VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

INTRODUCTION TO HIGH PERFORMANCE COMPUTING

PERFORMANCE ANALYSIS BASICS

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EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research, Development and Education

MINISTRY OF EDUCATION, YOUTH AND SPORTS

OUTLINE

Performance analysis and optimisation

- Motivation
- Hardware aspects
- Development process
- Best-practices

Performance tools and methodology

- Performance metrics
- CPU/GPU tools
- Live examples

POP CoE

Cray-1 supercomputer (source: wikipedia.org)

TECHNICAL NOTES

- All presented tools/examples can be accessed and reproduced at IT4I clusters **anytime**
- Please, setup your preferred GUI access:
  1. **VNC** - server on a Karolina login node + client on laptop
     - How to? https://docs.it4i.cz/general/accessing-the-clusters/graphical-user-interface/vnc/
     - Recommended client https://www.realvnc.com/en/connect/download/viewer/
  2. **OOD** - Open OnDemand GUI via web browser, **IT4I VPN required**
     - How to? https://docs.it4i.cz/general/accessing-the-clusters/graphical-user-interface/ood/
     - Connection link https://ood-karolina.it4i.cz/
  3. **X11** - Log in via terminal with X-Window system enabled
     - How to? https://docs.it4i.cz/general/accessing-the-clusters/graphical-user-interface/x-window-system/
     - Usually worse UX for GUI apps due to network latency
- Most of the presented tools provide a **remote profiling**, e.g., generate output remotely from CLI while analysis can be done locally in GUI - not covered today

PERFORMANCE ANALYSIS

Who has any experience with a performance analysis tool?

- What was the tool?

Objectives today?

- Not to become an expert analyst
- Not to reach an incredible performance improvement of example codes

- Rather to get idea about the domain and introduce some tools

EFFICIENT USE OF HPC

What does it mean?

- To get the most performance out of your hardware
- The process is called **Performance Optimisation**

Why should I care about performance?

- Industry – achieve goals faster and **cheaper**
- Academia – do **more science**
  - The trend in grant competition (resource allocation) is to prove performance, scalability, etc.

KEY INGREDIENTS

Know your application

- What does it compute? (domain, methods, algorithms)
- How is it parallelized? (programming models)
- What final performance is expected? (HW limits)

Know your hardware

- What are the target machines and how many? (laptop, workstation, cluster)
- Machine-specific optimisations?

Know your tools

- Strengths and weaknesses of each tool? (easy-to-use vs detailed information)
- Learn how to use them (examples with problems/patterns)

Know your process

- Constant learning

Apply the knowledge!

HARDWARE ASPECTS OF PERFORMANCE

Filesystem

- I/O operations

Network

- internode communication

Memory subsystem

- NUMA effect

CPU cores

- thread/process affinity, pinning, caches

Vector registers

- vectorization, vector instructions

Accelerators

- GPU/MIC utilization, host-device data transfers

GET READY

Connect to login node via GUI

```
salloc --account=DD-23-116 --reservation=dd-23-116_2024-06-05T09:00:00_2024-06-05T12:30:00_5_qgpu
```

Submit an interactive job

```
salloc --account=DD-23-116 --reservation=dd-23-116_2024-06-05T09:00:00_2024-06-05T12:30:00_5_qgpu
```

BASIC TOOLS

Useful to get familiar with the machine

`cat /proc/cpuinfo`

- processor : 71 -> 72 logical processors per node
- cpu cores : 18 -> 18 physical cores per socket
- siblings : 36 -> 36 logical processors per socket
- -> 2 hyperthreads per core
- -> 2 sockets per node

`cpuinfo` # Intel MPI utility

`cat /proc/meminfo`

- MemTotal: 196510848 kB -> 187 GB

BASIC TOOLS

Use HTOP tool for interactive jobs

`htop -d 5` # delay 0.5s

- Configurable (e.g. core id, threads, process tree)

```
  1  [|||||||||||||100.0%]   10 [|||||||||||||100.0%]   19 [|||||||||||||100.0%]   28 [|||||||||||||100.0%]
  2  [|||||||||||||100.0%]   11 [|||||||||||||100.0%]   20 [|||||||||||||100.0%]   29 [|||||||||||||100.0%]
  3  [|||||||||||||100.0%]   12 [|||||||||||||100.0%]   21 [|||||||||||||100.0%]   30 [|||||||||||||100.0%]
  4  [|||||||||||||100.0%]   13 [|||||||||||||100.0%]   22 [|||||||||||||100.0%]   31 [|||||||||||||100.0%]
  5  [|||||||||||||100.0%]   14 [|||||||||||||100.0%]   23 [|||||||||||||100.0%]   32 [|||||||||||||100.0%]
  6  [|||||||||||||100.0%]   15 [|||||||||||||100.0%]   24 [|||||||||||||100.0%]   33 [|||||||||||||100.0%]
  7  [|||||||||||||100.0%]   16 [|||||||||||||100.0%]   25 [|||||||||||||100.0%]   34 [|||||||||||||100.0%]
  8  [|||||||||||||100.0%]   17 [|||||||||||||100.0%]   26 [|||||||||||||100.0%]   35 [|||||||||||||100.0%]
  9  [|||||||||||||100.0%]   18 [|||||||||||||100.0%]   27 [|||||||||||||100.0%]   36 [|||||||||||||100.0%]
  Mem[|||||                              13.8G/187G]   Tasks: 79, 346 thr; 36 running
  Swp[                                        0K/0K]   Load average: 23.62 6.93 3.32
                                                       Uptime: 15 days, 12:06:32

  PID USER      PRI  NI  VIRT   RES   SHR S CPU% MEM%   TIME+  Command
11171 vav0038    35  15  296M 90236  7232 R 99.5  0.0  1:02.72 ../examples/wave_c 100
11203 vav0038    35  15  298M 90240  7244 R 99.5  0.0  1:03.07 ../examples/wave_c 100
11212 vav0038    35  15  322M 92280  7324 R 99.5  0.0  1:03.04 ../examples/wave_c 100
11162 vav0038    35  15  300M 90220  7272 R 99.5  0.0  1:03.10 ../examples/wave_c 100
11188 vav0038    35  15  323M 90236  7328 R 99.5  0.0  1:03.05 ../examples/wave_c 100
11207 vav0038    35  15  311M 92272  7296 R 99.5  0.0  1:03.04 ../examples/wave_c 100
11164 vav0038    35  15  326M 90232  7340 R 99.5  0.0  1:03.09 ../examples/wave_c 100
11195 vav0038    35  15  298M 90232  7232 R 99.5  0.0  1:03.09 ../examples/wave_c 100
11158 vav0038    35  15  319M 92284  7304 R 99.5  0.0  1:03.07 ../examples/wave_c 100
F1Help  F2Setup F3SearchF4FilterF5Tree  F6SortByF7Nice -F8Nice +F9Kill  F10Quit
```

BASIC TOOLS

nvidia-smi

PERFORMANCE-AWARE DEVELOPMENT PROCESS

1. Develop correct functionality (testing helps)
2. Identify bottlenecks (performance limiters) using performance tools
3. Optimise bottlenecks until satisfied
    1. Build a hypothesis (ask a question)
    2. Explain the behavior (answer the question)
    3. Change the code (double-check correct functionality)
    4. Verify optimisations using profiling tools
4. Repeat until job done

OPTIMISATION TIPS

- Do not optimise your code prematurely!
- Focus on main computational time-consuming phases (hotspots), omit preprocessing/postprocessing phases
- The 80/20 rule:
  - Programs typically spend 80% of their time in 20% of the code
  - Programmers typically spend 20% of their effort to get 80% of the total speedup possible for the application
- Keep track of your optimisation progress over time
- Always use compute nodes for profiling (not login nodes - shared)
- **Use SW libraries**

SOFTWARE LIBRARIES

General-purpose math libraries

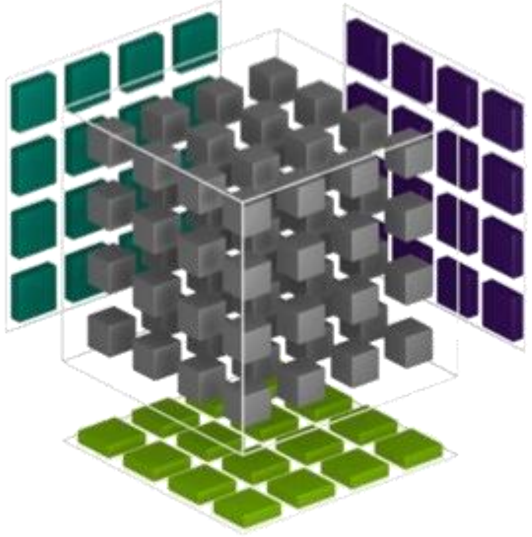
- BLAS (MKL, OpenBLAS, ATLAS, cuBLAS, ...)
- LAPACK (MKL, OpenBLAS, ATLAS, cuSolver, ...)
- FFT (MKL, cuFFT, ...)
- ...

Domain-specific libraries

- Chemistry, Bio, Geo, Physics, CAE, Big data, ML/DL

HW-specific libraries

- GPU/MIC, Intel/AMD/IBM



Optimized implementation

- Usually much better performance than a custom code
- Do NOT reinvent a wheel!
- (But avoid overkill)

PERFORMANCE METRICS

Execution time (time, time.h, ...)

- real 0m10.245s (elapsed real time)
- user 0m19.890s (user CPU time using OMP_NUM_THREADS=2)
- sys 0m0.285s (system CPU time)

Processor speed (flop/s) and Memory throughput (GB/s)

- Calculated operations per time (e.g. c = a + b + c -> 2 operations)
- Transferred bytes per time (e.g. c = a + b + c -> 3 RD + 1 WR * 8 bytes)

Speedup and Efficiency

- $S_P = T_1 / T_P$
- $E_P = S_P / P$

Scalability

- Strong vs weak scaling

Others: portability, programming ability, etc.

PEAK PERFORMANCE EXAMPLE

- The theoretical HW limits, e.g. AMD EPYC 7H12 (Rome)

Processor speed:

Number of compute nodes (Karolina-size machine)	720
Number of sockets (CPUs) per node	2
Frequency	2.6 GHz
Number of cores per socket	64
FMA instructions (**a** * **b** + **c**)	2
FMA units per core	2
SIMD (AVX2 256b) = 4x double precision	4
	3 833 856 Gflop/s
	3.8 Pflop/s
	(2.6 Tflop/s per socket)

PEAK PERFORMANCE EXAMPLE

Memory bandwidth:

- Number of compute nodes (Karolina-size machine) 720
- Number of sockets (CPUs) per node 2
- # channels per socket 8
- DDR4 bus width 8 B
- Frequency 3200 MT/s

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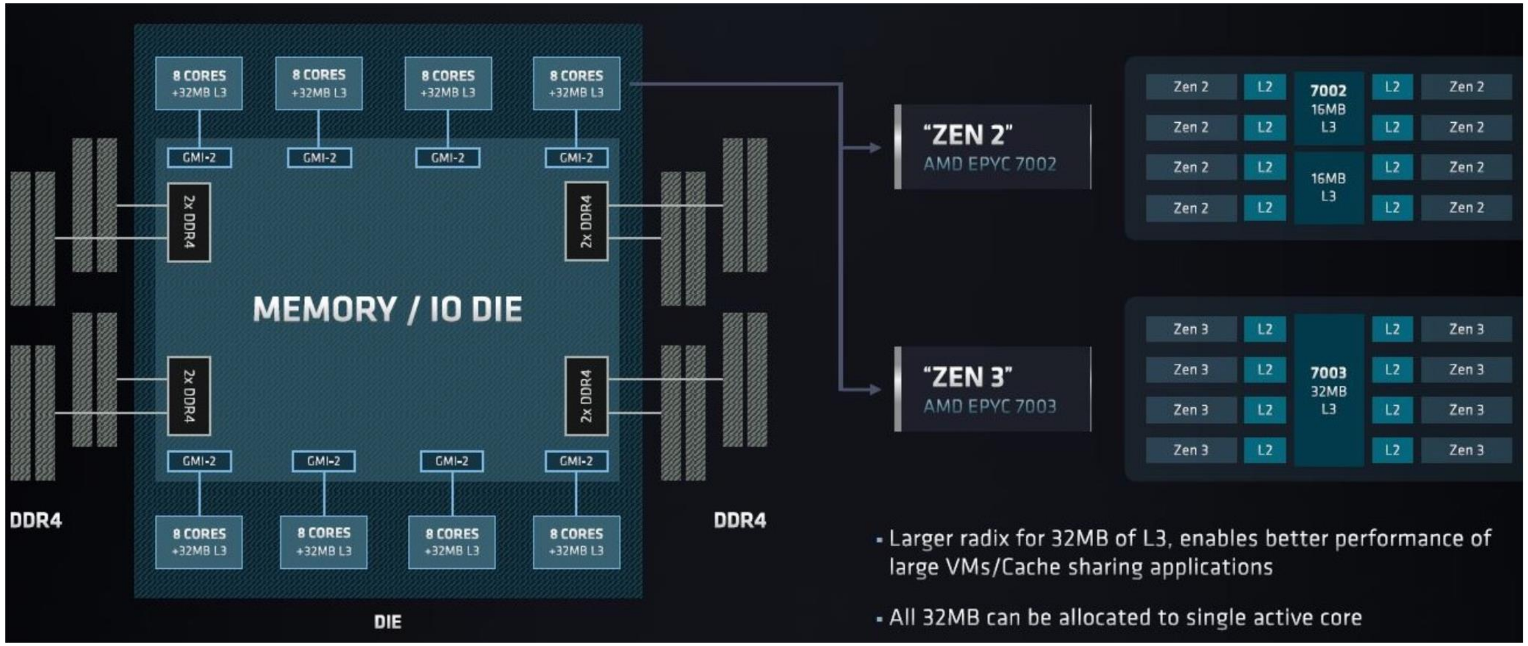
294 912 000 MB/s

294 TB/s

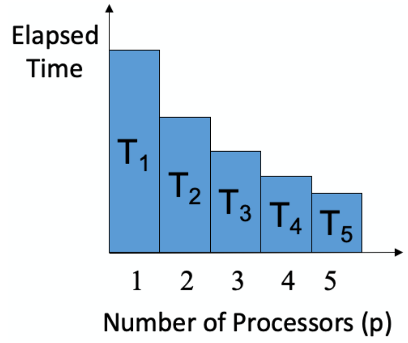
(204 GB/s per socket)



SPEEDUP EXAMPLE

- Assume the perfect speedup $\mathbf{S_P = P}$, perfect efficiency $\mathbf{E_P = 1}$ (100%)

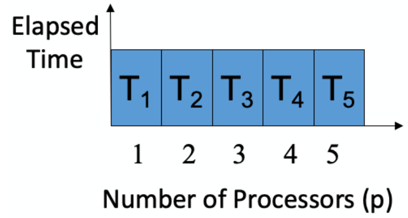
Strong scaling



$S_P = T_1 / T_P$ $S_{16} = T_1 / T_{16} = 32 / 2 = 16$

$E_P = S_P / P$ $E_{16} = S_{16} / 16 = 16 / 16 = 1$

Weak scaling



$S_P = T_1 / T_P$ $S_{16} = T_1 / T_{16} = 32 / 32 = 1$

$E_P = S_P / P$ $E_{16} = S_{16} / 16 = 1 / 16 = 0.0625$

- Perfect E = 6.25 % ? Not very intuitive, alternative:

$E_P = T_1 / T_P$ $E_{16} = T_1 / T_{16} = 32 / 32 = 1$

- “Perfect speedup” $\mathbf{S_P = 1}$

$S_P = 1 / E_P = T_P / T_1$ $S_{16} = T_{16} / T_1 = 32 / 32 = 1$

CLASSIFICATION OF PERFORMANCE TOOLS

- There are many tools that can be classified by the implemented approach

Data collecting mechanism

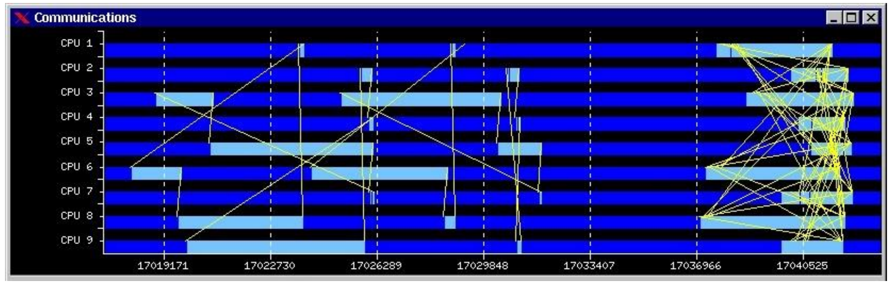
- Sampling - automatically collect data per time unit
- Instrumentation - manually/automatically add instructions to the source code to collect data - intrusive

Form of data presentation

- Reports - general overview of the whole application
- Profiling - accumulated characteristics of metrics
- Tracing - details about selected events - intrusive

Analysis of the collected data

- Online - during the execution - rare
- Post mortem - after the execution



Example of a trace, source: tools.bsc.es

Modeling - simulate state, ideal network, HW failure, etc.

PERFORMANCE TOOLS - CPU

- Single-node/parallel, architecture, language, programming model, focus (instrumentation, correctness checking, etc.)

Proprietary tools – licenses usually available on clusters

- ARM (~~Allinea~~) Performance Report
- ARM (Allinea) MAP
- Intel Application Performance Snapshot
- Intel Vtune
- AMD µProf
- Vampir

Open-source tools (VI-HPS)

- Extrae/Paraver
- Score-P/Scalasca/Cube
- MAQAO
- https://www.vi-hps.org/tools/tools.html (guide)

PERFORMANCE TOOLS – GPU

GUI tools

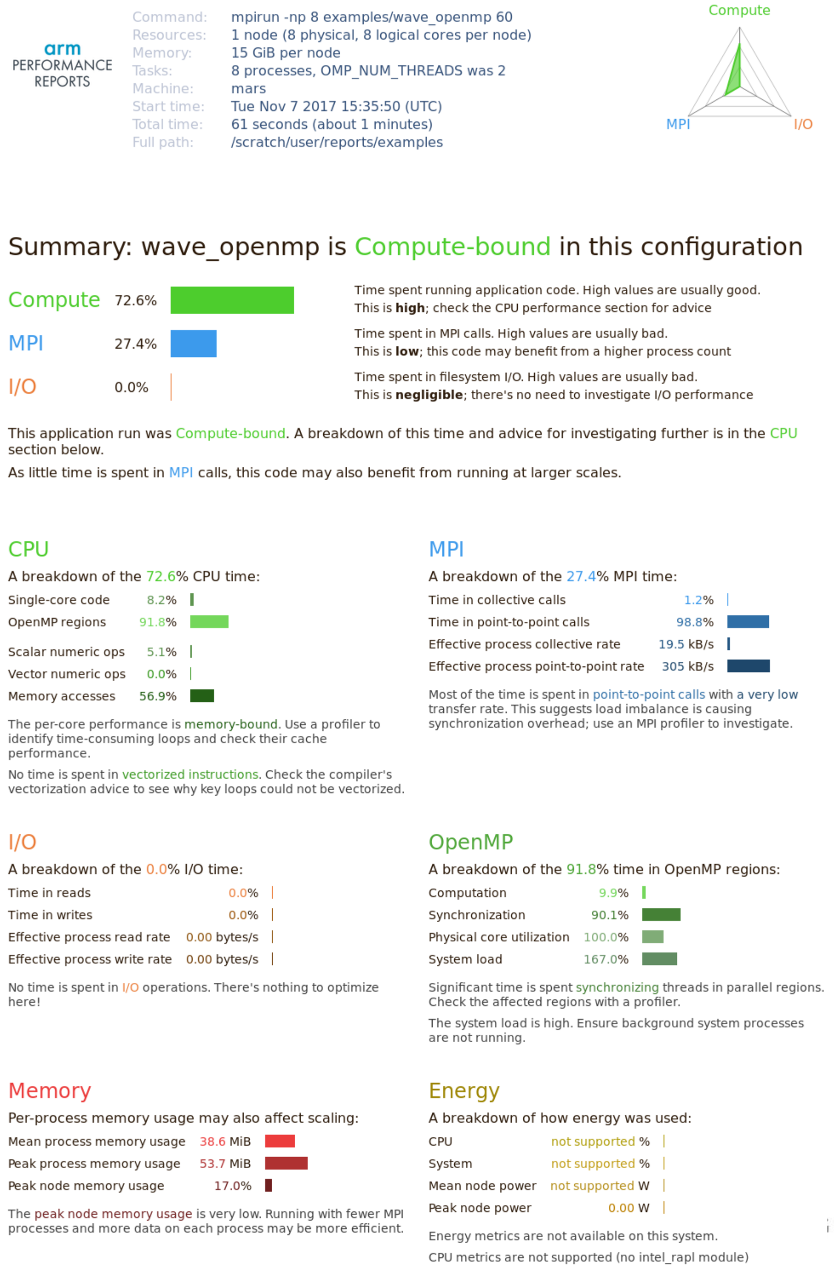
- NVIDIA Visual Profiler - deprecated
- NVIDIA Nsight Systems – system-level profiling
- NVIDIA Nsight Compute – CUDA kernel-level profiling

Command-line tools – useful if you cannot use GUI (e.g. batch job)

- NVIDIA nvprof - deprecated
- NVIDIA nsys
- AMD ROC-profiler – analogous to nvprof (Chrome for visualization)

ARM PERFORMANCE REPORTS

- Global high-level overview of the application
- No source code or recompilation required
- Run: **perf-report** mpirun -n <#procs> <app>
- Auto-generated text and HTML output
- Report summary (Compute, MPI, Input/Output)
- CPU, MPI, I/O, OpenMP, Memory, Energy, Accelerator breakdown sections
- Advanced configuration through command line flags possible


arm PERFORMANCE REPORTS

Command:	mpirun -np 8 examples/wave_openmp 60
Resources:	1 node (8 physical, 8 logical cores per node)
Memory:	15 GiB per node
Tasks:	8 processes, OMP_NUM_THREADS was 2
Machine:	mars
Start time:	Tue Nov 7 2017 15:35:50 (UTC)
Total time:	61 seconds (about 1 minutes)
Full path:	/scratch/user/reports/examples

Summary: wave_openmp is Compute-bound in this configuration

Compute	72.6%	Time spent running application code. High values are usually good. This is **high**; check the CPU performance section for advice
MPI	27.4%	Time spent in MPI calls. High values are usually bad. This is **low**; this code may benefit from a higher process count
I/O	0.0%	Time spent in filesystem I/O. High values are usually bad. This is **negligible**; there's no need to investigate I/O performance

This application run was Compute-bound. A breakdown of this time and advice for investigating further is in the CPU section below.

As little time is spent in MPI calls, this code may also benefit from running at larger scales.

CPU

A breakdown of the 72.6% CPU time:

Single-core code	8.2%
OpenMP regions	91.8%
Scalar numeric ops	5.1%
Vector numeric ops	0.0%
Memory accesses	56.9%

The per-core performance is memory-bound. Use a profiler to identify time-consuming loops and check their cache performance.

No time is spent in vectorized instructions. Check the compiler's vectorization advice to see why key loops could not be vectorized.

MPI

A breakdown of the 27.4% MPI time:

Time in collective calls	1.2%
Time in point-to-point calls	98.8%
Effective process collective rate	19.5 kB/s
Effective process point-to-point rate	305 kB/s

Most of the time is spent in point-to-point calls with a very low transfer rate. This suggests load imbalance is causing synchronization overhead; use an MPI profiler to investigate.

I/O

A breakdown of the 0.0% I/O time:

Time in reads	0.0%
Time in writes	0.0%
Effective process read rate	0.00 bytes/s
Effective process write rate	0.00 bytes/s

No time is spent in I/O operations. There's nothing to optimize here!

OpenMP

A breakdown of the 91.8% time in OpenMP regions:

Computation	9.9%
Synchronization	90.1%
Physical core utilization	100.0%
System load	167.0%

Significant time is spent synchronizing threads in parallel regions. Check the affected regions with a profiler.

The system load is high. Ensure background system processes are not running.

Memory

Per-process memory usage may also affect scaling:

Mean process memory usage	38.6 MiB
Peak process memory usage	53.7 MiB
Peak node memory usage	17.0%

The peak node memory usage is very low. Running with fewer MPI processes and more data on each process may be more efficient.

Energy

A breakdown of how energy was used:

CPU	not supported %
System	not supported %
Mean node power	not supported W
Peak node power	0.00 W

Energy metrics are not available on this system.
CPU metrics are not supported (no intel_rapl module)

ARM PERFORMANCE REPORTS - EXAMPLE

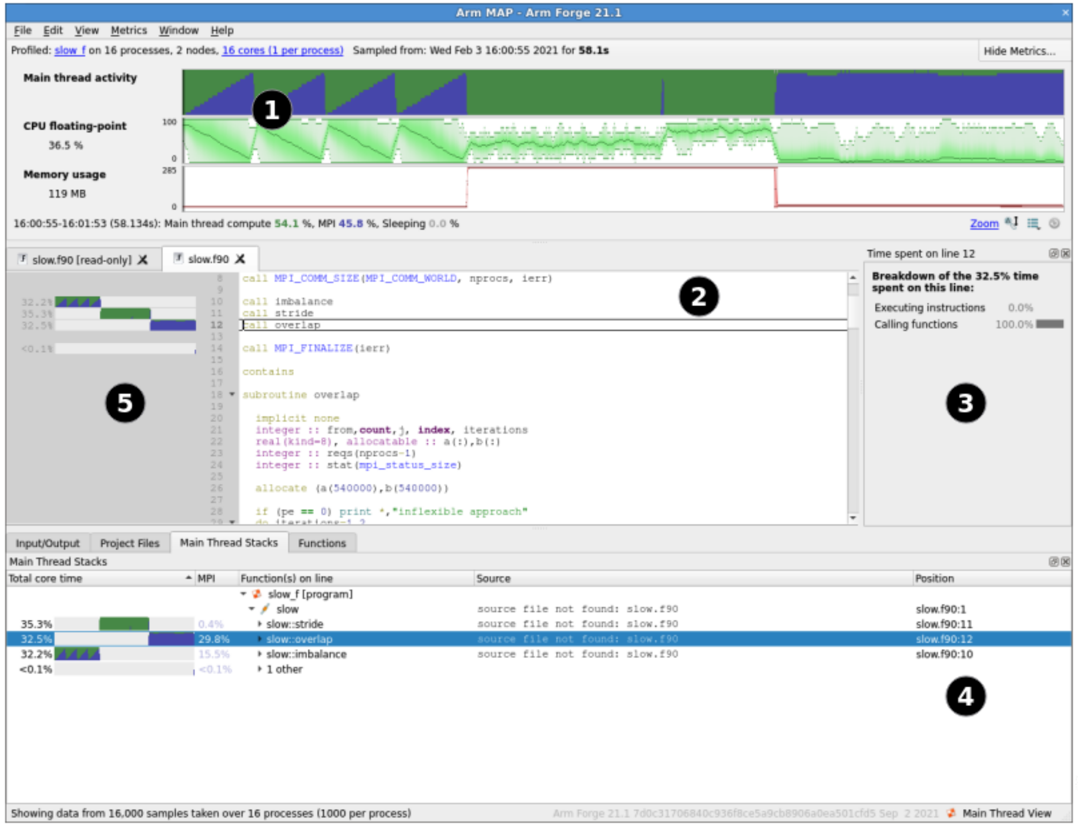
```
ml Forge/21.1.3 impi/2019.9.304-iccifort-2020.4.304
ml show Forge
cp -r /apps/all/Forge/21.1.3/examples ~/forge_examples
cd ~/forge_examples
make

mpirun -n 16 ./wave_c 10

mkdir perf_reports && cd perf_reports
perf-report mpirun -n 16 ../wave_c 10
firefox wave_c_16p_1n_YYYY-MM-DD_hh-mm.html &          # on login node
OMP_NUM_THREADS=8 perf-report mpirun -n 2 ../wave_openmp 10
firefox wave_openmp_2p_1n_8t_YYYY-MM-DD_hh-mm.html &
```

ARM MAP

- Low overhead sampling profiler for localisation of bottlenecks
- No recompilation required, only debugging symbols are useful (-g)

1. Metrics view (CPU, MPI, I/O, memory, vectorization)
2. Source code viewer
3. Selected lines view
4. Output, files, callpaths
5. Sparkline charts

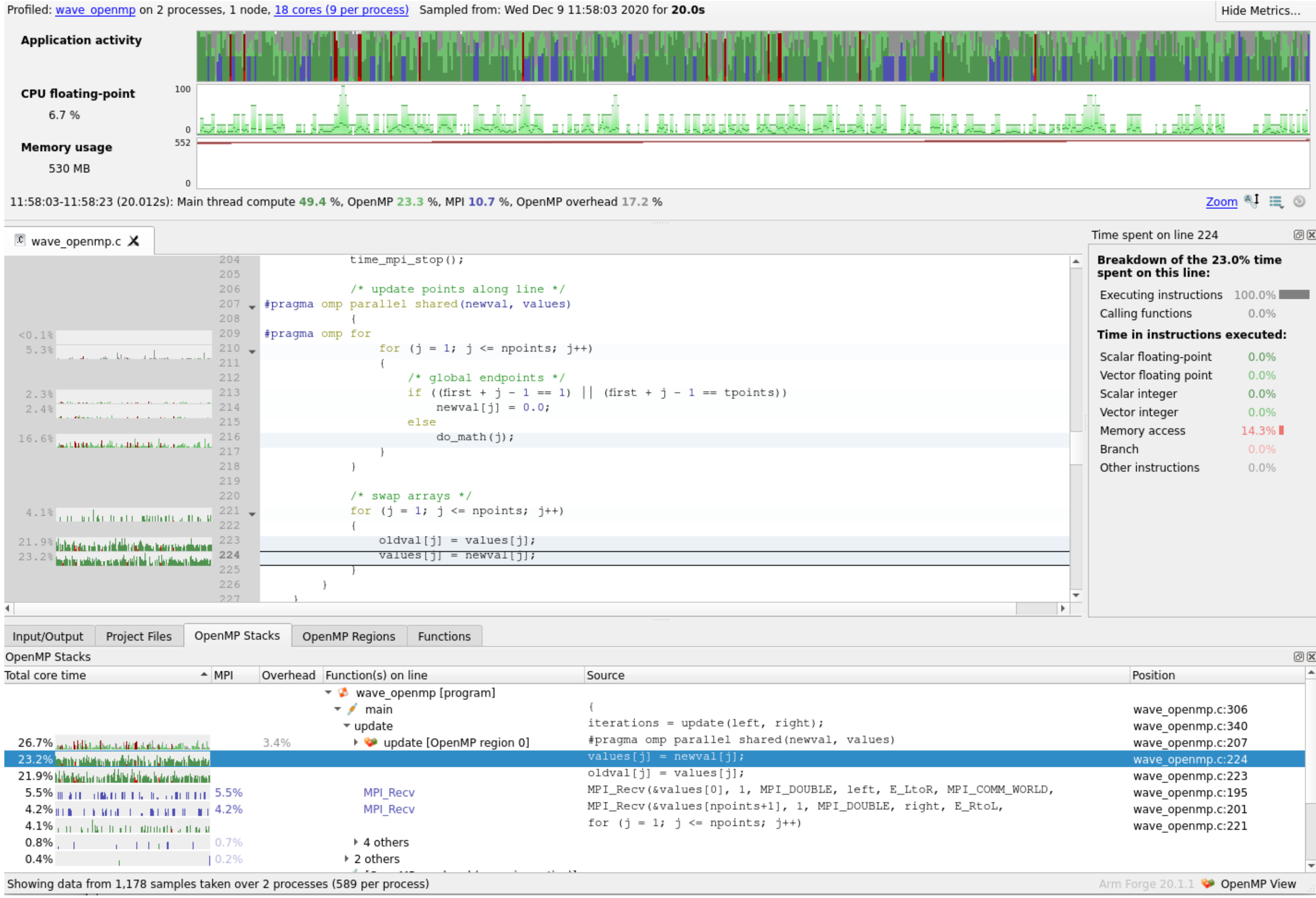
```
map
map mpirun -n <#procs> <app> [args]
map --profile mpirun -n <#procs> …
map <profile.map>
perf-report <profile.map>
```



ARM MAP

- All charts are timelines
  - Horizontal axis time
- Vertical axis are processes
- Useful code is green
- MPI is blue
- breakout recalculated

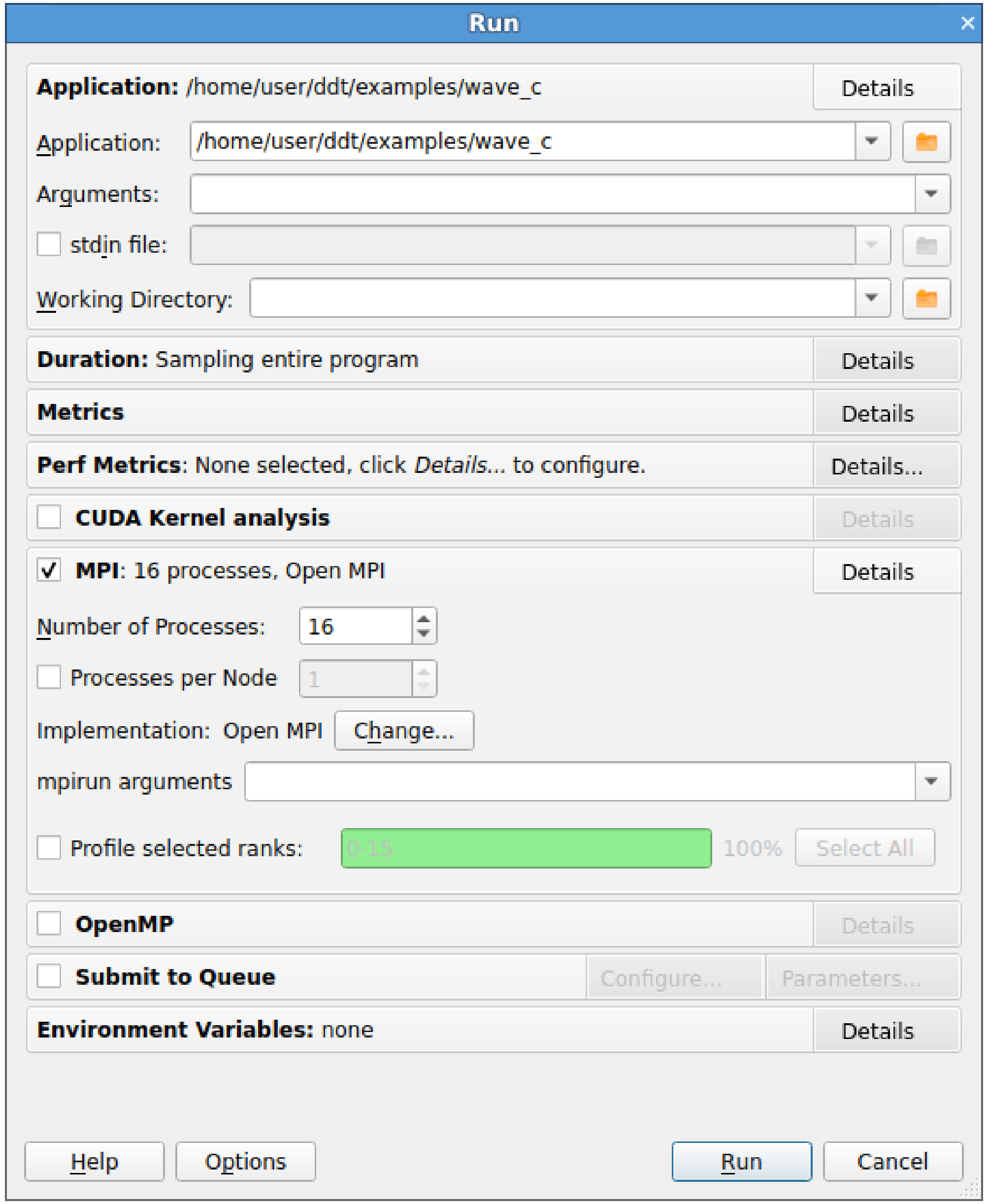
  when zooming
- Multiple presets available
  - CPU
  - MPI
  - I/O
  - memory
  - …



ARM MAP - EXAMPLE

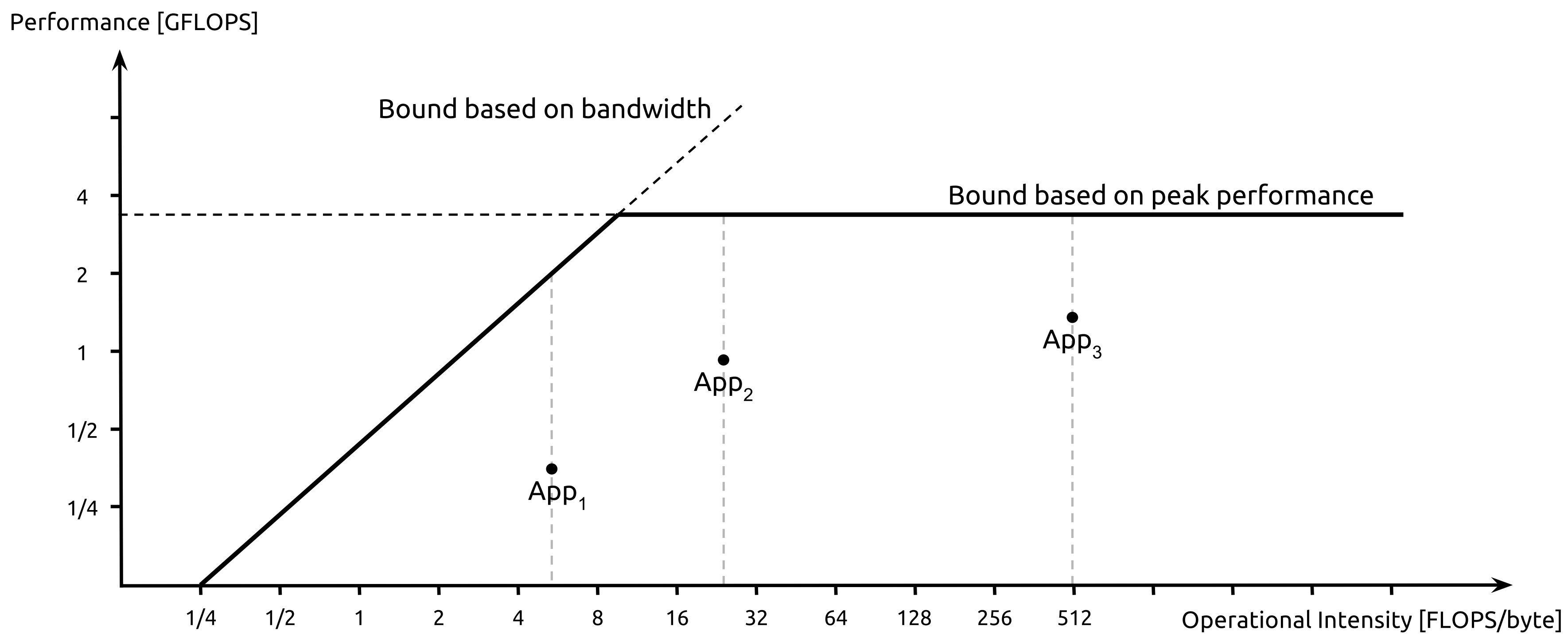
- `ml Forge/21.1.3 impi/2019.9.304-iccifort-2020.4.304`
- `mkdir ~/forge_examples/map && cd ~/forge_examples/map`
- `OMP_NUM_THREADS=8 map mpirun -n 2 ../wave_openmp 10`

- Optionally limit duration
- Optionally adapt metrics
- Click Run



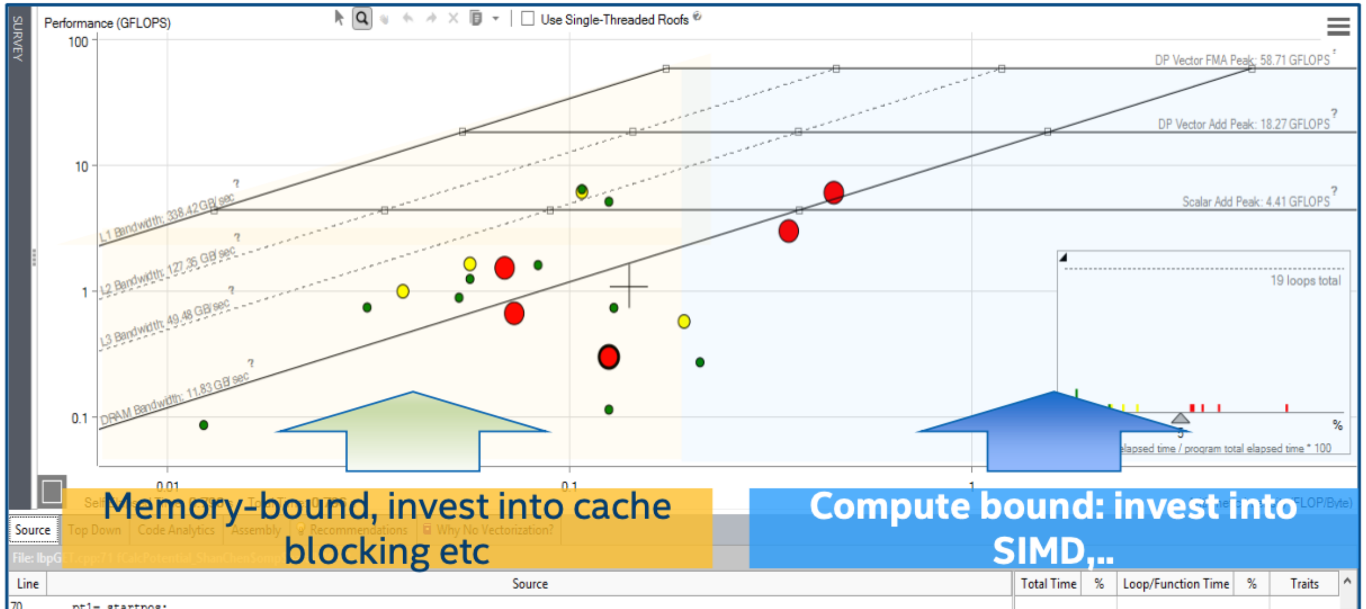
ROOFLINE MODEL

- Shows the performance of an algorithm (application) with respect to the HW limits of the architecture
- Identify if an algorithm is **compute bound** or **memory bound**
- Based on **Operational intensity** - a ratio of FLOPS (arithmetic operations) performed with required amount of data (operands)



INTEL ADVISOR

- Primarily to support vectorization of codes
- Performs dynamic analysis of codes
- Identify data access patterns
- But also computes Operational intensity vs. Performance (flops)
- It helps to identify what loops to focus on (Big red dots first)
- Ideally, during optimisations the dot moves top right



INTEL ADVISOR - EXAMPLE

```
mkdir ~/forge_examples/advisor
```

```
ml Advisor
```

- To analyse MPI application:

```
mpirun -n 2 advixe-cl --collect survey --project-dir advisor/wave_c/ -- ./wave_c 10
```

```
mpirun -n 2 advixe-cl --collect tripcounts --project-dir advisor/wave_c/ --flop --no-trip-counts -- ./wave_c 10
```

```
advixe-gui advisor/wave_c/
```

- Show my results -> Summary -> Survey & Roofline

INTEL ADVISOR - EXAMPLE

Maqao?

likwid?

NVIDIA NSIGHT SYSTEMS

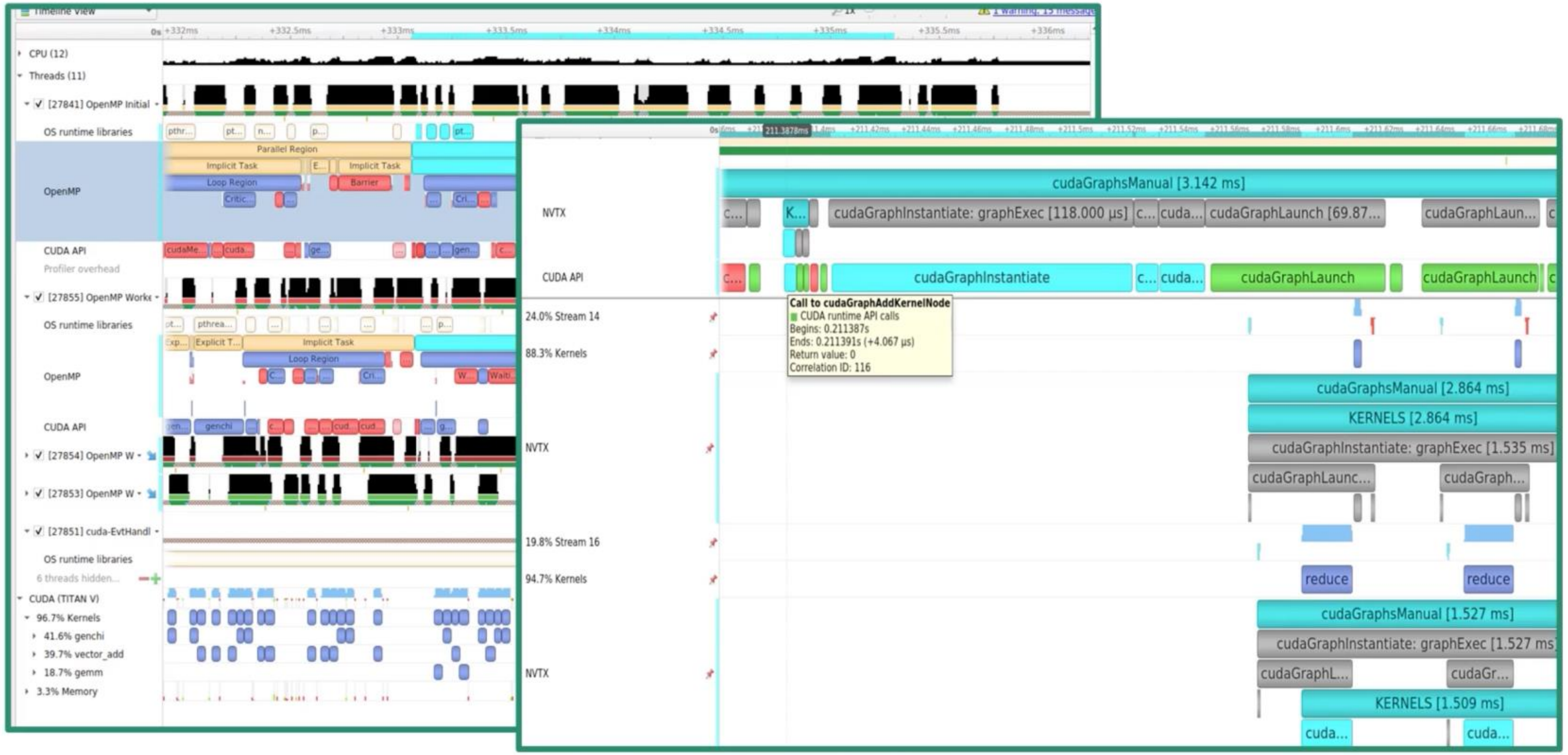
Scalable system-wide performance analysis tool

- Low-overhead multi-node, multi-GPU profiling
- Assess on timeline to narrow down frames/areas of the app to focus
- Locate optimization opportunities
- Determine CPU vs. GPU bottlenecks, idle time
- Visualize millions of events on a very fast GUI timeline
- Or gaps of unused CPU and GPU time
- Balance your workload across multiple CPUs and GPUs
- Expert system GPU utilization analysis
- Detailed information, documentation, free download
  https://developer.nvidia.com/nsight-systems

NVIDIA NSIGHT SYSTEMS

Multi-level information

- CPU cores utilization
- MPI calls
- Threading
- OS runtime calls
- NVTX
- CUDA API calls
- HtD / DtH data transfers
- CUDA kernels / OpenACC
- CUDA streams
- CUDA libraries (cuBLAS, …), GPU HW metrics, UCX, NIC, …



NVIDIA NSIGHT SYSTEMS

PROFILING WITH NSIGHT SYSTEMS

GUI profiling and analysis

| `nsight-sys`

- File -> New Project
- **Select target for profiling... -> acnXX.karolina.it4i.cz** (your allocated GPU node)
- Enter **Command line** and **Working directory** (absolute path to the binary required)
- Select tracing modules (CPU, OS, CUDA, GPU, ...)
- Start

Cmd line profiling + GUI analysis

| **`nsys profile -t cuda,osrt --stats=true -o simpleMultiGPU`** `./simpleMultiGPU`

| `nsight-sys`

- File -> Open -> Select simpleMultiGPU.nsys-rep

NVIDIA NSIGHT SYSTEMS - EXAMPLE

```
git clone https://github.com/NVIDIA/cuda-samples.git
ml CUDAcore/11.6.0 Qt5/5.14.2-GCCcore-10.2.0
cd cuda-samples/Samples/0_Introduction/concurrentKernels/
make SMS=70
```

- Perform profiling of **concurrentKernels** example with:
  - CPU context switch
  - OS runtime libraries
  - CUDA
  - GPU metrics

- An extra example:

```
cd cuda-samples/Samples/0_Introduction/simpleMultiGPU/
simpleMultiGPU                                    # at least 2 GPUs required
make SMS=70
```

POP COE

An EU H2020 **Centre of Excellence** (CoE)

- On **Performance Optimisation and Productivity**
- Promoting **best practices** in parallel programming

Providing **FREE Services**

- Precise understanding of application and system behaviour
- Suggestion/support on how to refactor code in the most productive way

Horizontal

- Transversal across application areas, platforms, scales

For EU **academic AND industrial codes and users**

www.pop-coe.eu pop@bsc.es @POP_HPC youtube.com/POPHPC

POP COE

Performance Assessment

- Primary service
- Identifies performance issues of customer code
- If needed, identifies the root causes of the issues found and qualifies and quantifies approaches to address them (recommendations)
- Medium effort (1-3 months)
- Performance report

Proof-of-Concept

- Follow-up service
- Experiments and mock-up tests for customer codes
- Kernel extraction, parallelisation, mini-apps experiments to show effect of proposed optimisations
- Larger effort (3-6 months)

Note: Effort shared between our analysts and customer

USEFUL LINKS

VI-HPS – Association of institutions developing tools and providing training

- Overview of the tools with a description: https://www.vi-hps.org/cms/upload/material/general/ToolsGuide.pdf

Intel performance tools: VTune and Advisor

- Running VTune on IT4I systems requires loading of special kernel modules, see the docs

Nvidia tools for GPUs: Nsight Systems and Nsight Compute

Database of code patterns and best practices developed in POP: co-design

Further reading:

- https://software.intel.com/content/www/us/en/develop/articles/predicting-and-measuring-parallel-performance.html
- https://developer.arm.com/documentation/101136/2020/Performance-Reports?lang=en
- https://developer.arm.com/documentation/101136/2020/MAP?lang=en
- https://software.intel.com/content/www/us/en/develop/articles/intel-advisor-roofline.html
- https://scc.ustc.edu.cn/zlsc/tc4600/intel/2018.1.163/advisor/welcomepage/get_started.htm
- https://llvm.org/docs/Benchmarking.html

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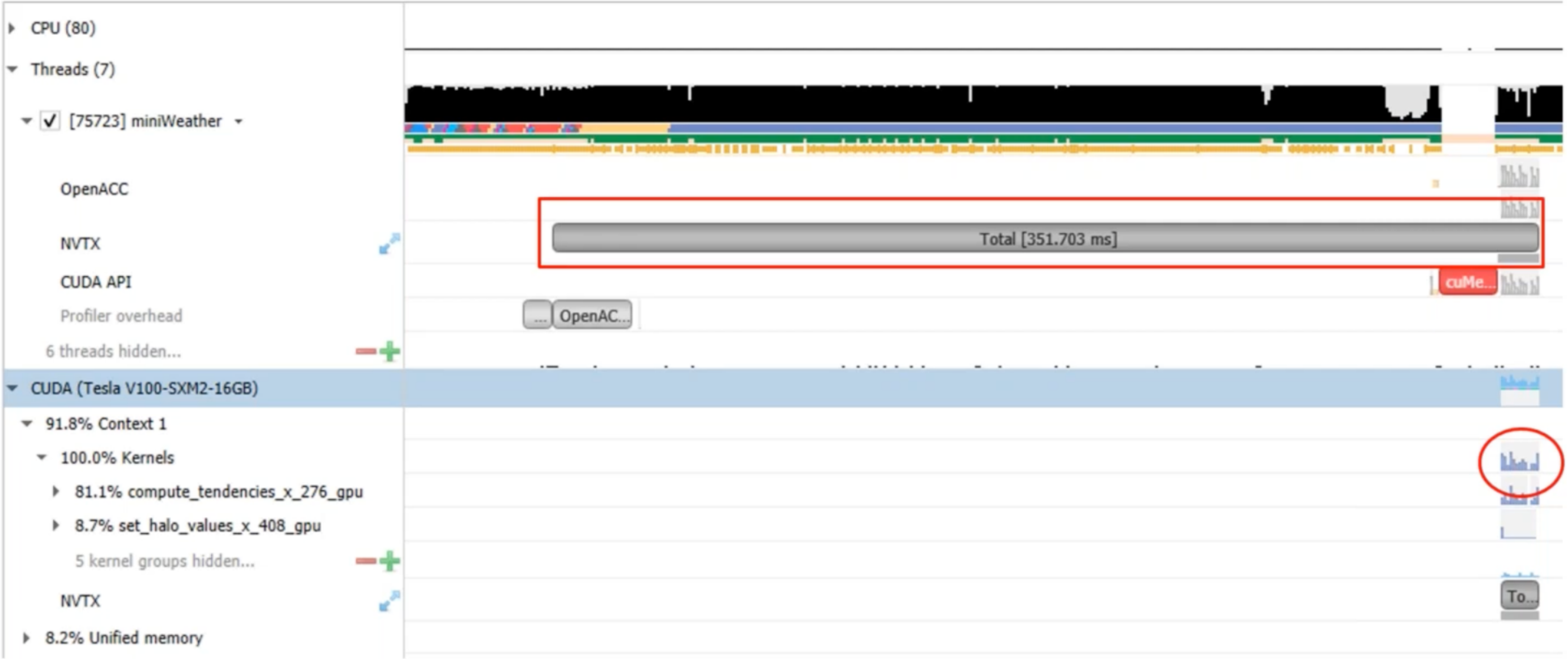
MINISTRY OF EDUCATION, YOUTH AND SPORTS

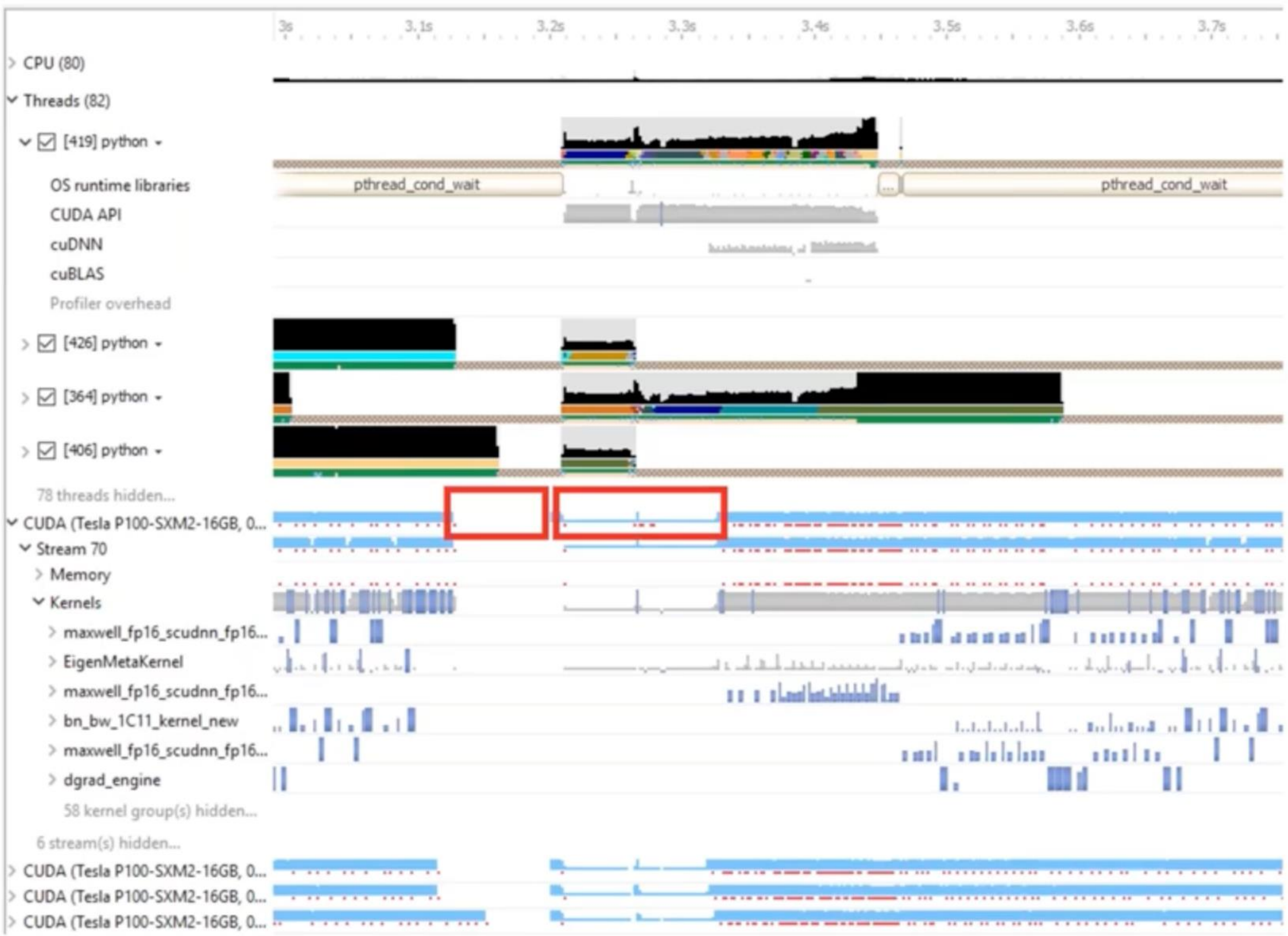
ANALYSIS WITH NSIGHT SYSTEMS

Only small portion of application accelerated



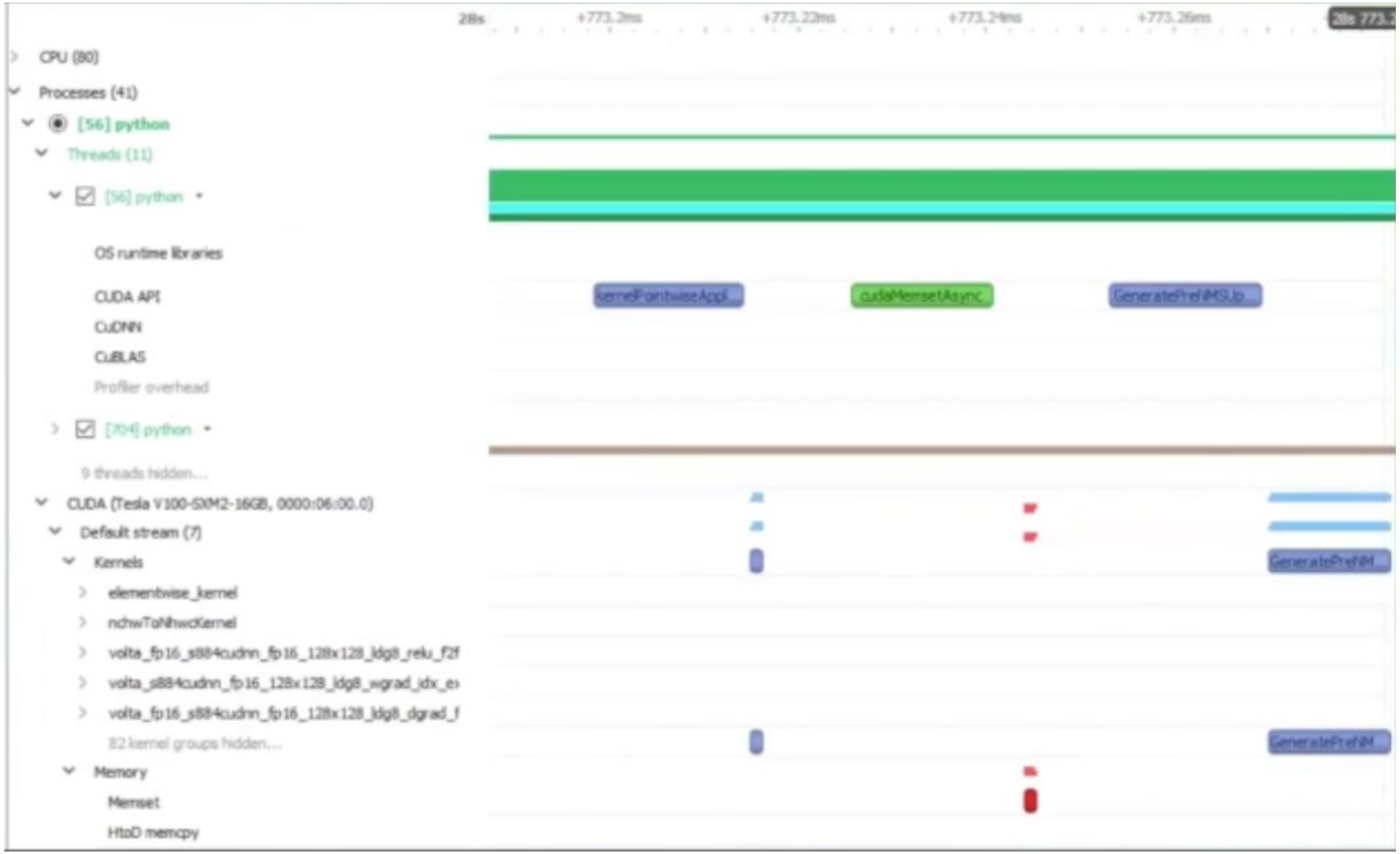
ANALYSIS WITH NSIGHT SYSTEMS

GPU idle or low utilization level of details (because of pthread creation)



ANALYSIS WITH NSIGHT SYSTEMS

Fusion opportunities: CPU launch cost + small GPU work size ~ GPU idle



ANALYSIS WITH NSIGHT SYSTEMS

cudaMemcpyAsync behaving synchronous – DtH pageable memory -> Mitigate with pinned memory

ANALYSIS WITH NSIGHT SYSTEMS

GPU idle caused by stream synchronization