

# OpenACC Performance Optimization Workflow

Markus Hrywniak, Senior DevTech Compute | JSC OpenACC course, October 2023

### Before We Start

#### Content and expectations

- Workflow focus
  - Data-driven via tools
  - Memory coalescing
  - Loop optimizations
- Goal: Understand how tools (compiler output/profiler) can help
- Performance optimization Now vs. Then
  - GPUs are *a lot* faster than even 2, 3 years ago
  - Not just FLOPs, also larger caches, ...
  - Programmability even more improved
- Example application: Realism vs. Learning
- Performance optimization is very seldomly a straightfoward process
  - Tinker and experiment this is what makes it fun!

### General notes

- Important flags for NVHPC Compiler
- Building with lightweight debug information:
  - -gpu=lineinfo -gopt
- Check compiler output: -Minfo=accel

#### **NVHPC Runtime Measurements**

- For quick sanity checks
- Applications compiled with NVHPC compiler: Analyze via environment variables
- Maybe simplest/quickest check
- Set NV\_ACC\_TIME=1 for lightweight profiler on time of data movements and kernels
  - NV\_ACC\_NOTIFY=1 gives a detailed breakdown of kernel launches and data transfers (bit field)
- More details at <a href="https://docs.nvidia.com/hpc-sdk/compilers/openacc-gs/index.html#env-vars">https://docs.nvidia.com/hpc-sdk/compilers/openacc-gs/index.html#env-vars</a>

#### NVHPC Runtime Measurements

```
$ NV_ACC_TIME=1 srun -n1 ./spmv
Runtime 0.007972 s.
Accelerator Kernel Timing data
/p/home/jusers/hrywniak1/jusuf/openacc-4/C/task0/spmv.c
 main NVIDIA devicenum=0
    time(us): 307,478
   37: data region reached 2 times
       37: data copyin transfers: 168
            device time(us): total=222,883 max=1,527 min=143 avg=1,326
        57: data copyout transfers: 4
            device time(us): total=5,145 max=1,312 min=1,277 avg=1,286
   41: compute region reached 10 times
       41: kernel launched 10 times
           grid: [63443] block: [128]
            device time(us): total=79,450 max=7,948 min=7,940 avg=7,945
            elapsed time(us): total=79,667 max=8,011 min=7,957 avg=7,966
```



## Nsight Profiler Suite





- Comes with HPC SDK, also standalone
- Profiles application, including CUDA Kernels and API calls
- Supports OpenACC
- Systems for whole application, Compute for kernel tuning
- Generates performance reports, timelines; measures events and metrics

https://developer.nvidia.com/tools-overview



## **Nsight Systems on the Command Line**

\$ srun -n1 nsys profile -t cuda, openacc \
-f true -o spmv --stats=true ./spmv

- Always records a report (\*.nsys-rep)
- Reports customizable
- Forgot --stats?
   nsys stats can post-process any report

Time(%)	Total	Time	(ns)	Num C	Calls	Average	Minimum	Maximum	Name
60.4		822	200447		12	6850037.3	1272194	7950555	cuStreamSynchronize
25.3		343	383053		172	199901.5	1560	6964642	cuEventSynchronize
10.0		135	578282		1	13578282.0	13578282	13578282	cuMemHostAlloc
2.7		37	721103		6	620183.8	143751	1490944	cuMemAlloc_v2
0.7		Ç	954802		168	5683.3	4600	27610	cuMemcpyHtoDAsync_v2
0.4		5	533741		1	533741.0	533741	533741	cuMemAllocHost_v2
0.3		3	364570		174	2095.2	1820	4311	cuEventRecord
0.1		1	119510		1	119510.0	119510	119510	cuModuleLoadDataEx
0.1		1	114440		10	11444.0	8460	32760	cuLaunchKernel
0.0			28350		4	7087.5	4810	11910	cuMemcpyDtoHAsync_v2
0.0			16230		1	16230.0	16230	16230	cuStreamCreate
0.0			5380		4	1345.0	450	2530	cuEventCreate

CUDA Kernel Statistics:

Time(%)	Total Time (ns)	Instances	Average	Minimum	Maximum	Name
100.0	79415454	10	7941545.4	7932394	7948329	main_41_gpu

CUDA Memory Operation Statistics (by time):

Time(%)	Total Time (ns)	Operations	Average	Minimum	Maximum	Operation
97.8	220817077	168	1314387.4	138847	1522486	[CUDA memcpy HtoD]
2.2	4926174	4	1231543.5	1111096	1271928	[CUDA memcpy DtoH]

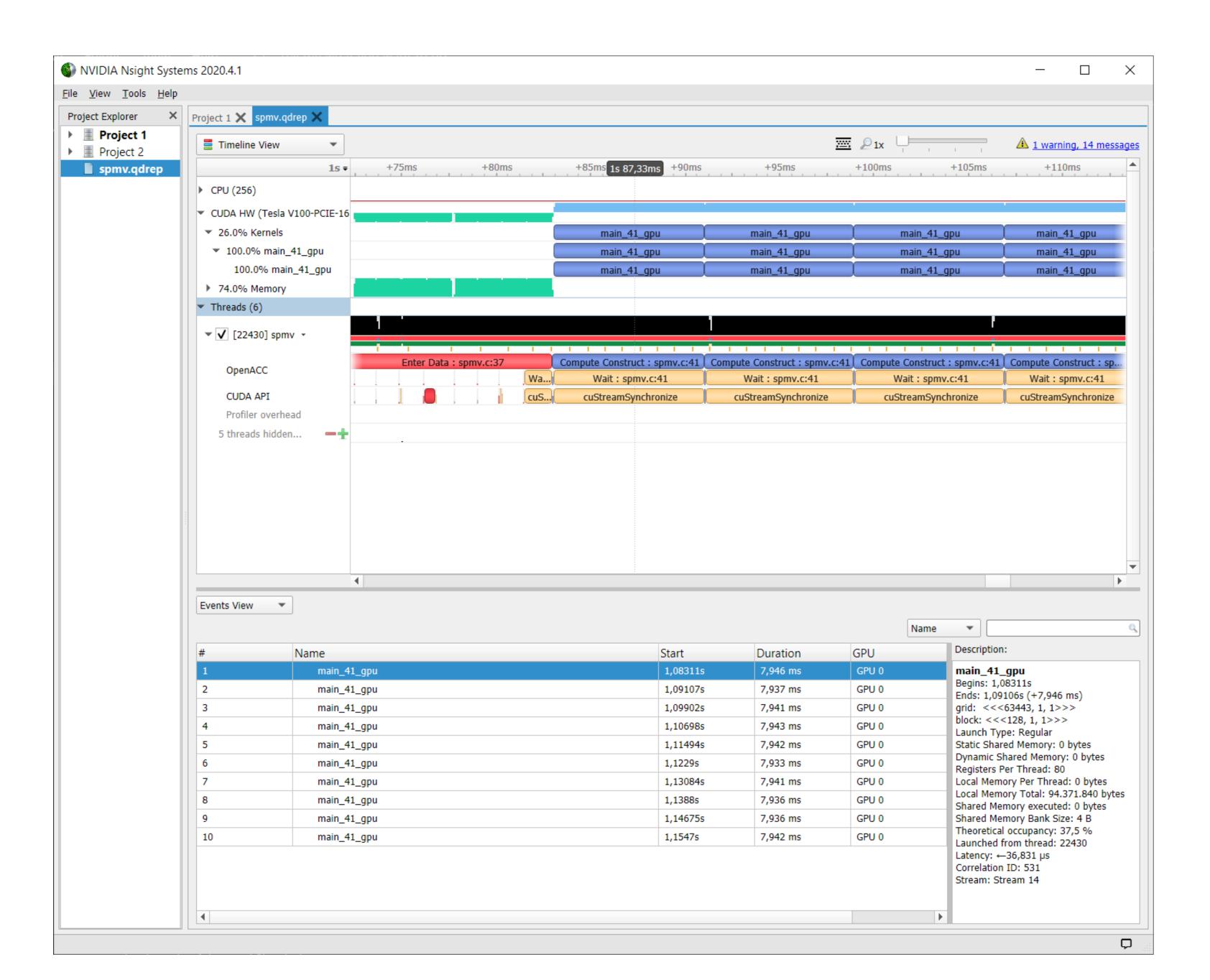
CUDA Memory Operation Statistics (by size in KiB):

Total	Operations	Average	Minimum	Maximum	Operation
63442.195					[CUDA memcpy DtoH]
2719562.816	168	16187.874	1684.441	16384.000	[CUDA memcpy HtoD]

## Nsight Systems GUI

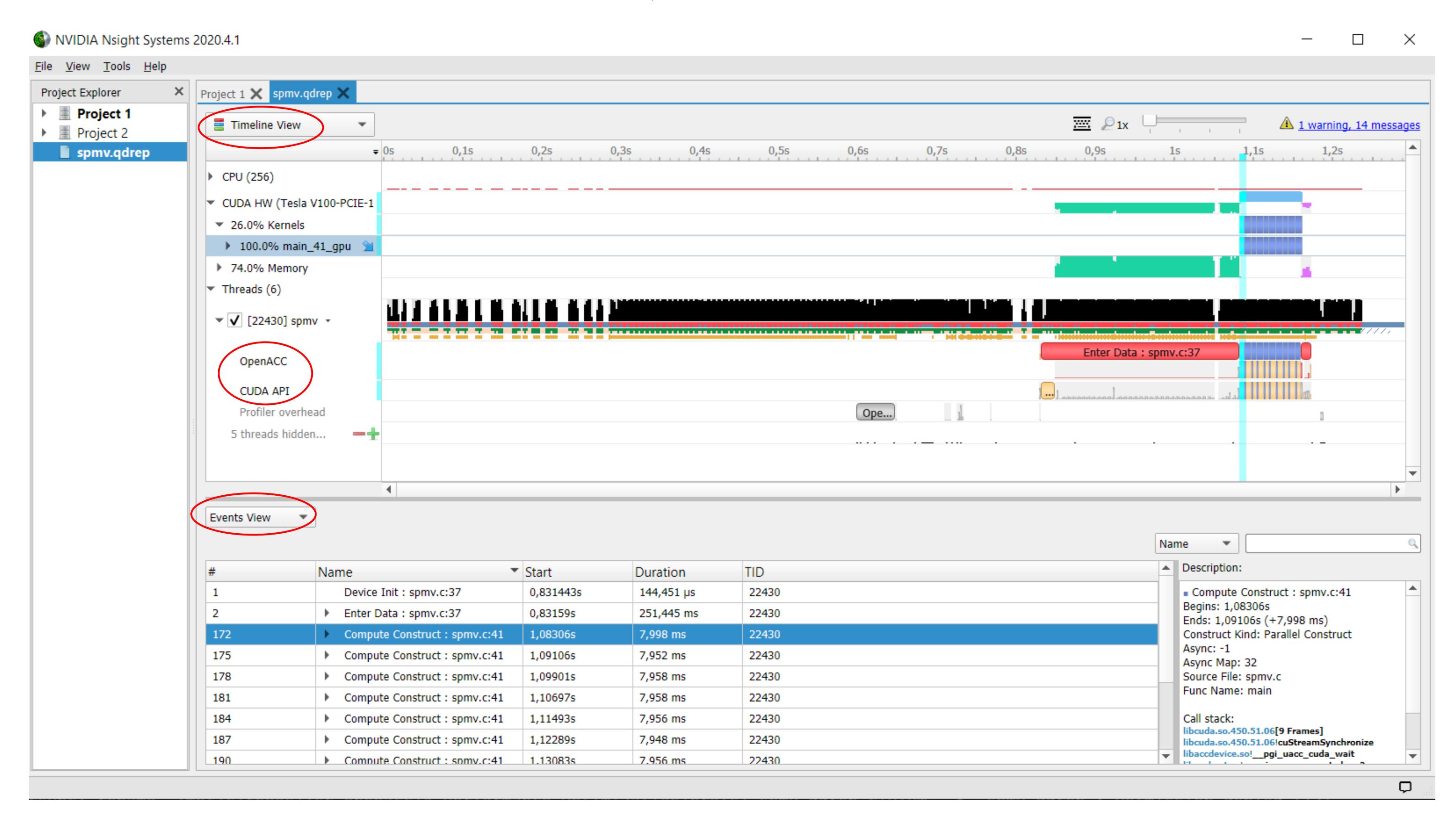
- Graphical, interactive profiler
- Comes with HPC SDK, also standalone
- High-level, whole-program visualization for quick insight
- Timeline traces for OpenACC, OpenMP, CUDA, MPI, etc.

https://docs.nvidia.com/nsight-systems/UserGuide/index.html



# Nsight Systems GUI

Timeline, Traces and Events View



# Implementing a Convolution

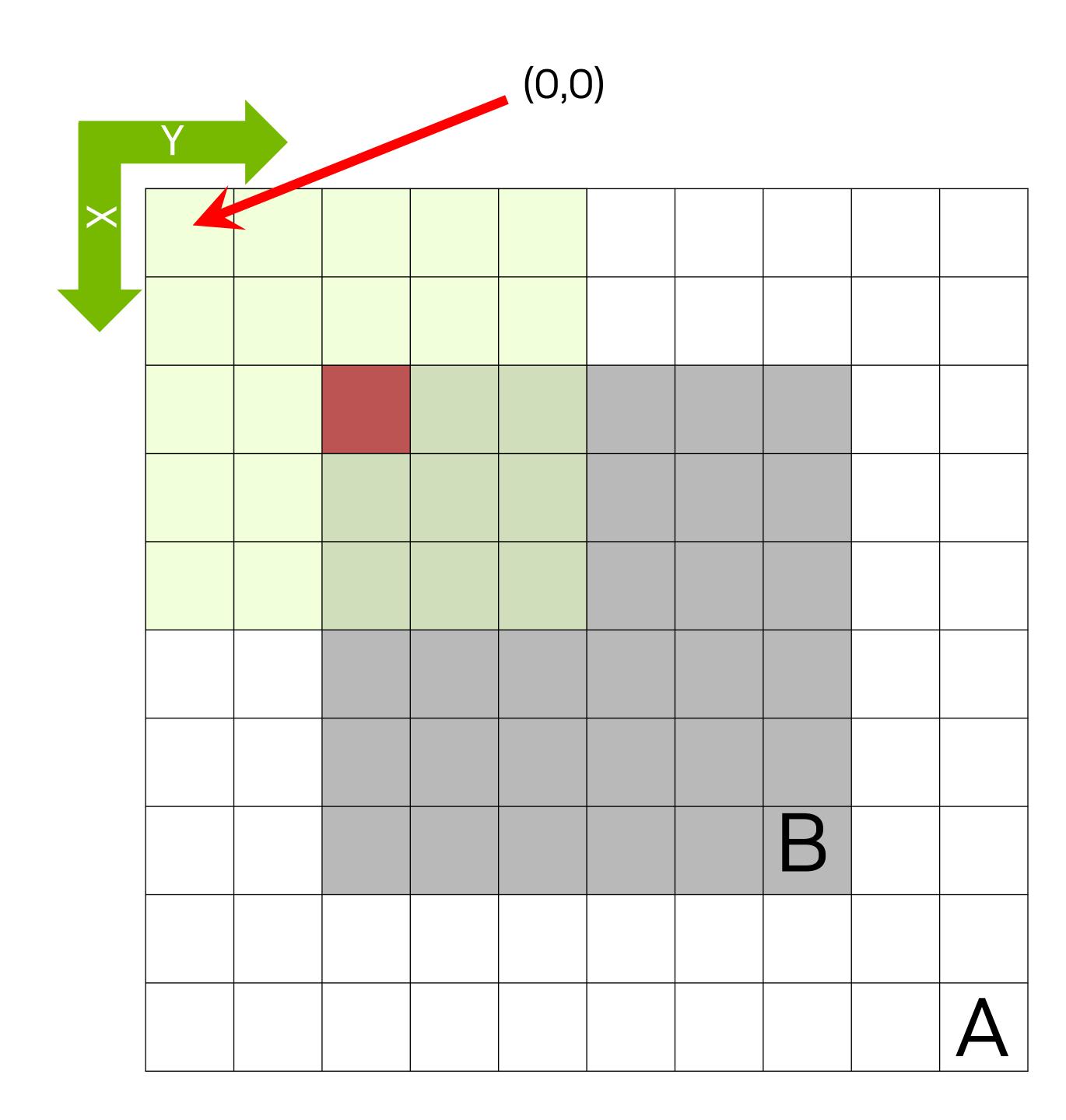
- Weighted summation over local neighborhood ("stencil")
  - Input A, output B (inner grey block)

• 
$$x = 0 \dots N_x - 1, y = 0 \dots N_y - 1$$

- stencil coefficients  $\omega$  for local neighborhood around x and y
- Halo area at borders

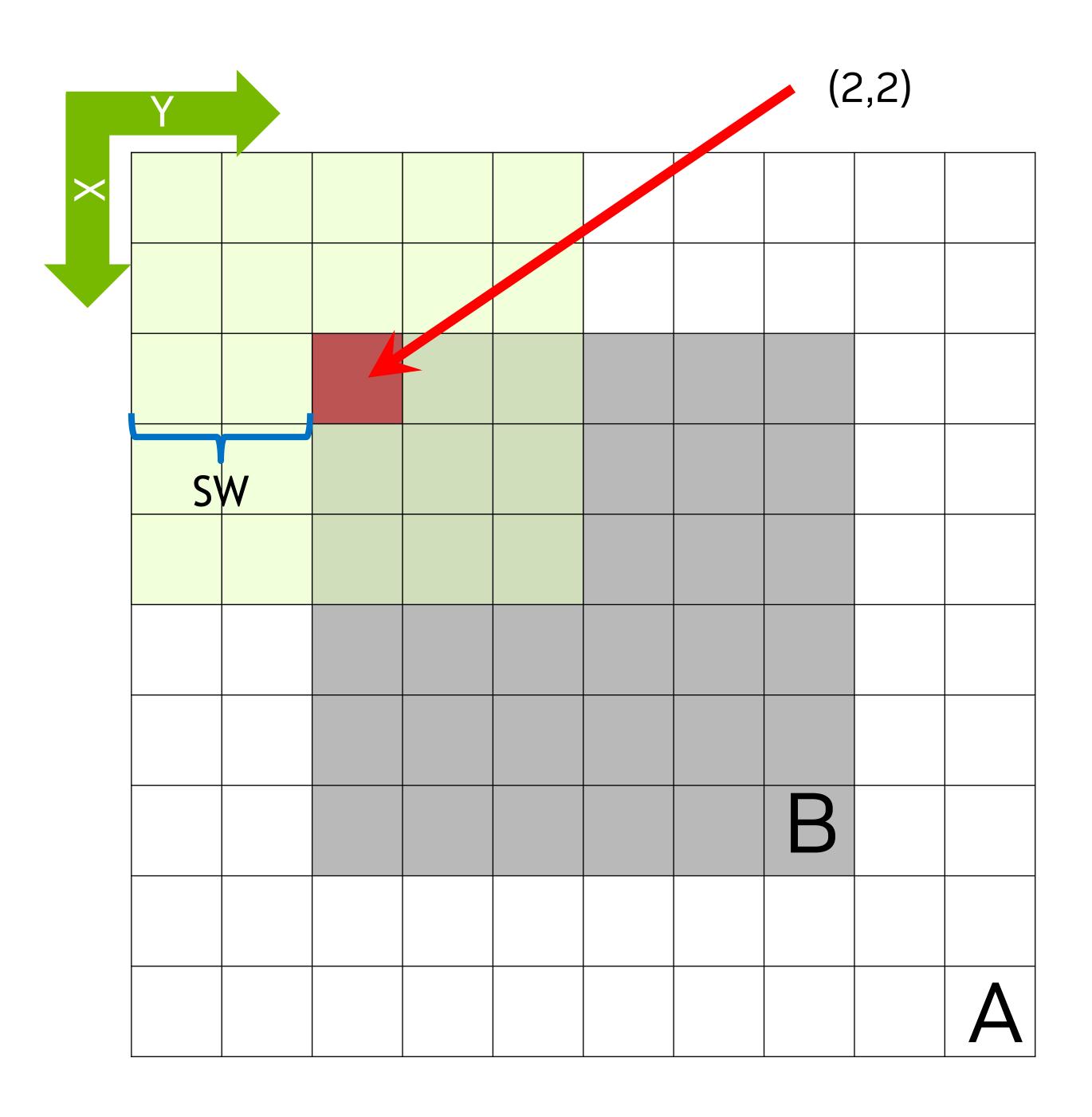
$$B(x,y) = \sum_{sx} \sum_{sy} \omega(sx,sy)A(x+sx,y+sy)$$

- Jacobi "generalized" could also be written that way
- "Filter kernel", "stencil", name depends on context
  - size of the stencil etc.
- Image filter applications
  - border detection, gaussian softening



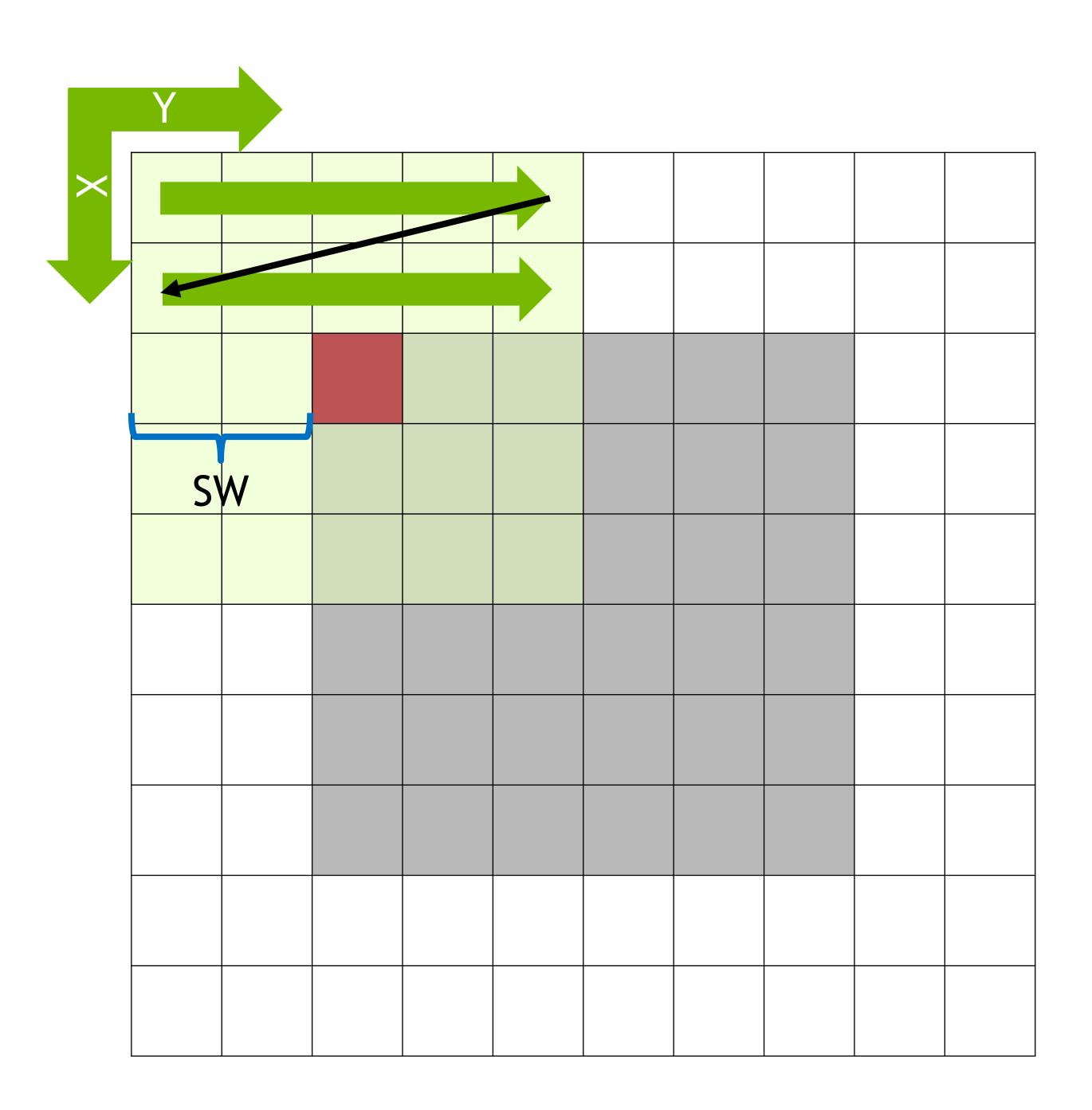
## Implementing a Convolution

- Stencil width: Go SW pixels into all directions
  - sum up contributions
  - repeat for all pixels
- Total points  $(2 sw + 1)^2$
- Example on the right: sw = 2, red square at (x=2, y=2)
  - Note: zero-based indexing below



# Implementing a Convolution

- Configurable stencil width
- Explicit looping, no unrolling, for simplicity



## Parallelizing on CPU

Via -acc=multicore

- Always: Checking correctness
  - Easy to go fast by computing nonsense
- Recall: NV\_ACC\_TIME for simple measurements
- Code example uses manual timing: Repetitions for averaging
- Exercise in each task folder
  - Original task file: .taskN.conv.c
  - Solution file: .solutionN.conv.c

#### Task 0

#### Get familiar with the code and establish a baseline

- Directory: task0/
- 2. There are several variants you can build. Try "make all"
  - 1. Launching any of the built executable variants will print a help
  - 2. NOTE: We will use SW=3 for all tasks the Makefile targets do this automatically
- 3. Generate reference data. Use "make create\_ref"
  - 1. This will run the serial version and output the expected data in a .bin file, as we have not yet verified any of the parallel versions
  - 2. Note the command line, you can run this yourself with any version

```
$ make create_ref
srun [...] ./conv_serial 3 yes
Recreating reference data...
Using stencil width = 3
Runtime 1194.230588 ms
```

- 4. Inspect the Makefile, the source conv.c and look for the TODO
  - 1. Use the correct #pragma to parallelize the outer loop
  - 2. Compare runtimes of all versions. You can use "make run\_all". Write down the runtimes.

#### Task 0 - Results

- Reference results: Simplest way is to dump data and compare (or run known-good implementation afterwards)
  - Only serial known-good for task 0 for other tasks, we can copy/link .bin file or use existing GPU version
- Roughly, you should see
  - Serial, Multicore, GPU
  - 1200 ms vs 165 ms vs 56 ms
- Now, to make it faster, look for first clues
- Compiler output
- Profilers: Nsight Systems should usually be your first step!

## Task 0 - Compiler output

Via -Minfo=accel

```
run_convolution_kernel_and_time:
    49, Generating copyout(B[:4096][:]) [if not already present]
        Generating copyin(stencil[:stencil_dim][:stencil_dim],A[:4096][:]) [if not already present]
    51, Generating NVIDIA GPU code
        56, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
        57, #pragma acc loop seq
        59, #pragma acc loop seq
        60, #pragma acc loop seq
    57, Complex loop carried dependence of B->, A->, stencil prevents parallelization
    59, Complex loop carried dependence of stencil prevents parallelization
        Loop carried dependence of B-> prevents parallelization
        Loop carried backward dependence of B-> prevents vectorization
        Complex loop carried dependence of B->, A-> prevents parallelization
    60, Complex loop carried dependence of stencil, B->, A-> prevents parallelization
        Loop carried dependence of B-> prevents parallelization
        Loop carried backward dependence of B-> prevents vectorization
```

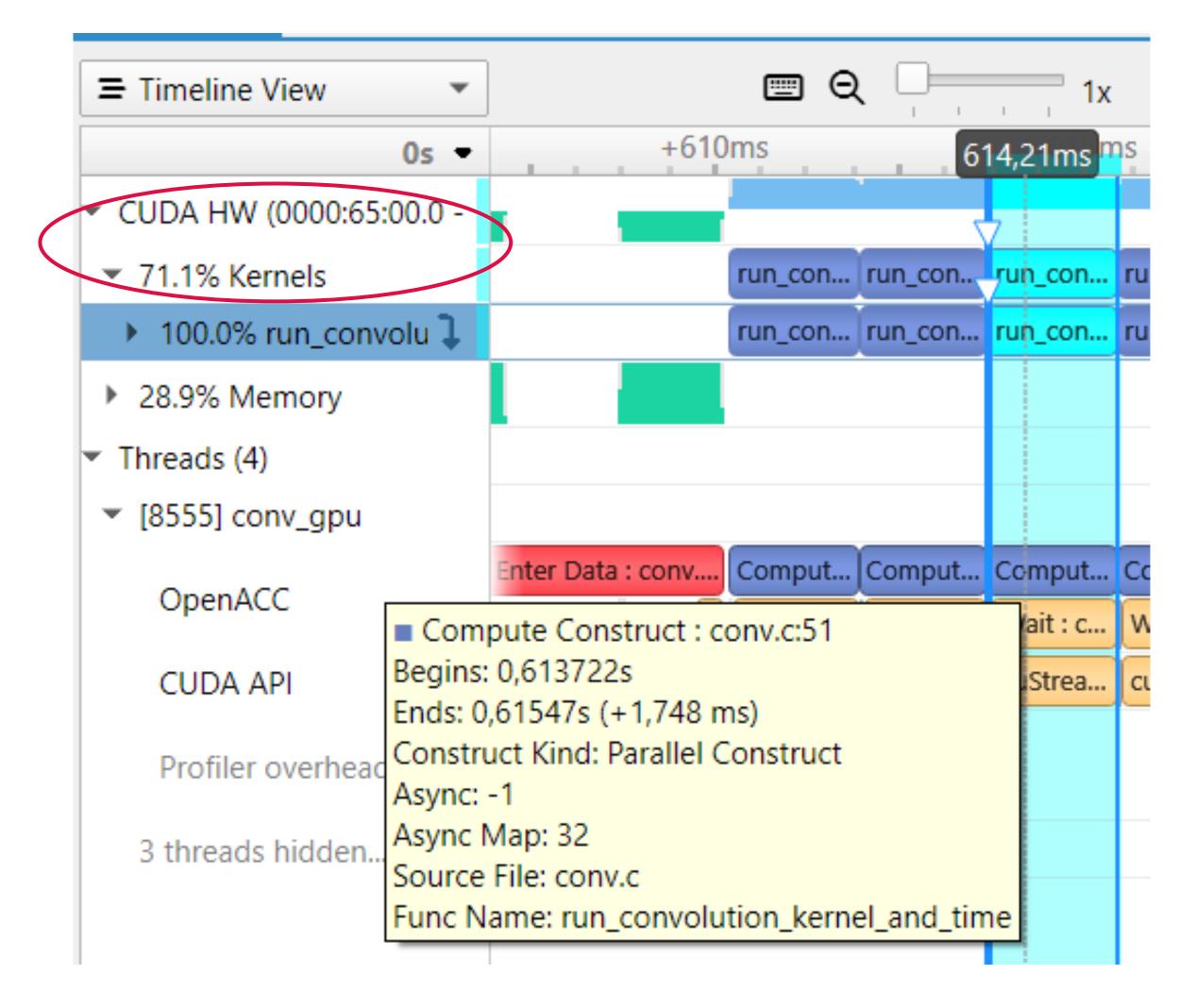
## Locating kernels - Nsight Systems timeline

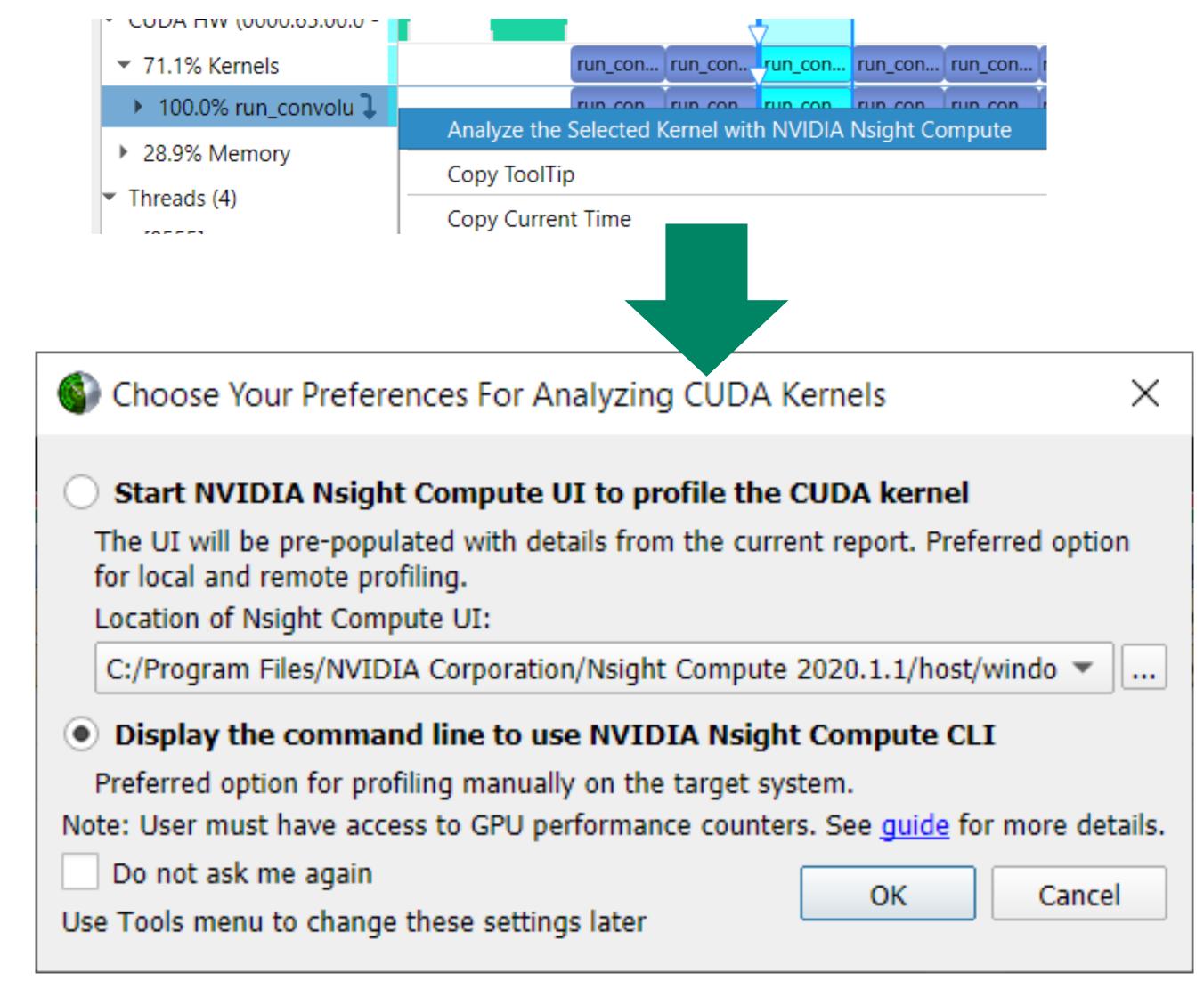
...and how to get to Nsight Compute for kernels

- Record timeline
  - nsys profile -t cuda, openacc -o task1\_initial ./conv\_gpu 3
- Locate kernel and get command line

• ncu --kernel-name run\_convolution\_kernel\_and\_time\_51\_gpu --launch-skip 2 --launch-count 1

"./conv\_gpu" 3







## Using Nsight Compute

- Very powerful and configurable tool
- Command line mode: Useful for quick experiments
- Export into report file, "-o output\_filename"
  - Transfer report to local machine, inspect metrics, charts, etc.
- Other recommended options:
  - "--set full" ensures you record all metrics (collections takes longer)
  - "--import-source on" ensures the report embeds source file in current optimization state
- Ensure you only record what you need, use the "skip" and "count" options, short -s and -c

### Task 1

- 1. Directory task 1/
- 2. Run the GPU version: Just type "make" (and look at the executed command line)
- 3. Identify potential issues
  - 1. Check profiler output, "make ncu"
  - 2. Also try "make NV\_ACC\_TIME=1" (or NOTIFY)
  - 3. Closely look at compiler output.
- 4. Look for TODO and implement collapse clause
- 5. Note down new time, and also record a profile via "make profile" (you will need it later)

#### Task 1 - Results

NCU output:

Section: Launch Statistics

Block Size 128

Function Cache Configuration cudaFuncCachePreferNone

Grid Size 32

Registers Per Thread register/thread 38

Shared Memory Configuration Size Kbyte 32.77

Driver Shared Memory Per Block Kbyte/block 1.02

Dynamic Shared Memory Per Block byte/block 0

Static Shared Memory Per Block byte/block 0

Threads thread 4096

Waves Per SM 0.02

\_\_\_\_\_\_

WRN The grid for this launch is configured to execute only 32 blocks, which is less than the GPU's 108 multiprocessors.

#### Task 1 - Results

```
    NV_ACC_TIME command line output:

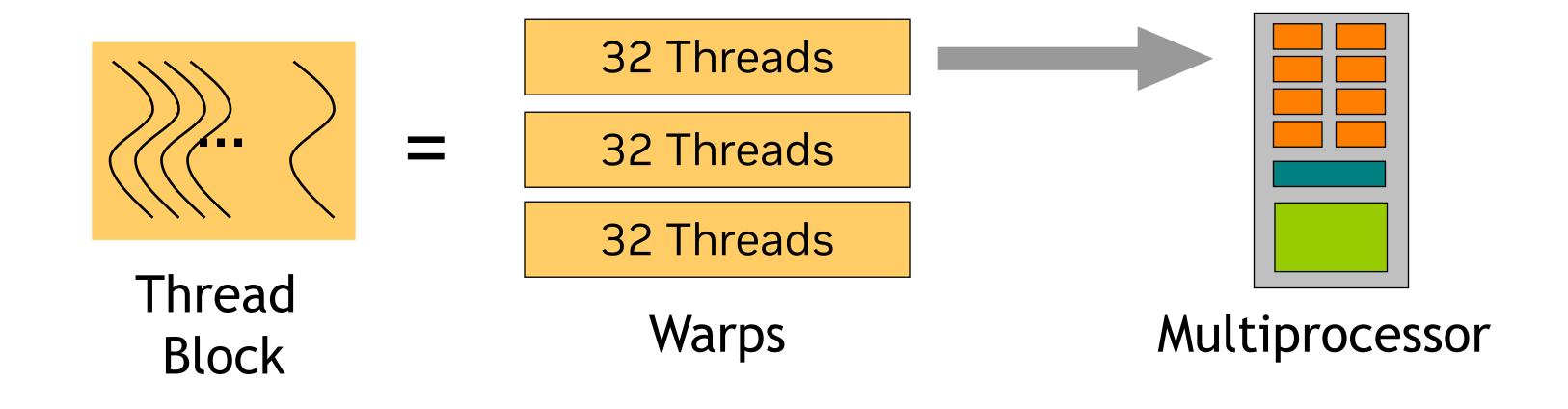
$ make NV_ACC_TIME=1
./conv_gpu 3
    51: compute region reached 15 times
        51: kernel launched 15 times
            grid: [32] block: [128]
            elapsed time(us): total=842,551 max=74,560 min=50,411 avg=56,170

    Before/after: 56 ms vs. 2.4 ms!

    Relevant profiler output

 51, Generating NVIDIA GPU code
         56, #pragma acc loop gang, vector(128) collapse(2) /* blockIdx.x threadIdx.x */
               /* blockIdx.x threadIdx.x collapsed */
         59, #pragma acc loop seq
         60, #pragma acc loop seq
```

## CUDA Warps



A thread block consists of a groups of warps

A warp is executed physically in parallel (SIMT) on a multiprocessor

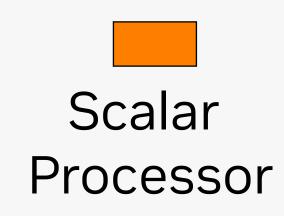
Currently all NVIDIA GPUs use a warp size of 32

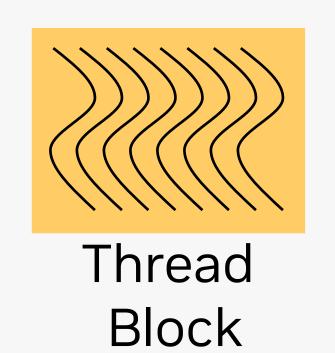
#### CUDA Execution Model

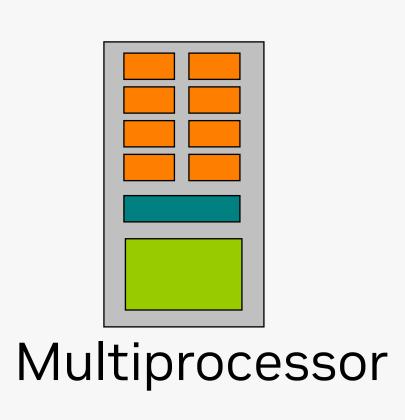
#### Software

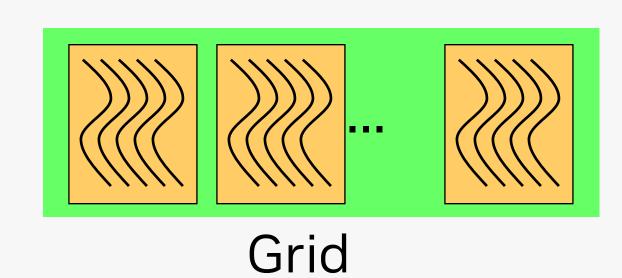
#### Hardware

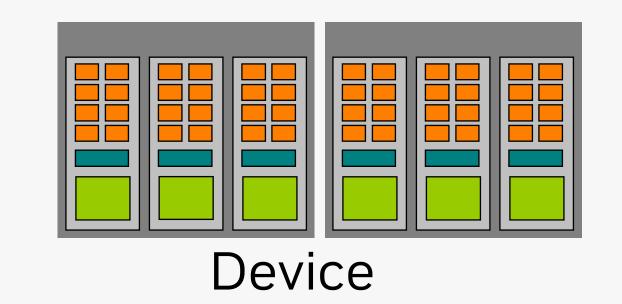












Threads are executed by scalar processors

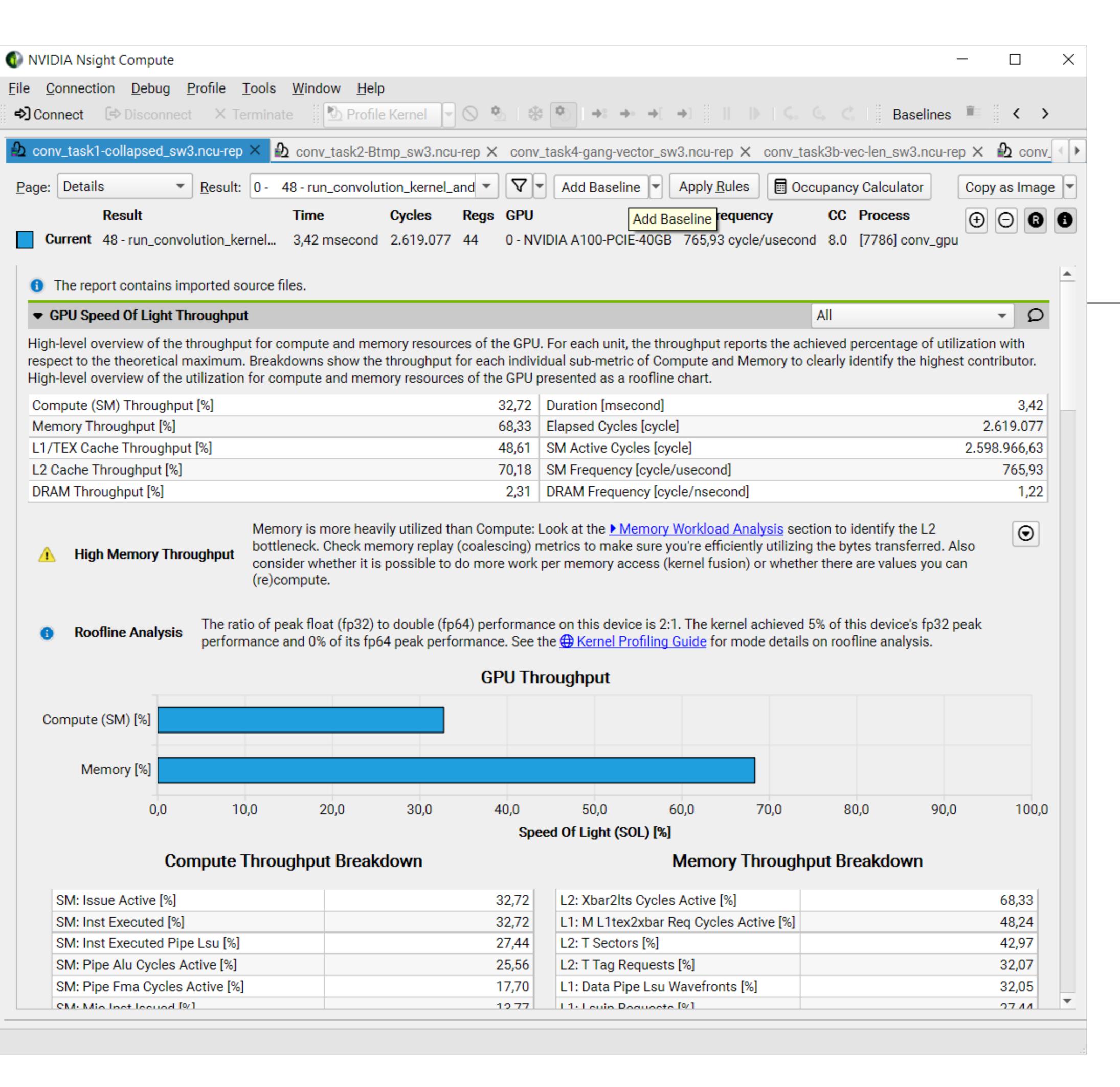
Thread blocks are executed on multiprocessors (SMs)

Thread blocks do not migrate

Several concurrent thread blocks can reside on one multiprocessor - limited by multiprocessor resources (shared memory and register file)

A kernel is launched as a grid of thread blocks

Blocks and grids can be multi dimensional (x,y,z)



## Using the Nsight Compute GUI

Profile from task 1

- Baseline feature compare results
- Data-driven,
- SoL throughput: Tables
- Consider warnings/hints from rules

## What is a loop-carried dependence?

- Compiler output:
  - 59, Complex loop carried dependence of stencil prevents parallelization Loop carried dependence of B-> prevents parallelization Loop carried backward dependence of B-> prevents vectorization Complex loop carried dependence of B->, A-> prevents parallelization
    60, Complex loop carried dependence of stencil, B->, A-> prevents parallelization
- Loop carried dependence of B-> prevents parallelization

  Loop carried backward dependence of B-> prevents vectorization
- Code this refers to

## Task 2: Remove the dependence

- Directory task2/
- 2. Check compiler output: loop carried dependence
- 3. Look for TODOs and break the dependency
- 4. What is the new runtime? Can you see why?
- 5. Record a profile via "make profile"
  - 1. Try to compare it with the profile from task 1

#### Task 2 - Results

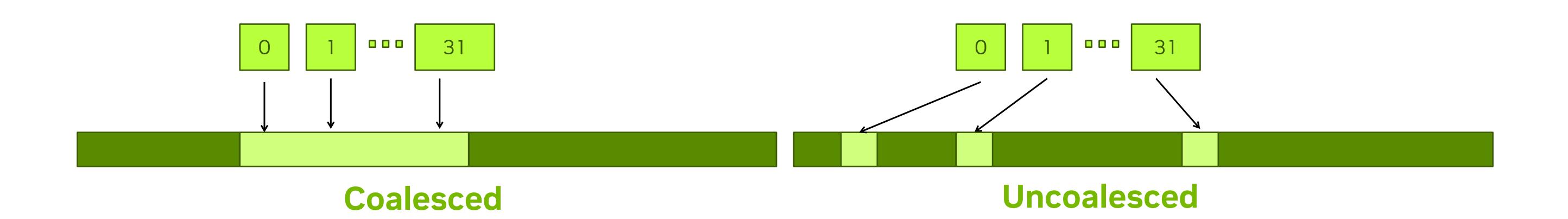
- Code should've gotten much slower again, about 180 ms
- The compiler was able to parallelize the inner loop
- 51, Generating NVIDIA GPU code

```
56, #pragma acc loop gang collapse(2) /* blockIdx.x */
```

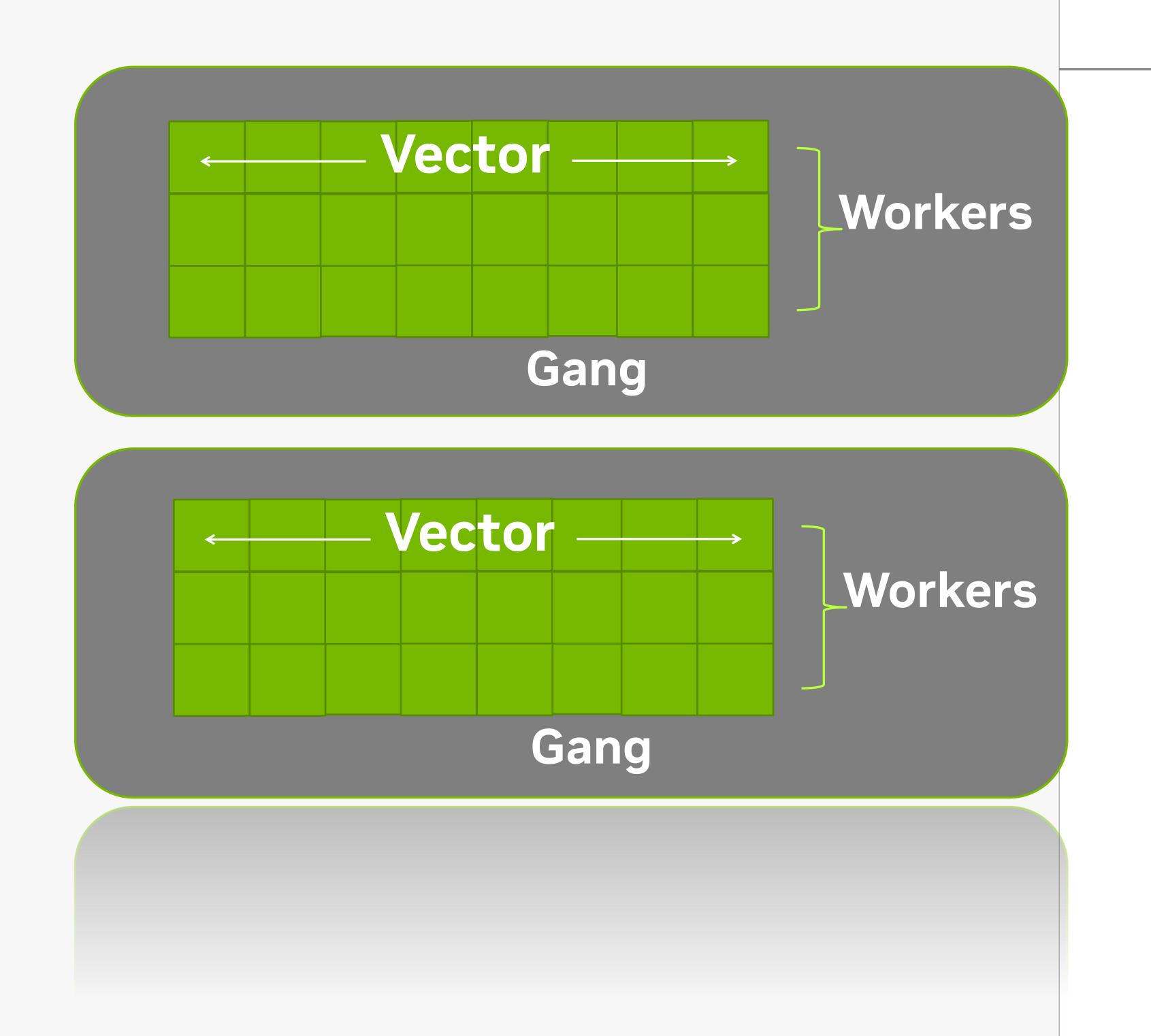
- 57, /\* blockIdx.x collapsed \*/
- 59, #pragma acc loop seq
- 60, #pragma acc loop vector(128) /\* threadIdx.x \*/
  Generating implicit reduction(+:B\_tmp)
- 59, Loop is parallelizable
- 60, Loop is parallelizable
- But why is this slower?
  - Memory access patterns
  - Extra reduction

# Memory Coalescing

- Coalesced access:
  - A group of 32 contiguous threads ("warp") accessing adjacent elements
  - Few transactions and high utilization
- Uncoalesced access:
  - A warp of 32 threads accessing scattered elements
  - Many transactions and low utilization
- For best performance threadIdx.x should access contiguously



## OpenACC: 3 Levels of Parallelism



- Vector threads work in lockstep (SIMD/SIMT parallelism)
- Workers have 1 or more vectors
- Gangs have 1 or more workers and share resources (such as a cache, the SM, etc.)
- Multiple gangs work independently of each other

## Mapping OpenACC to CUDA

- The compiler is free to do what it wants
- In general

gang: mapped to blocks (COARSE GRAIN)

worker: mapped to threads (FINE GRAIN)

vector: mapped to threads (FINE SIMD/SIMT)

- Exact mapping is compiler dependent
- Performance Tips
  - Use a vector size that is divisible by 32
  - Block size is num\_workers \* vector\_length

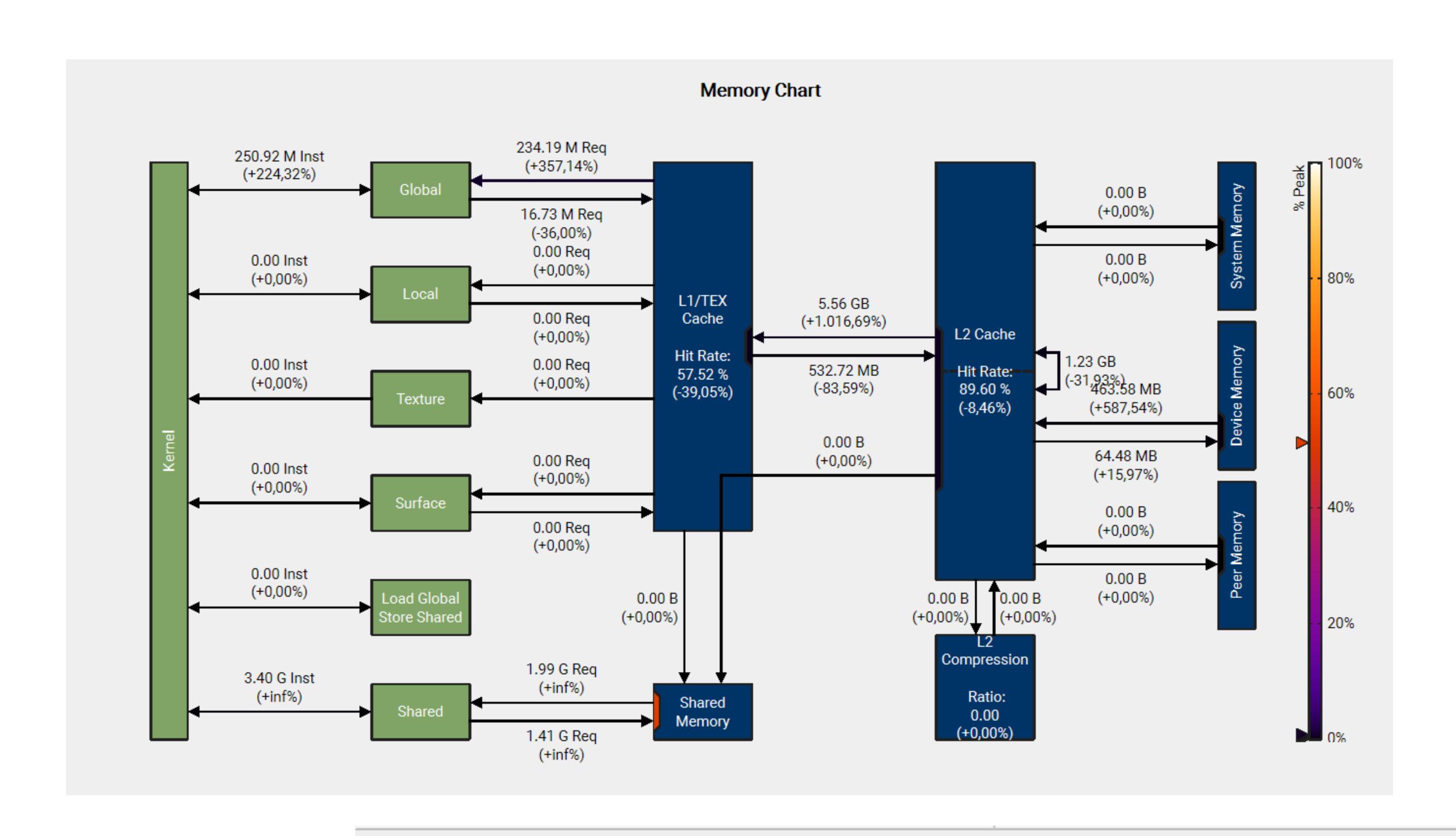
## OpenACC gang, worker, vector clauses

- Gang, worker, vector can be added to a loop clause
- Control the size using the following clauses on the parallel region
  - Parallel: num\_gangs(n), num\_workers(n), vector\_length(n)
  - Kernels: gang(n), worker(n), vector(n)
  - Note: We have not used "worker" parallelism in our example



## Nsight Compute profile

A closer look at Task 2





Uncoalesced Global Accesses

This kernel has uncoalesced global accesses resulting in a total of 188148180 excessive sectors (43% of the total 439069680 sectors). Check the L2 Theoretical Sectors Global Excessive table for the primary source locations. The 

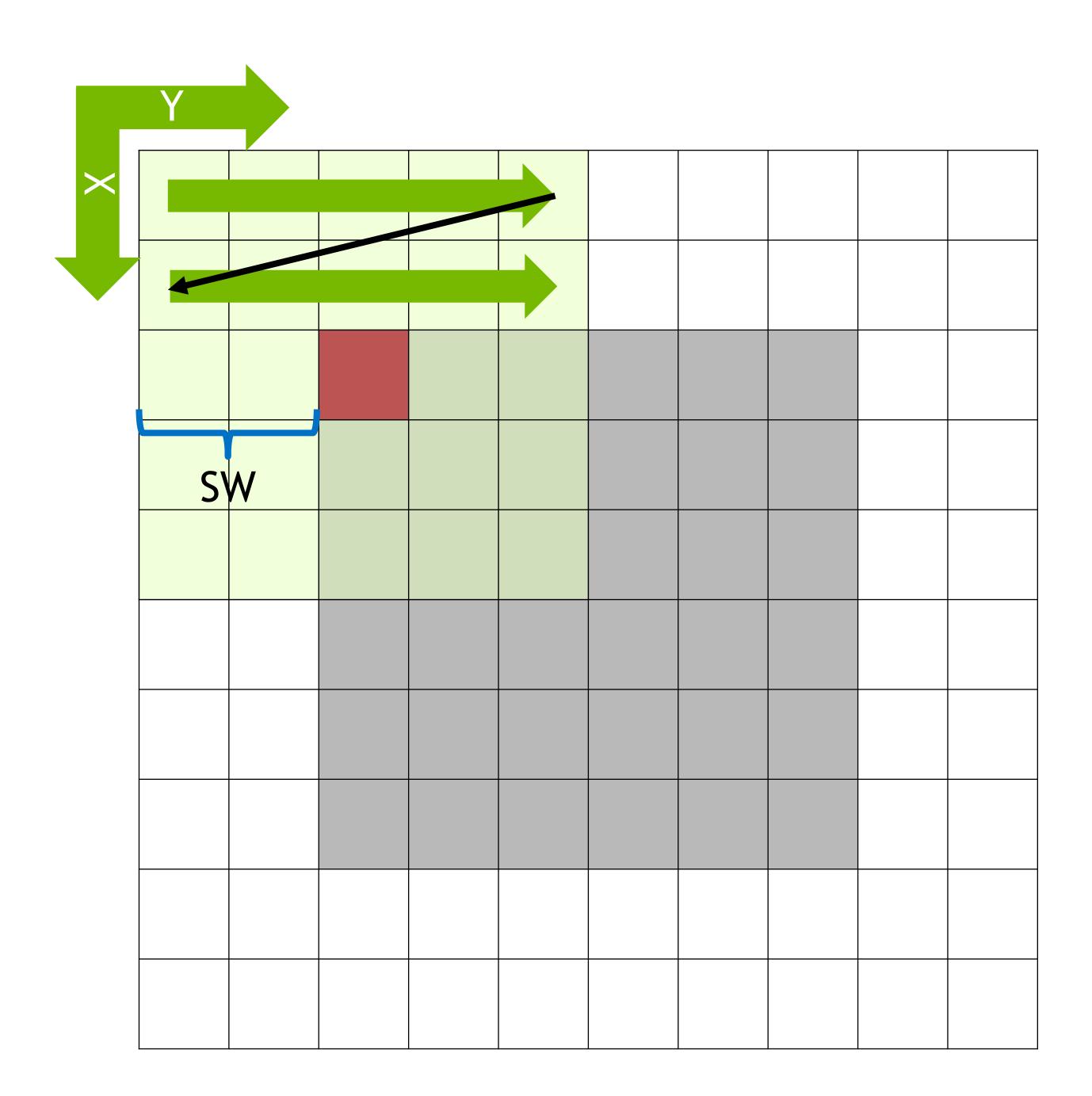
CUDA Programming Guide had additional information on reducing uncoalesced device memory accesses.

#### Task 3: Understand slowdown and test fixes

- 1. Directory task3/
- 2. Use compiler output, and Nsight Compute, try to undestand memory access patterns
  - 1. Look for memory traffic, worse cache hit rates, uncoalesced access %,
    - 1. also mem tables: global load vs. store less stores (reduction), but a lot more loads
- 3. See TODOs to implement one variant (optionally: draw yourself a diagram on paper!)
  - 1. Outer stencil as vector loop
  - 2. Add vector\_length(32)
- 4. Record a profile and compare again

## Task 3 - Results

- Outer stencil as vector loop: 47 ms
  - Add vector\_length(32): 17.3 ms
  - Still: Have not recovered original performance
- Why does length help?
  - Only 49 points, i.e. (3+1+3)^2



## Task 4: Recover and improve performance

- 1. Directory task4/ (and solution/)
- 2. Follow the single TODO and measure the runtime
- 3. Record a profile (again "make profile")
- 4. Can you find clues on the optimality of the solution?
  - 1. Hint: look at the roofline diagram
- 5. Can you improve it further?

## Task 4 - Results

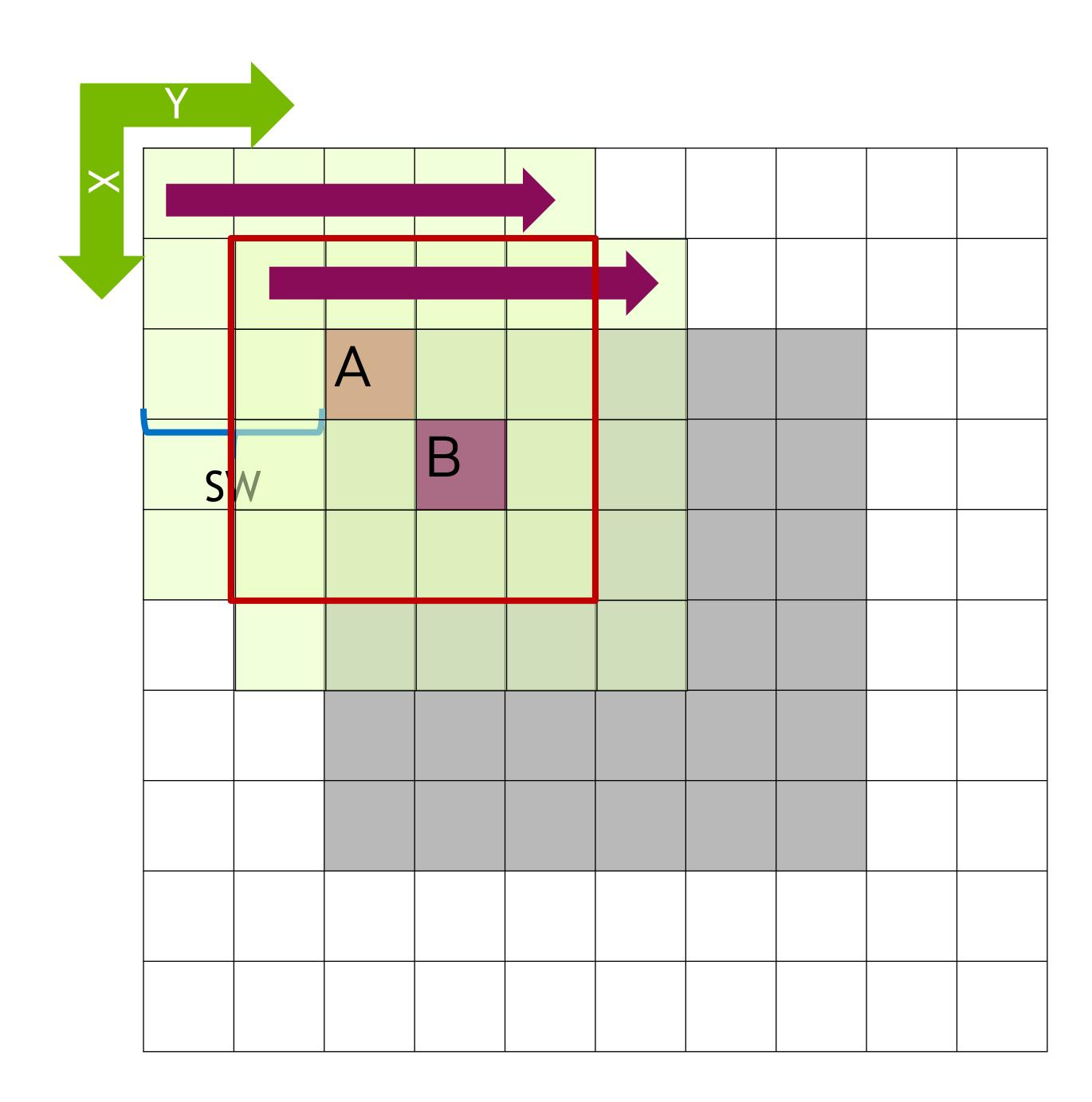
- Runtime about 1.5 ms
- Memory is now (again) more cache-friendly
  - 56, #pragma acc loop gang, vector(128) collapse(2) /\* blockldx.x threadldx.x \*/

```
56: for (int x = sw; x < N - sw; ++x) {
57: for (int y = sw; y < N - sw; ++y) {
```

Accesses to input data:

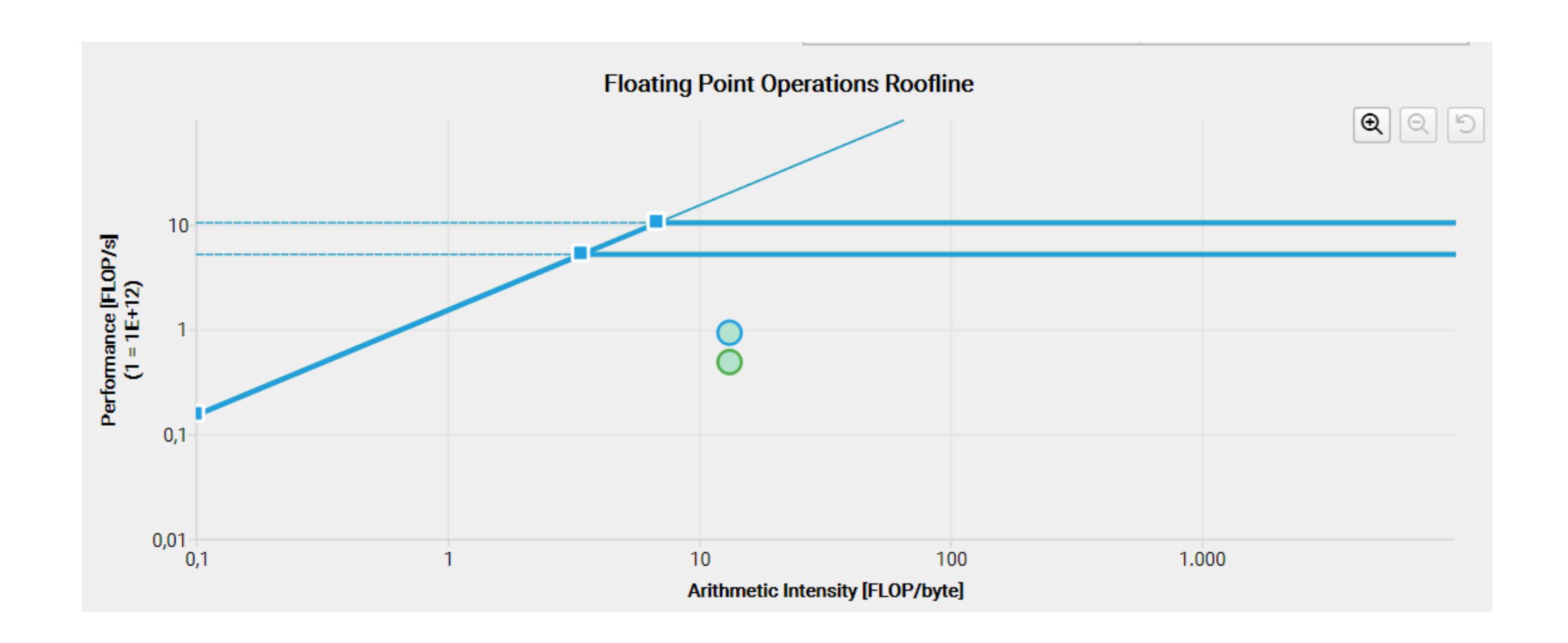
$$A[x + sx][y + sy];$$

- Outer loop over rows, inner loop over columns
- Temporal and spatial locality: Each thread loops over its stencil area
  - Neighboring threads from surrounding blocks share cached data



## Roofline model

- Powerful tool to judge how well hardware is utilized
- FLOPs vs. Al "how often is each transferred byte used"
- Compute bound, but below roof
  - Inefficiencies in memory accesses



# Summarizing the Steps

Task	Action taken	Time [ms]
Serial version, starting point	None	1200
Task 0	Add "parallel loop"	165 (multicore) 56 (GPU)
Task 1	Collapse outer loops, expose parallelism	2.4
Task 2	Break loop-carried dependency with B_tmp, causes compiler to apply "vector" to innermost loop, add reduction	
Task 3a	Move "vector" to second- outermost loop	46
Task 3b	Use shorter vector_length(32)	17.3
Task 4	Outermost collapsed loop as "gang vector" on top of B_tmp	1.5

## Further tinkering

- Compare stencil size: How does runtime scale with it?
  - small size sw=2, latency effects
- Experiment with different stencil sizes (2, 3, 5)
  - don't forget reference data
- You can adapt the stencil to actually perform image filtering operations
  - Simple image loading libraries available
  - Note: We did not normalize stencil coefficients don't forget to do so

#### Conclusion

- The Nsight Profilers can be used to identify performance bottlenecks in applications and OpenACC Kernels
  - But most importantly, combine with knowledge of code
  - Closely look at compiler output
- Coalescing memory accesses is important for performance
  - Ordering of loop clauses can have large impact
- Iterative methods and workflow look for clues, experiment, compare!

