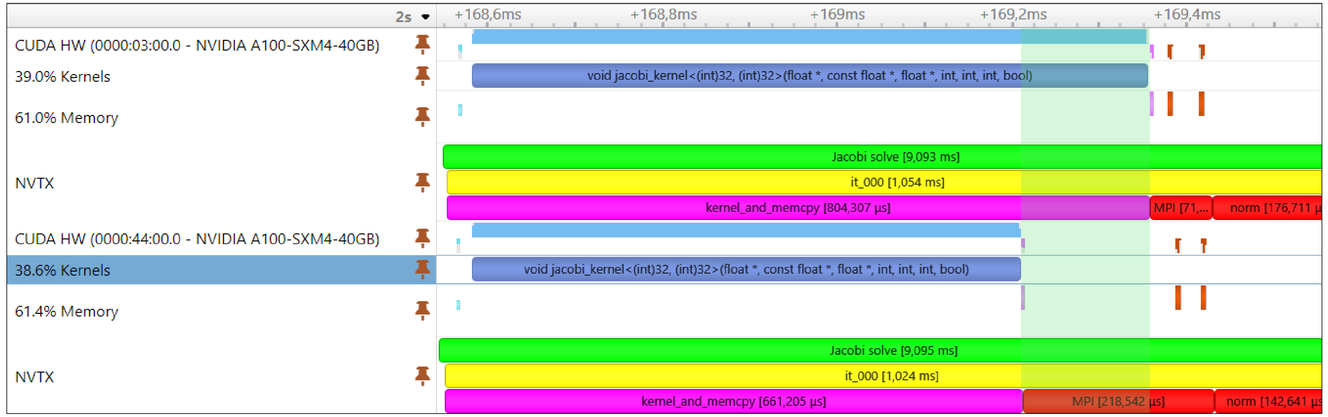


MULTI-PROCESS GPU ANALYSIS

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







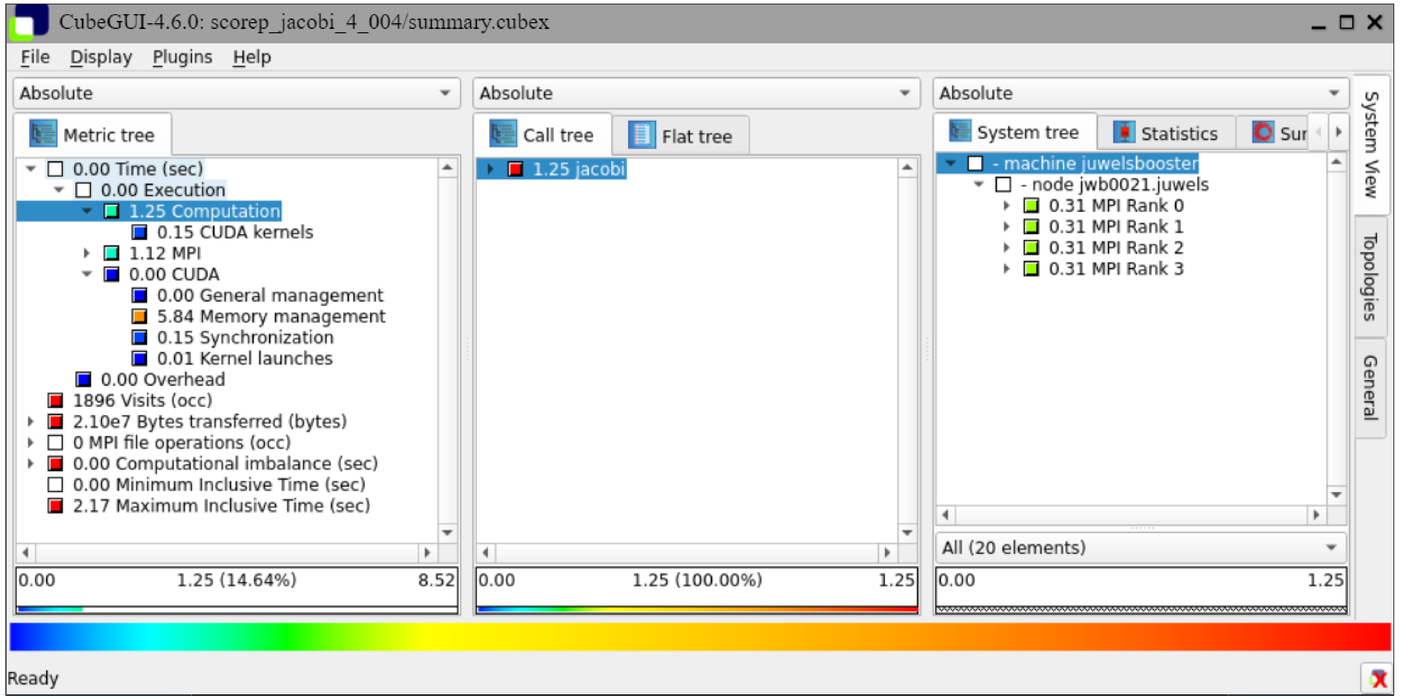
COMMUNITY PROFILING TOOLS

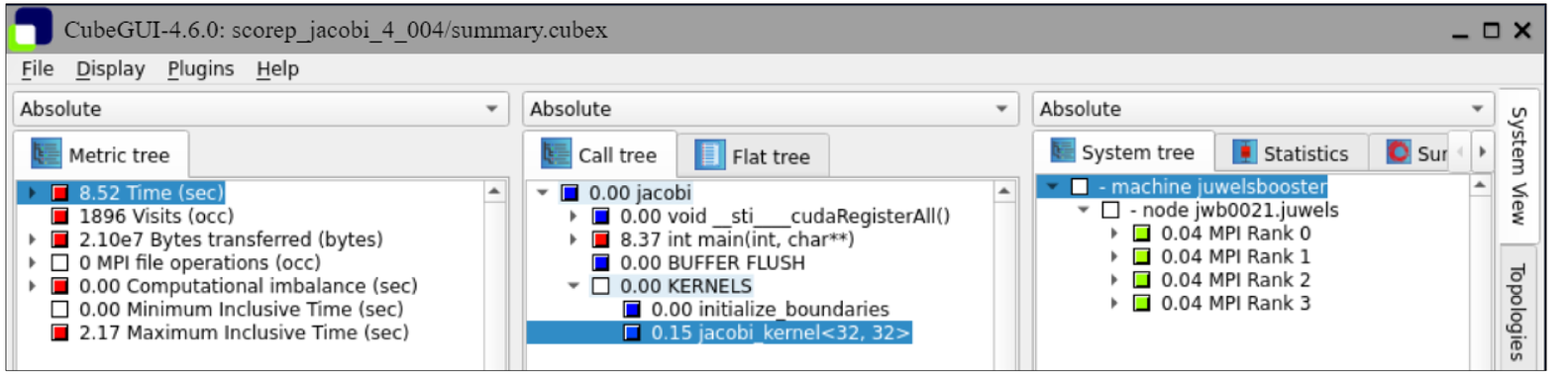
Specialized for large-scale distributed analysis

- 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/

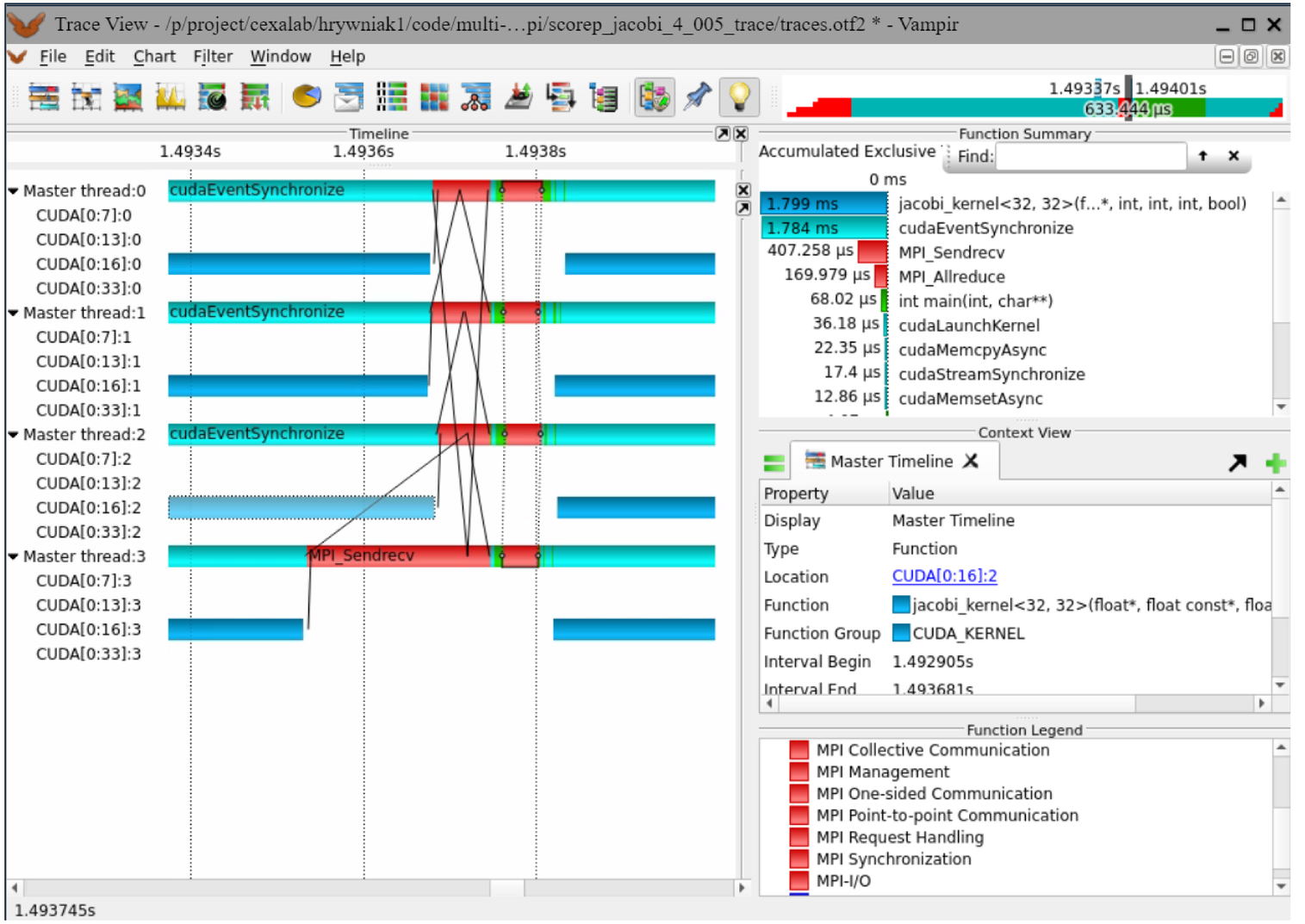




VAMPIR TRACE

- 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/

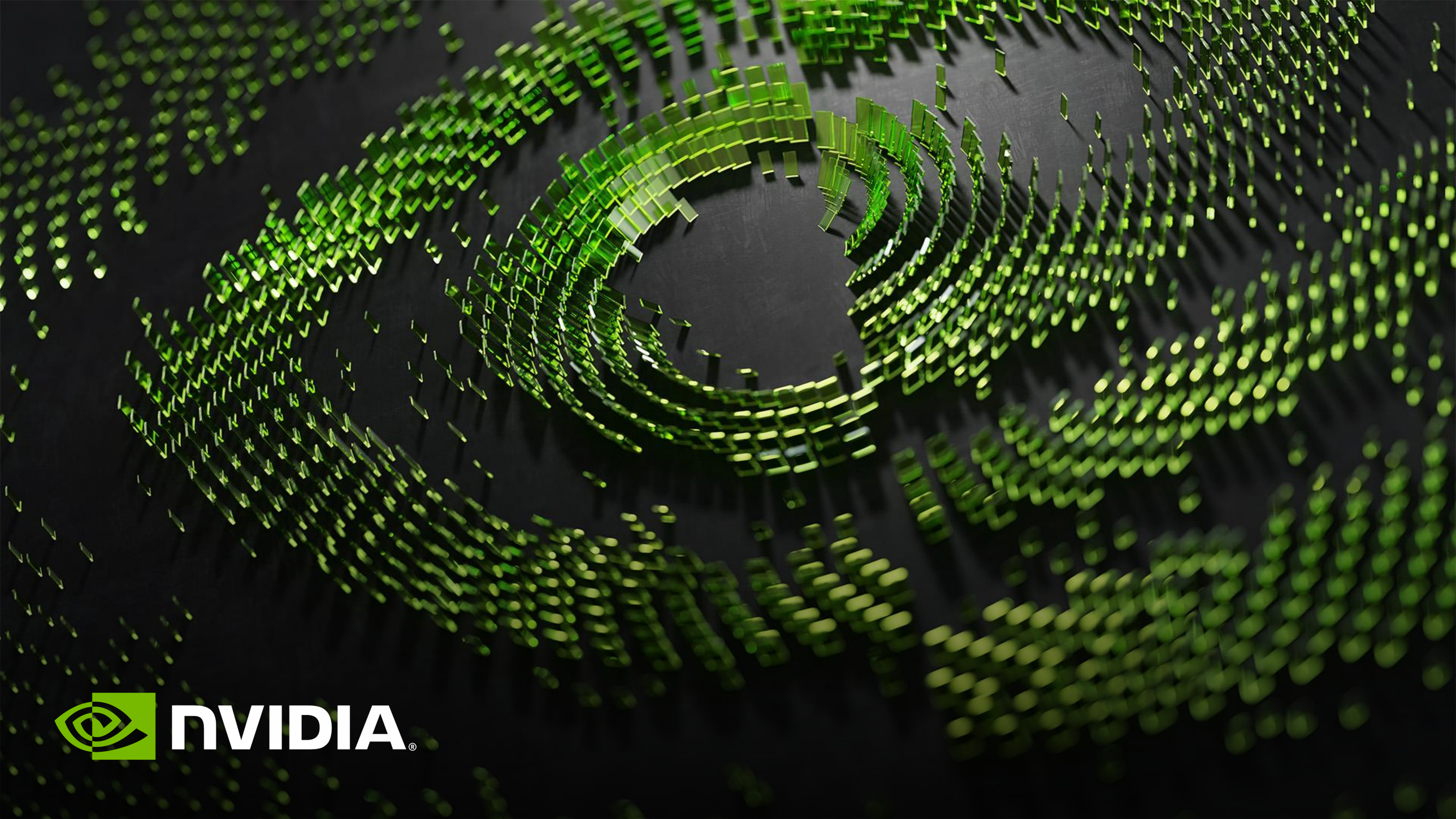


SUMMARY

- 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
- GTC labs from Nsight teams: https://github.com/NVIDIA/nsight-training
- GPU bootcamp material, e.g., https://github.com/gpuhackathons-org/gpubootcamp/tree/master/hpc/multi_gpu_nways


NVIDIA