

Porting Jacobi on Perlmutter using OpenMP and OpenACC

Lecture 11

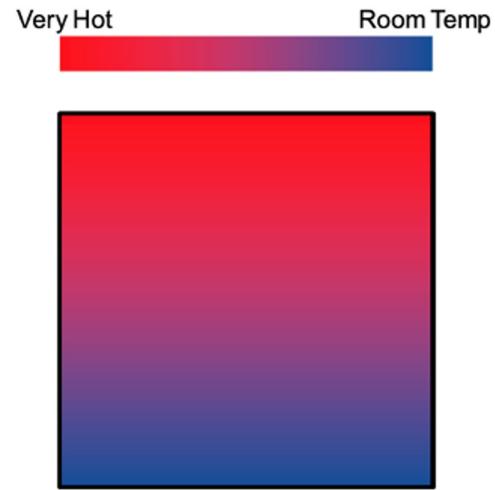
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PDC Summer School, Aug 2023
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- Laplace Serial code – example

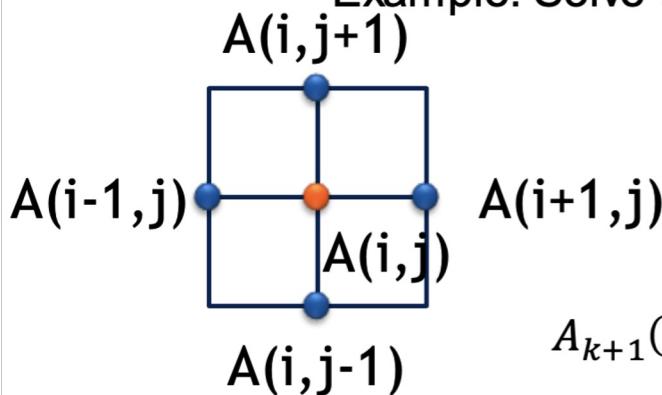
Laplace Heat Transfer

- A simple simulation of heat distributing across a metal plate
- Apply a consistent heat to the top of the plate
- Simulating the heat distribution across the plate



EXAMPLE: JACOBI ITERATION

- Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.
- Common, useful algorithm
 - Example: Solve Laplace equation in 2D: $\nabla^2 f(x, y) = 0$



$$A_{k+1}(i, j) = \frac{A_k(i - 1, j) + A_k(i + 1, j) + A_k(i, j - 1) + A_k(i, j + 1)}{4}$$

```
while ( error > tol && iter < iter_max )  
{  
    error = 0.0;
```

Iterate until converged

```
for( int j = 1; j < n-1; j++ )  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1] + A[j-1][i] + A[j+1][i]);  
        error = fmax( error, fabs(Anew[j][i] - A[j][i]));  
    }  
}
```

Iterate across matrix elements

Calculate new neighbors

Compute max error for convergence

```
for( int j = 1; j < n-1; j++ )  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        A[j][i] = Anew[j][i];  
    }  
}
```

Swap input/output arrays

Profiling Sequential Code

Profile your code to obtain detailed information about how does the code runs:

- Total runtime
- runtime of routines
- Hardware counters

Identify portions that took longer to execute. These are the portions that you will want to parallelize.

LLVM

```
$ clang -Ofast -fopenmp -fno-inline -pg -o jacobi-serial jacobi.c
Jacobi relaxation Calculation: 4096 x 4096 mesh
    0, 0.250000
    100, 0.002397
    200, 0.001204
    300, 0.000804
    400, 0.000603
    500, 0.000483
    600, 0.000403
    700, 0.000345
    800, 0.000302
    900, 0.000269
total: 25.557923 s
```

to use gprof
add **-pg** to
compile the
application

Serial code with Nvidia nvc, performs similar to LLVM

NVC

```
$ nvc -O3 -o jacobi-serial jacobi.c
Jacobi relaxation Calculation: 4096 x 4096 mesh
    0, 0.250000
    100, 0.002397
    200, 0.001204
    300, 0.000804
    400, 0.000603
    500, 0.000483
    600, 0.000403
    700, 0.000345
    800, 0.000302
    900, 0.000269
total: 23.364053 s
```

Table of content

- Laplace Serial code – example
- Parallelization using target parallel for

```
while ( error > tol && iter < iter_max )  
{  
    error = 0.0;
```

Parallelize first loop next
OpenMP requires reduction
clause

```
//#pragma acc parallel loop copy(A[ :m*n],Anew[ :m*n])  
#pragma omp target parallel for map(tofrom: A[ :m*n],Anew[ :m*n]) \  
reduction(max:error)  
for( int j = 1; j < n-1; j++)  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1] + A[j-1][i] + A[j+1][i]);  
        error = fmax( error, fabs(Anew[j][i] - A[j][i]));  
    }  
}
```

```
//#pragma acc parallel loop copy(A[ :m*n],Anew[ :m*n])  
#pragma omp target parallel for map(tofrom: A[ :m*n],Anew[ :m*n])  
for( int j = 1; j < n-1; j++)  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        A[j][i] = Anew[j][i];  
    }  
}
```

Parallelize second loop

Build and run the code

- Using Perlmutter
- Module load nvhpc/23.1
- Target which architecture you want to use to compile and execute the code; for example
- Using OpenMP offloading
 - nvc -fast **-mp=gpu** -Minfo=all <source_code.c> -o <executable>
 - **-mp=gpu**: denotes that the target gpu
 - -fast: an optimization flag that you can add to your compilation command
 - -Minfo=all: gives you information about what parts of the code were accelerated
- Check for
 - “Generating GPU kernel”
 - Proof that your code generated GPU code

NVC

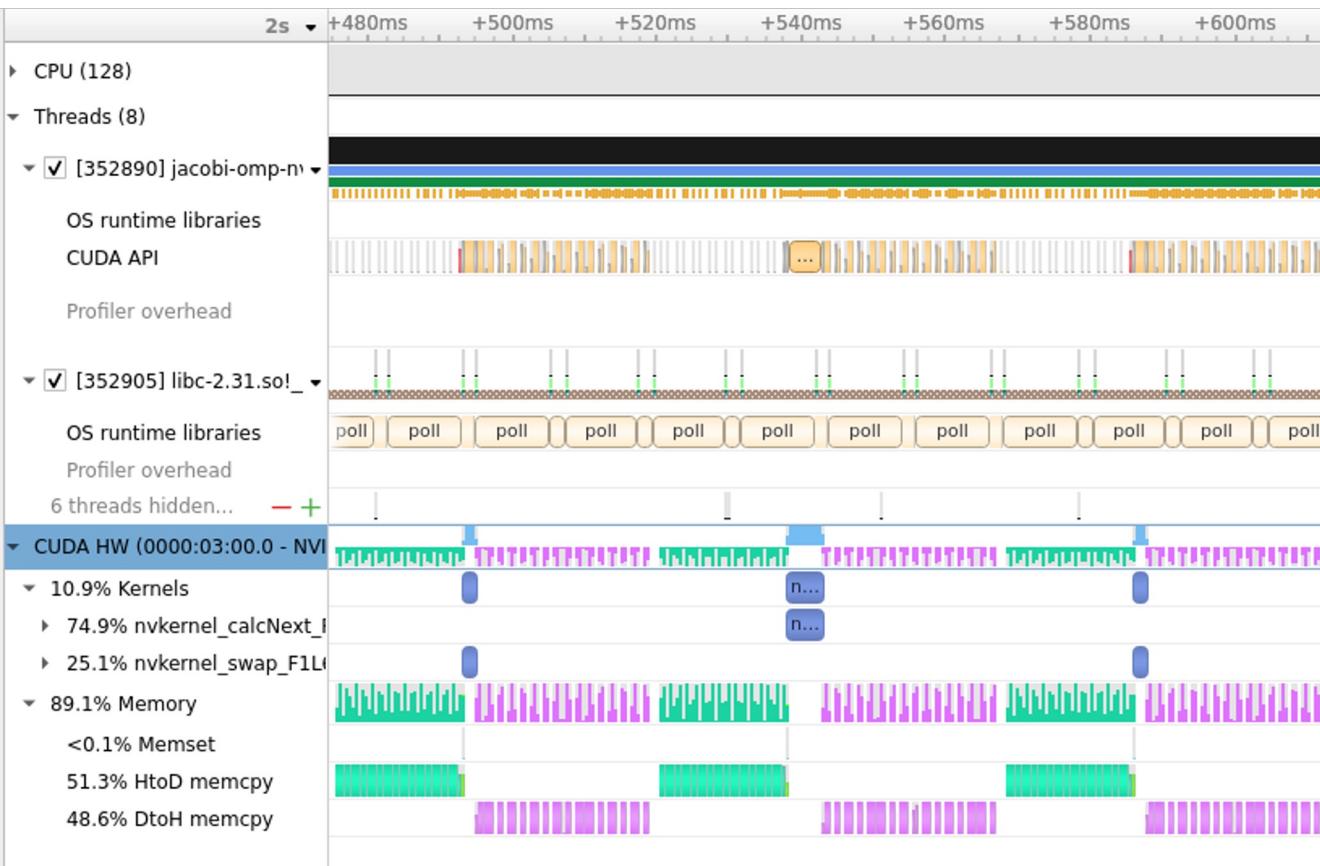
```
$ nvc -fast -mp=gpu -Minfo=all -o jacobi-omp-nvc-loop jacobi.c
initialize:
    41, Generated vector SIMD code for the loop
calcNext:
    52, #omp target parallel do
        52, Generating "nvkernel_calcNext_F1L52_2" GPU kernel
            Generating reduction(max:error)
            Loop parallelized across threads(128), schedule(static)
    52, Generating map(tofrom:A[:n*m],Anew[:n*m],error)
        Loop not vectorized/parallelized: not countable
    54, Generated vector SIMD code for the loop containing
reductions
    60, Loop not vectorized/parallelized: not countable
swap:
    65, #omp target parallel do
        65, Generating "nvkernel_swap_F1L65_5" GPU kernel
        68, Loop parallelized across threads(128), schedule(static)
    65, Generating map(tofrom:Anew[:n*m],A[:n*m])
    70, Memory copy idiom, loop replaced by call to __c_mcopy8
main:
    113, initialize inlined, size=10 (inline) file jacobi.c (37)
        41, Loop not fused: function call before adjacent loop
            Generated vector SIMD code for the loop
    121, Loop not vectorized/parallelized: potential early exits
    136, deallocate inlined, size=2 (inline) file jacobi.c (78)
```

```
Jacobi relaxation
Calculation: 4096 x 4096
mesh
    0, 0.250000
    100, 0.002397
    200, 0.001204
    300, 0.000804
    400, 0.000603
    500, 0.000483
    600, 0.000403
    700, 0.000345
    800, 0.000302
    900, 0.000269
total: 89.513495 s
```

Using OpenMP offloading -

Accelerated code using parallel and no data clauses takes 89.51 on GPUs
about 4 times slower than serial

Using Nsight System



nvkernel_calcNext_F1L52_2
Begins: 2.63115s
Ends: 2.63503s (+3.885 ms)
grid: <<<108, 1, 1>>>
block: <<<128, 1, 1>>>
Launch Type: Regular
Static Shared Memory: 16 bytes
Dynamic Shared Memory: 1,656 bytes
Registers Per Thread: 54
Local Memory Per Thread: 0 bytes
Local Memory Total: 127,401,984 bytes
Shared Memory executed: 65,536 bytes
Shared Memory Bank Size: 4 B
Theoretical occupancy: 56.25 %
Launched from thread: 352890
Latency: ~7.512 µs
Correlation ID: 716
Stream: Stream 16

Using LLVM OpenMP Offloading and NVIDIA A100

LLVM

```
$ clang -Ofast -fopenmp --offload-arch=native -g -Rpass=openmp-opt -Rpass-missed=openmp-opt -Rpass-analysis=openmp-opt -o jacobi-omp-llvm-loop jacobi.c
remark: Found thread data sharing on the GPU. Expect degraded performance due to data
globalization. [OMP112] [-Rpass-missed=openmp-opt]
```

Jacobi relaxation
Calculation: 4096 x 4096
mesh
0, 0.250000
100, 0.002397
200, 0.001204
300, 0.000804
400, 0.000603
500, 0.000483
600, 0.000403
700, 0.000345
800, 0.000302
900, 0.000269
total: 242.194770 s

<https://openmp.llvm.org//remarks/OptimizationRemarks.html>

<https://openmp.llvm.org//remarks/OMP112.html#omp112>

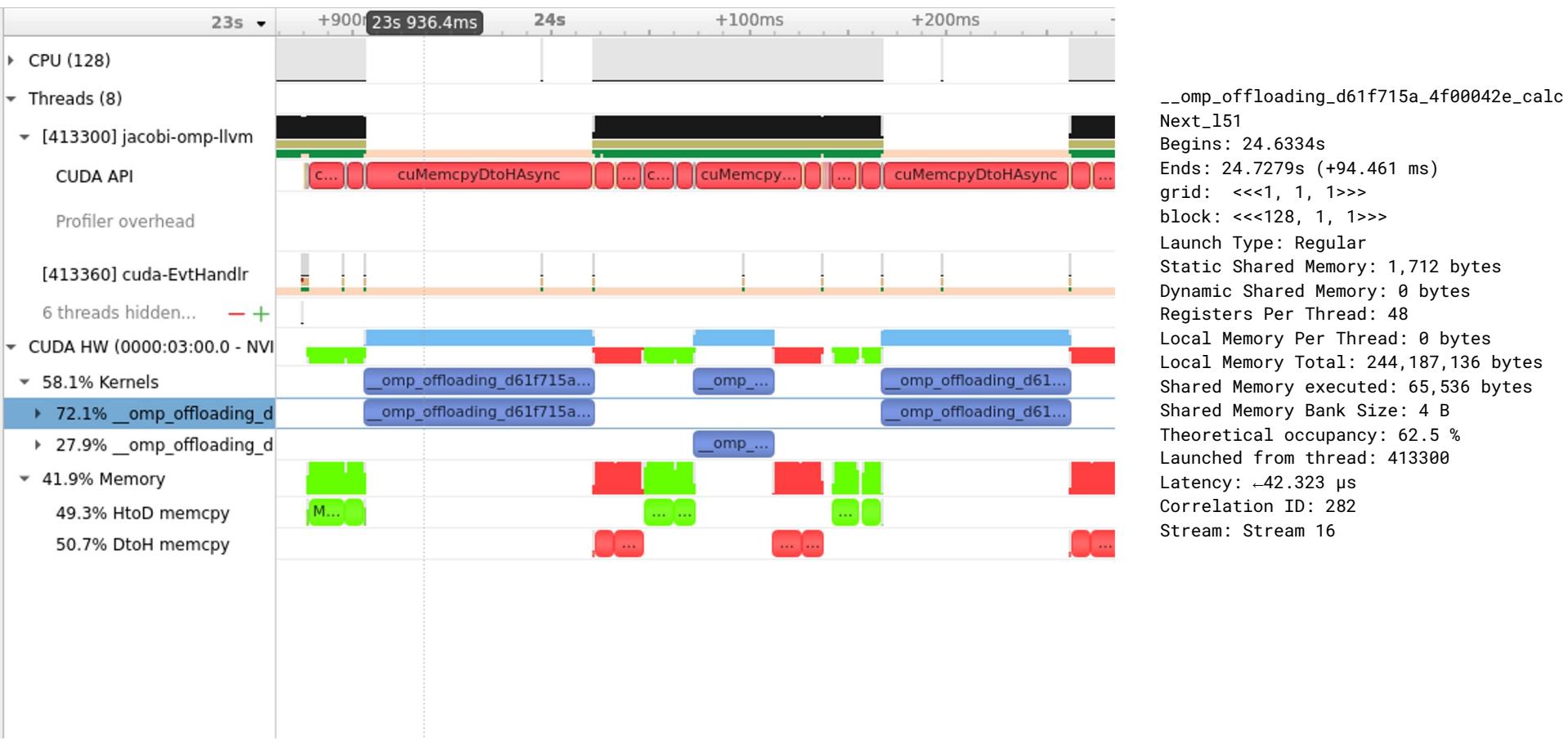
This missed remark indicates that a globalized value was found on the target device that was not either replaced with stack memory by [OMP110](#) or shared memory by [OMP111](#). Globalization that has not been removed will need to be handled by the runtime and will significantly impact performance.

...

Using OpenMP offloading:

Accelerated code using parallel and no data clauses takes 242.19
on GPUs **about 10 times slower than serial**

Using Nsight System



Improving first openMP version

- The LLVM OpenMP offloading version is really slow
- Adding **teams distribute**, improves it significantly

```
while ( error > tol && iter < iter_max )  
{  
    error = 0.0;
```

Parallelize first loop adding
teams distribute
OpenMP requires reduction
clause

```
##pragma acc parallel loop copy(A[:m*n],Anew[:m*n])  
#pragma omp target teams distribute parallel for \  
map(tofrom: A[:m*n],Anew[:m*n]) reduction(max:error)  
for( int j = 1; j < n-1; j++)  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1] + A[j-1][i] + A[j+1][i]);  
        error = fmax( error, fabs(Anew[j][i] - A[j][i]));  
    }  
}
```

```
##pragma acc parallel loop copy(A[:m*n],Anew[:m*n])  
#pragma omp target teams distribute parallel for \  
map(tofrom: A[:m*n],Anew[:m*n])  
for( int j = 1; j < n-1; j++)  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        A[j][i] = Anew[j][i];  
    }  
}
```

Parallelize second loop

NVC

```
$ nvc -fast -mp=gpu -Minfo=all -o jacobi-omp-nvc-loop jacobi.c
initialize:
    41, Generated vector SIMD code for the loop
calcNext:
    52, #omp target teams distribute parallel for
        52, Generating "nvkernel_calcNext_F1L52_2" GPU kernel
            Loop parallelized across teams and threads(128),
schedule(static)
    Generating reduction(max:error)
    52, Generating map(tofrom:A[:n*m],Anew[:n*m],error)
        Loop not vectorized/parallelized: not countable
    54, Generated vector SIMD code for the loop containing
reductions
    60, Loop not vectorized/parallelized: not countable
swap:
    65, #omp target teams distribute parallel for
        65, Generating "nvkernel_swap_F1L65_6" GPU kernel
        68, Loop parallelized across teams and threads(128),
schedule(static)
    65, Generating map(tofrom:Anew[:n*m],A[:n*m])
    70, Memory copy idiom, loop replaced by call to __c_mcopy8
main:
    113, initialize inlined, size=10 (inline) file jacobi.c (37)
        41, Loop not fused: function call before adjacent loop
            Generated vector SIMD code for the loop
    121, Loop not vectorized/parallelized: potential early exits
    136, deallocate inlined, size=2 (inline) file jacobi.c (78)
```

Jacobi relaxation
Calculation: 4096 x 4096
mesh

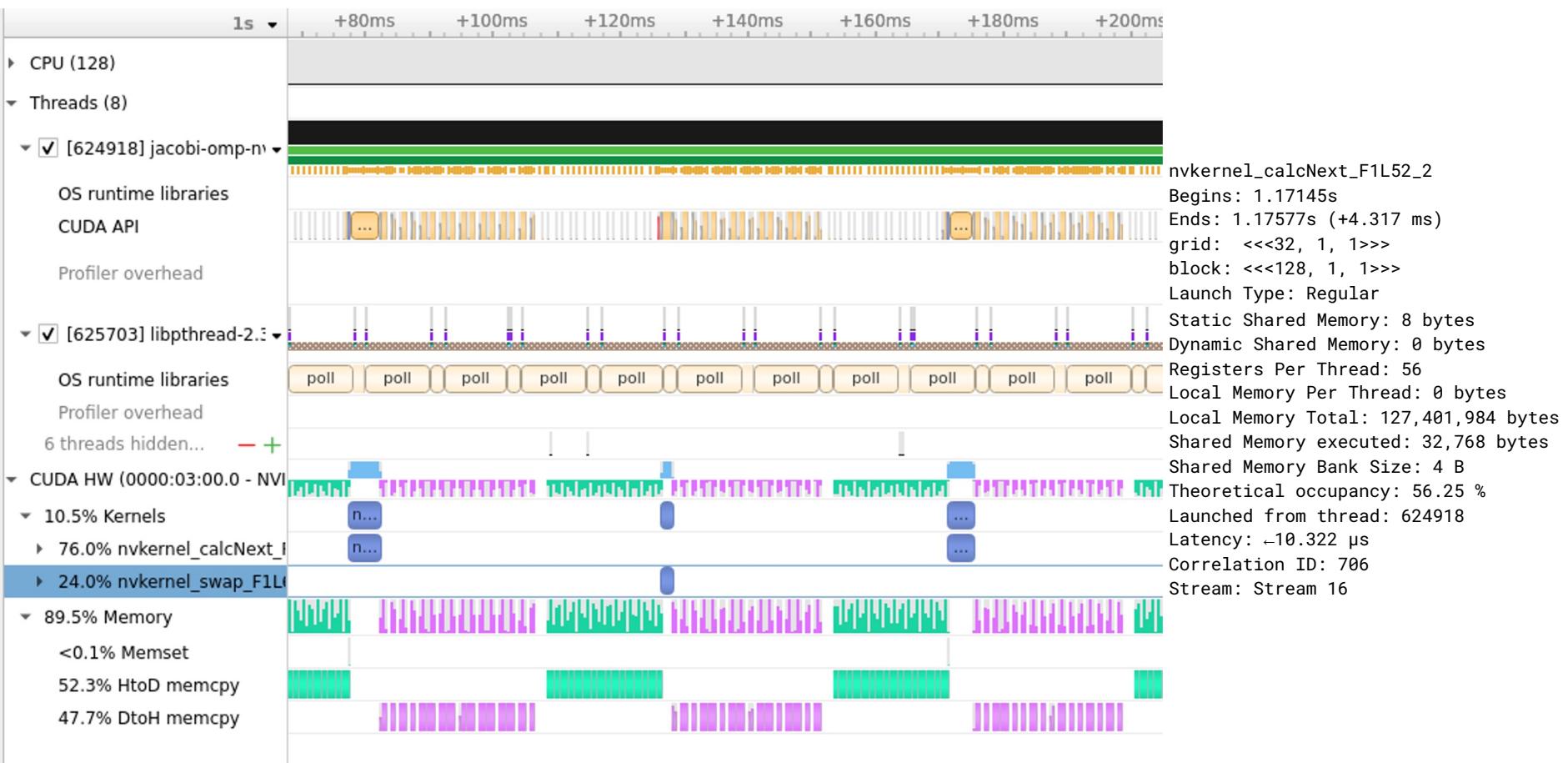
0,	0.250000
100,	0.002397
200,	0.001204
300,	0.000804
400,	0.000603
500,	0.000483
600,	0.000403
700,	0.000345
800,	0.000302
900,	0.000269

total: 89.992197 s

Using OpenMP Offloading:

Accelerated code using parallel and no data clauses takes 89.51 on GPUs
about 4 times slower than serial

Using Nsight System



Using LLVM OpenMP Offloading and NVIDIA A100

LLVM

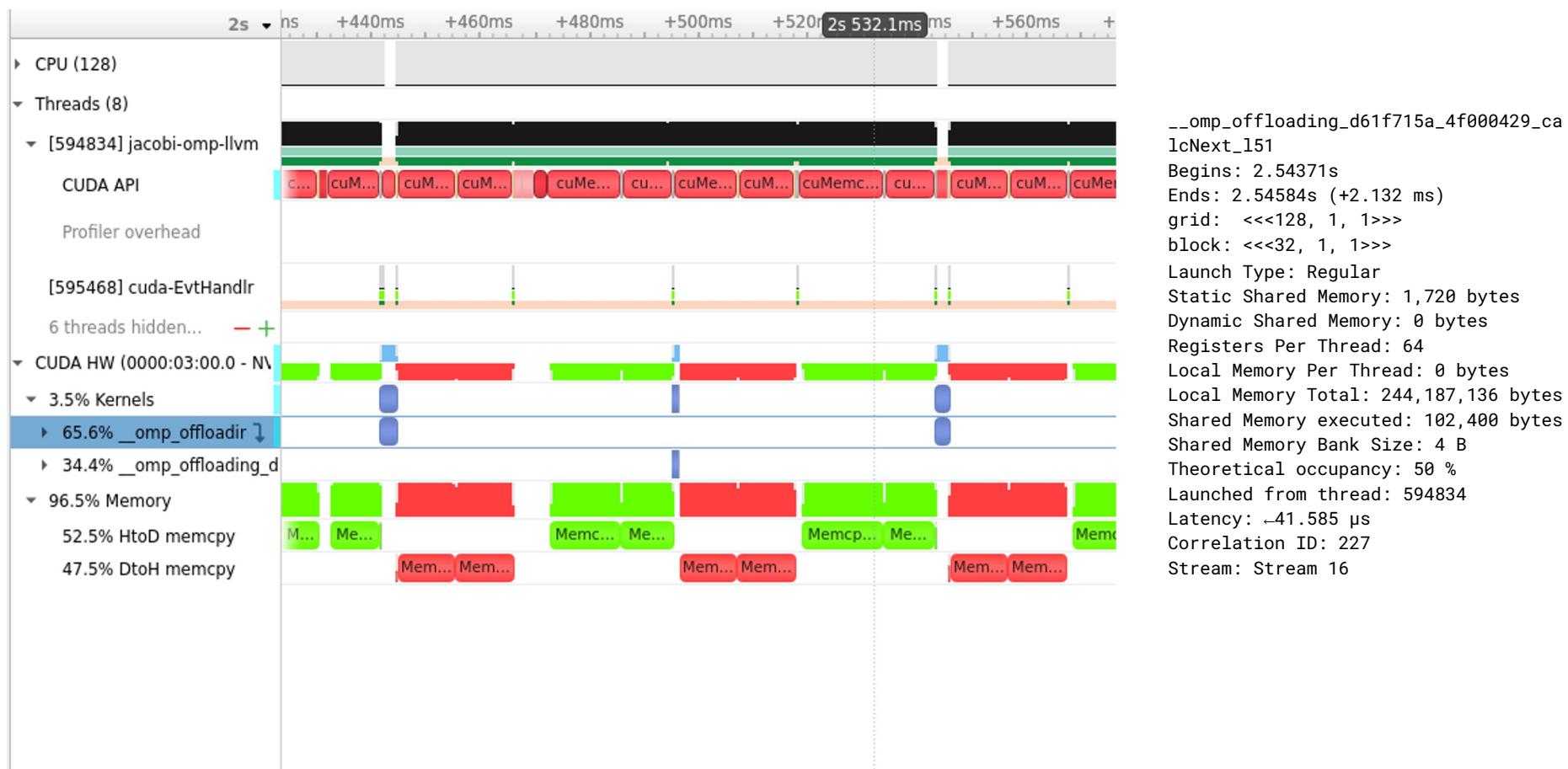
```
$ clang -Ofast -fopenmp --offload-arch=native -g -Rpass=openmp-opt -Rpass-missed=openmp-opt -Rpass-analysis=openmp-opt -o jacobi-omp-llvm-loop jacobi.c
remark: Found thread data sharing on the GPU. Expect degraded performance due to data
globalization. [OMP112] [-Rpass-missed=openmp-opt]
```

```
Jacobi relaxation
Calculation: 4096 x 4096
mesh
  0, 0.250000
  100, 0.002397
  200, 0.001204
  300, 0.000804
  400, 0.000603
  500, 0.000483
  600, 0.000403
  700, 0.000345
  800, 0.000302
  900, 0.000269
total: 100.463713 s
```

Using OpenMP offloading:

Accelerated code using parallel and no data clauses takes 242.19 on GPUs
about 10 times slower than serial

Using Nsight System



What was missing in the previous code?

Our next goal is to add data clauses to our code



Table of content

- Laplace Serial code – example
- Parallelization using target parallel for
- Parallelization with target parallel and data constructs

```
//#pragma acc data copy(A[:n*m]) create(Anew[:n*m])
#pragma omp target data map(to:A[:m*n],Anew[:m*n])
while ( error > tol && iter < iter_max )
{
    error = 0.0;
```

Create data on the GPUs

```
//#pragma acc parallel loop reduction(max:error) copy(A[:m*n],Anew[:m*n])
#pragma omp target teams distribute parallel for map(tofrom:
A[:m*n],Anew[:m*n]) reduction(max:error)
for( int j = 1; j < n-1; j++)
{
    for( int i = 1; i < m-1; i++ )
    {
        Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1] + A[j-1][i] + A[j+1][i]);
        error = fmax( error, fabs(Anew[j][i] - A[j][i]));
    }
}
```

Parallelize and
max reduction

```
//#pragma acc parallel loop copy(A[:m*n],Anew[:m*n])
#pragma omp target teams distribute parallel for
map(tofrom: A[:m*n],Anew[:m*n])
for( int j = 1; j < n-1; j++)
{
    for( int i = 1; i < m-1; i++ )
    {
        A[j][i] = Anew[j][i];
    }
}
```

Parallelize second loop

```
$ nvc -fast -mp=gpu -Minfo=all -o jacobi-omp-nvc-copy jacobi.c
initialize:
    41, Generated vector simd code for the loop
calcNext:
    52, #omp target teams distribute parallel for
        52, Generating "nvkernel_calcNext_F1L52_2" GPU kernel
            Loop parallelized across teams and threads(128),
schedule(static)
    Generating reduction(max:error)
    52, Generating map(tofrom:A[:n*m],Anew[:n*m],error)
        Loop not vectorized/parallelized: not countable
    54, Generated vector simd code for the loop containing
reductions
    60, Loop not vectorized/parallelized: not countable
swap:
    65, #omp target teams distribute parallel for
        65, Generating "nvkernel_swap_F1L65_6" GPU kernel
        68, Loop parallelized across teams and threads(128),
schedule(static)
    65, Generating map(tofrom:Anew[:n*m],A[:n*m])
    70, Memory copy idiom, loop replaced by call to __c_mcopy8
main:
    113, initialize inlined, size=10 (inline) file jacobi.c (37)
        41, Loop not fused: function call before adjacent loop
            Generated vector simd code for the loop
    122, Generating map(to:Anew[:m*n],A[:m*n])
        Loop not vectorized/parallelized: potential early exits
    137, deallocate inlined, size=2 (inline) file jacobi.c (78)
```

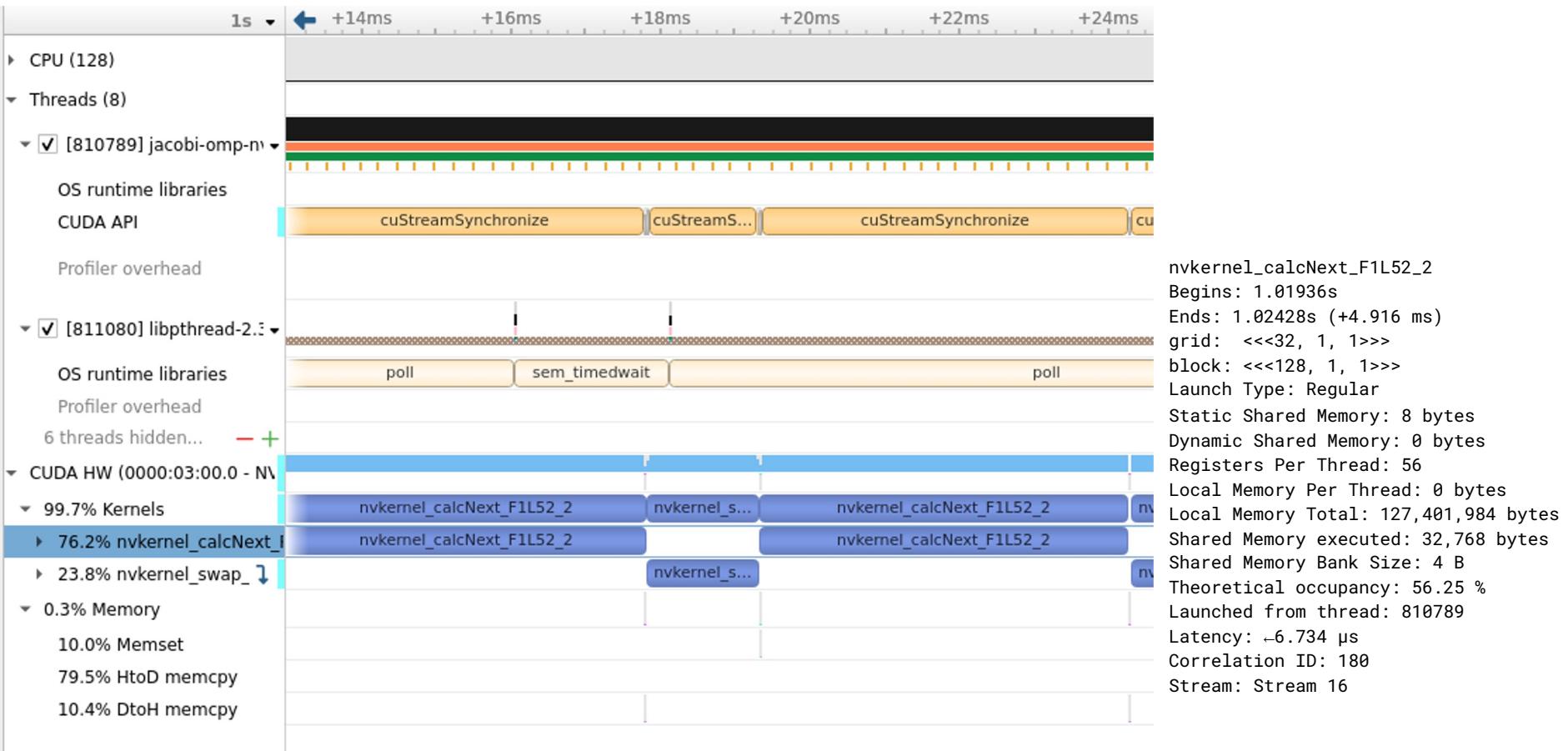
```
Jacobi relaxation
Calculation: 4096 x 4096
mesh
    0, 0.250000
    100, 0.002397
    200, 0.001204
    300, 0.000804
    400, 0.000603
    500, 0.000483
    600, 0.000403
    700, 0.000345
    800, 0.000302
    900, 0.000269
total: 6.215937 s
```

Using OpenMP offloading:

Accelerated code using parallel and data clauses taking 6.21s on GPUs using OpenMP offloading

OpenACC version 1.58s on GPUs

Using Nsight System



Using LLVM OpenMP Offloading and NVIDIA A100

```
$ clang -Ofast -fopenmp --offload-arch=native -g -o jacobi-omp-llvm-copy jacobi.c
```

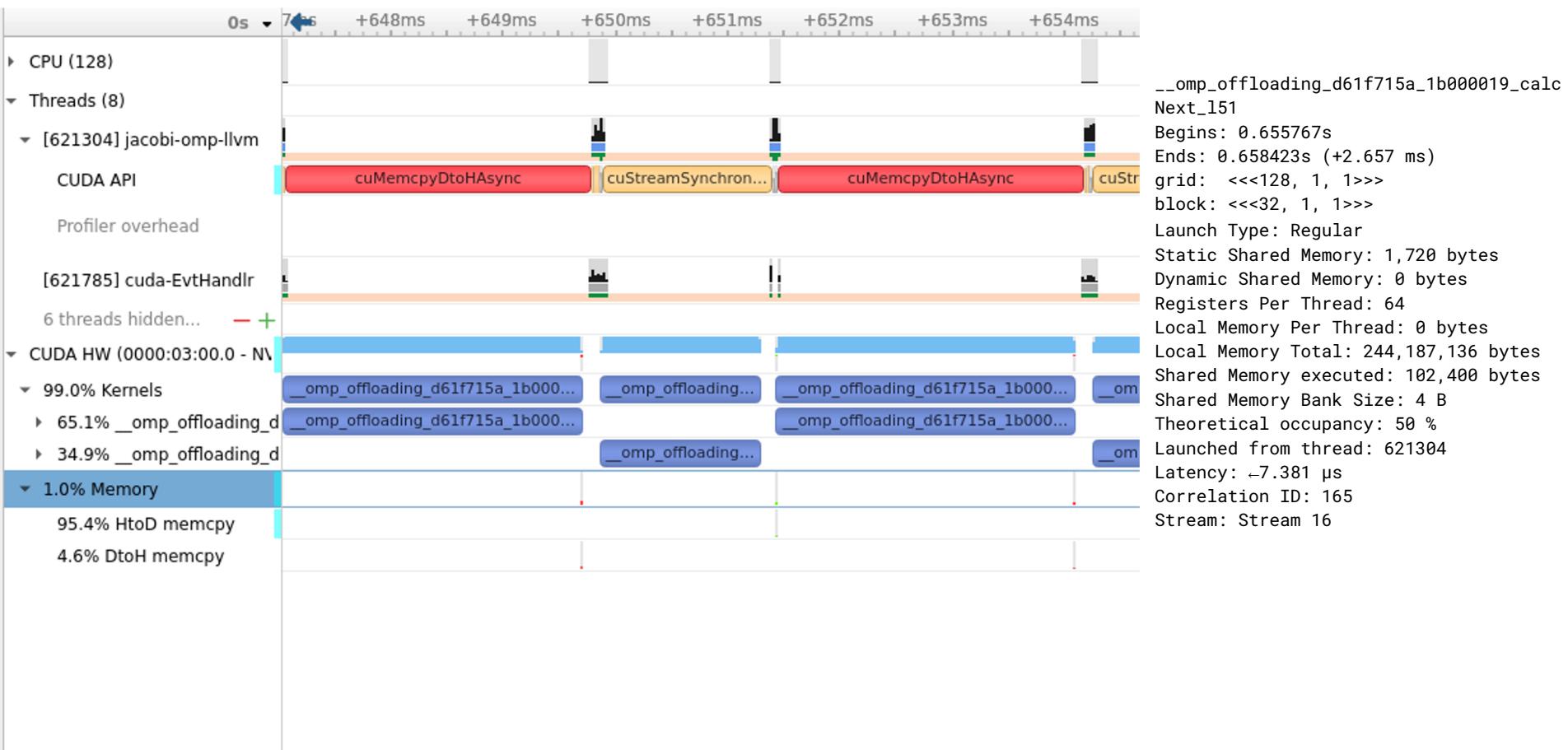
```
Jacobi relaxation
Calculation: 4096 x
4096 mesh
    0, 0.250000
    100, 0.002397
    200, 0.001204
    300, 0.000804
    400, 0.000603
    500, 0.000483
    600, 0.000403
    700, 0.000345
    800, 0.000302
    900, 0.000269
total: 3.666144 s
```

Using OpenMP offloading:

Accelerated code using parallel and data clauses taking 3.66s on GPUs

OpenACC version 1.58s on GPUs

Using Nsight System



OpenMP collapse

- In order to improve the code, and obtain more parallelism, the collapse() clause

```
//#pragma acc data copy(A[ :n*m]) create(Anew[ :n*m])
#pragma omp target data map(to:A[ :m*n],Anew[ :m*n])
while ( error > tol && iter < iter_max )
{
    error = 0.0;
```

Create data on the GPUs

```
//#pragma acc parallel loop reduction(max:error) copy(A[ :m*n],Anew[ :m*n])
#pragma omp target teams distribute parallel for map(tofrom:
A[ :m*n],Anew[ :m*n]) reduction(max:error) collapse(2)
for( int j = 1; j < n-1; j++)
{
    for( int i = 1; i < m-1; i++ )
    {
        Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1] + A[j-1][i] + A[j+1][i]);
        error = fmax( error, fabs(Anew[j][i] - A[j][i]));
    }
}
```

Parallelize and
max reduction

```
//#pragma acc parallel loop copy(A[ :m*n],Anew[ :m*n])
#pragma omp target teams distribute parallel for
map(tofrom: A[ :m*n],Anew[ :m*n]) collapse(2)
for( int j = 1; j < n-1; j++)
{
    for( int i = 1; i < m-1; i++ )
    {
        A[j][i] = Anew[j][i];
    }
}
```

Parallelize second loop

```
$ nvc -fast -mp=gpu -Minfo=all -o jacobi-omp-nvc-copy-collapse
jacobi.c
initialize:
    41, Generated vector SIMD code for the loop
calcNext:
    52, #omp target teams distribute parallel for
        52, Generating "nvkernel_calcNext_F1L52_2" GPU kernel
            Loop parallelized across teams and threads(128),
schedule(static)
    Generating reduction(max:error)
    52, Generating map(tofrom:A[:n*m],Anew[:n*m],error)
    54, Loop not vectorized/parallelized: not countable
    60, Loop not vectorized/parallelized: not countable
swap:
    65, #omp target teams distribute parallel for
        65, Generating "nvkernel_swap_F1L65_6" GPU kernel
        68, Loop parallelized across teams and threads(128),
schedule(static)
    65, Generating map(tofrom:Anew[:n*m],A[:n*m])
    70, Loop not vectorized/parallelized: not countable
main:
    113, initialize inlined, size=10 (inline) file jacobi.c (37)
        41, Loop not fused: function call before adjacent loop
            Generated vector SIMD code for the loop
    122, Generating map(to:Anew[:m*n],A[:m*n])
        Loop not vectorized/parallelized: potential early exits
    137, deallocate inlined, size=2 (inline) file jacobi.c (78)
```

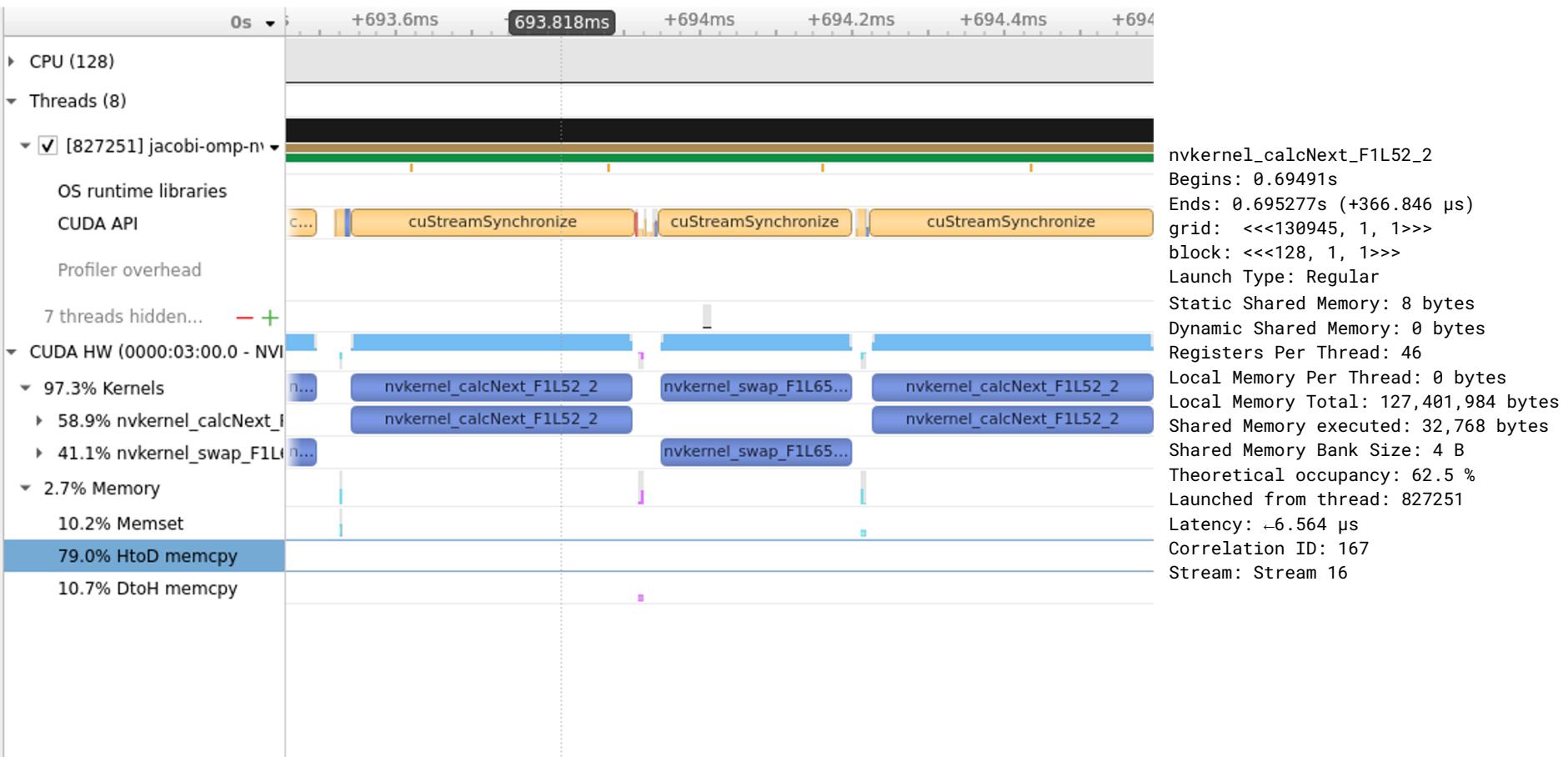
```
Jacobi relaxation
Calculation: 4096 x 4096
mesh
    0, 0.250000
    100, 0.002397
    200, 0.001204
    300, 0.000804
    400, 0.000603
    500, 0.000483
    600, 0.000403
    700, 0.000345
    800, 0.000302
    900, 0.000269
total: 1.604023 s
```

Using OpenMP offloading:

Accelerated code using parallel and data clauses taking 1.6s on GPUs

OpenACC version 1.58s on GPUs

Using Nsight System



Using LLVM OpenMP Offloading and NVIDIA A100

```
$ clang -Ofast -fopenmp --offload-arch=native -g -o jacobi-omp-  
llvm-copy-collapse jacobi.c
```

```
Jacobi relaxation  
Calculation: 4096 x  
4096 mesh  
0, 0.250000  
100, 0.002397  
200, 0.001204  
300, 0.000804  
400, 0.000603  
500, 0.000483  
600, 0.000403  
700, 0.000345  
800, 0.000302  
900, 0.000269  
total: 1.222854 s
```

Using OpenMP offloading:

Accelerated code using parallel and data clauses taking 1.22s on GPUs

OpenACC version 1.58s on GPUs

Using Nsight System

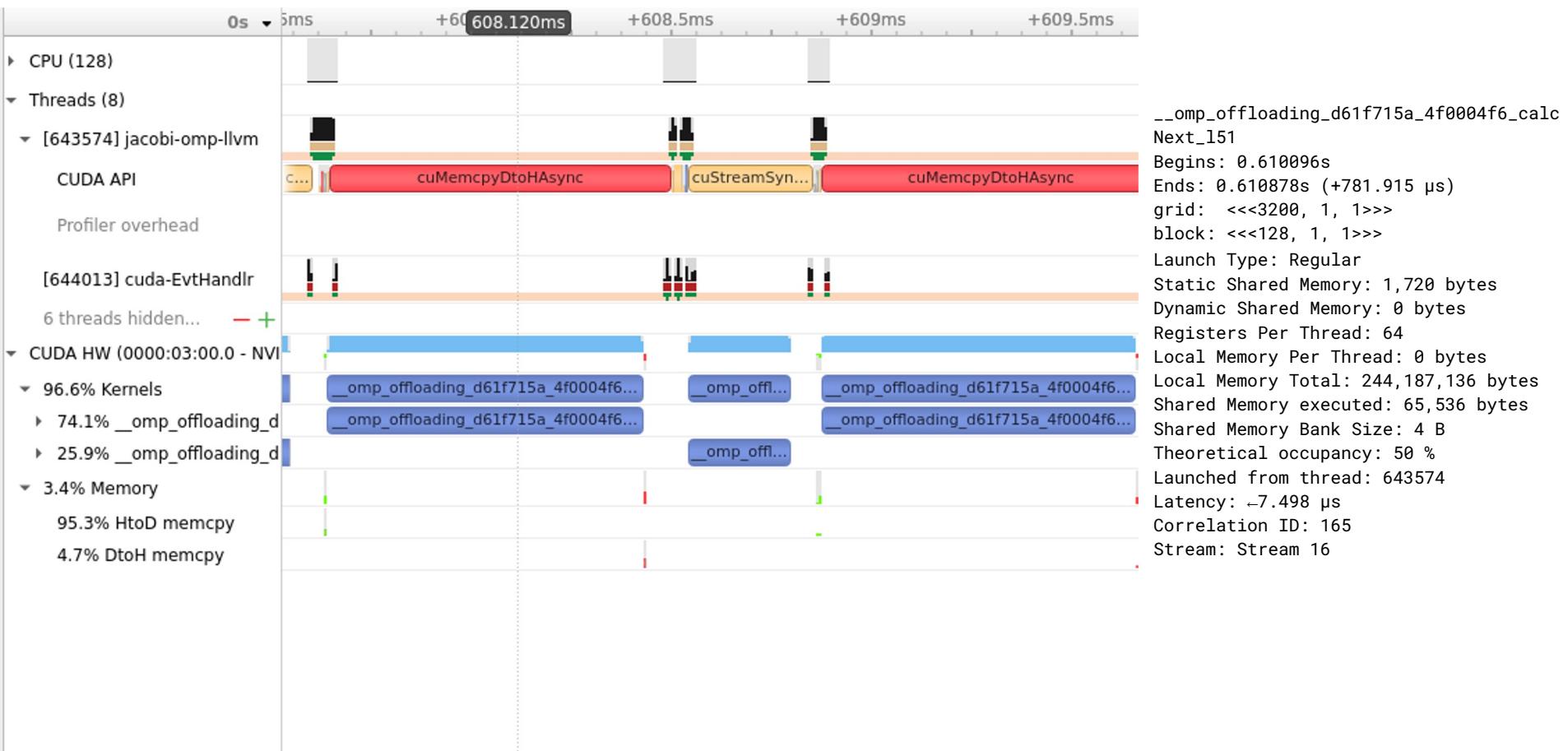


Table of content

- Laplace Serial code – example
- Parallelization using target parallel for
- Parallelization with target parallel and data constructs
- Parallelization using offload to host =CPU

Use multicore flag

```
$ nvc -fast -mp=multicore -Minfo=all -o jacobi-omp-nvc-host jacobi.c
initialize:
    41, Generated vector SIMD code for the loop
calcNext:
    52, #omp target teams distribute parallel for
        52, Loop parallelized across teams and threads,
schedule(static)
    Generating reduction(max:error)
    54, Loop not vectorized: unknown
        Loop not vectorized: may not be beneficial for target
    60, Loop not vectorized/parallelized: not countable
swap:
    65, #omp target teams distribute parallel for
        68, Loop parallelized across teams and threads,
schedule(static)
    70, Loop not vectorized: unknown
        Loop not vectorized: may not be beneficial for target
main:
    113, initialize inlined, size=10 (inline) file jacobi.c (37)
        41, Loop not fused: function call before adjacent loop
            Generated vector SIMD code for the loop
    122, Loop not vectorized/parallelized: potential early exits
    137, deallocate inlined, size=2 (inline) file jacobi.c (78)
```

Set cores

```
$ OMP_NUM_THREADS=128
./jacobi-omp-nvc-host
Calculation: 4096 x 4096
mesh
    0, 0.250000
    100, 0.002397
    200, 0.001204
    300, 0.000804
    400, 0.000603
    500, 0.000483
    600, 0.000403
    700, 0.000345
    800, 0.000302
    900, 0.000269
total: 2.269870 s
```

Parallelized code using parallel construct
took 2.269870 s on 64 core CPU
AMD EPYC 7763 64-Core Processor

Using LLVM OpenMP Offloading and NVIDIA A100

Use multicore flag

Set cores

```
$ clang -Ofast -g -fopenmp --target=x86_64-pc-linux-gnu -o jacobi-omp-llvm-host
```

```
$ OMP_NUM_THREADS=128 jacobi-omp-llvm-host jacobi.c
Jacobi relaxation Calculation: 4096 x 4096 mesh
  0, 0.250000
 100, 0.002397
 200, 0.001204
 300, 0.000804
 400, 0.000603
 500, 0.000483
 600, 0.000403
 700, 0.000345
 800, 0.000302
 900, 0.000269
total: 2.277123 s
```

Using OpenMP offloading:

Parallelized code using parallel construct took 0.852s on 64 core CPU

AMD EPYC 7763 64-Core Processor

Increasing the size of the mesh size

4096 x 4096 GRID

OpenACC

16384 x 16384 GRID

Accelerated code using parallel and data clauses take **1.589625s** on GPUs

Parallelized code using parallel construct took **0.852060s** on 64 core multicore CPUs

4096 x 4096 GRID

OpenMP

16384 x 16384 GRID

NVC **1.604023 s**, and LLVM **1.222854s** on GPUs

NVC **2.269870s** and LLVM **2.277123s** on 64 core multicore CPUs

Accelerated code using parallel and data clauses take **9.582822 s** on GPUs

Parallelized code using parallel construct took **356.332373 s** on 64 core multicore CPUs

NVC **8.966994 s** and LLVM **12.720154** on GPUs

NVC **372.458698 s** and LLVM **393.499142 s** on 64 core multicore CPUs

	OpenMP		OpenACC
	nvc	llvm	nvc
Serial	23.364053s	25.557923	23.364053s
parallel for	89.513495	242.194770	84.040213
Teams distribute	89.992197	100.463713	
copy teams parallel for	6.215937	3.666144	1.589625
copy teams parallel for collapse	1.604023	1.222854	
multicore	2.269870	2.277123	0.852060