Running Jacobi using OpenACC on LBNL's Perlmutter system

Lecture 4

Sunita Chandrasekaran
Associate Professor, University of Delaware
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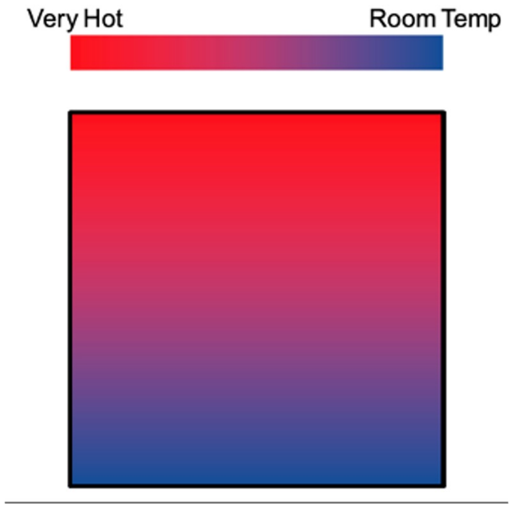
Materials also prepared by Dr. Felipe Cabarcas,
Postdoctoral Fellow, UDEL

Table of content

Table of content

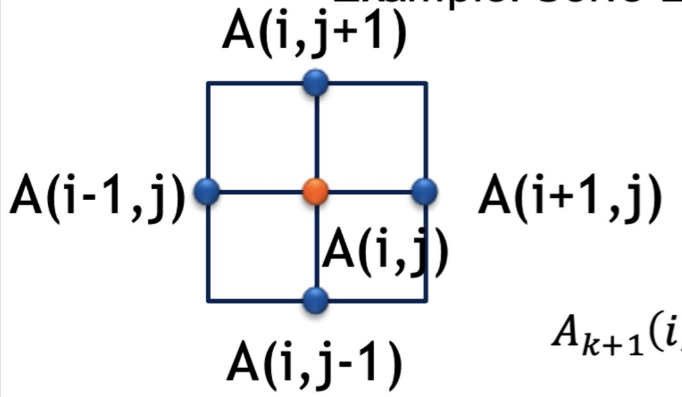
Laplace Heat Transfer

- 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: $\boldsymbol{\nabla^2 f(x, y) = 0}$



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

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

Iterate until converged

Iterate across matrix elements

Calculate new neighbors

```
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]));
  }
}
```

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

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

Parallelize first loop next

```
#pragma acc parallel loop copy(A[:m*n],Anew[:m*n])
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])
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

We didn't detail *how* to parallelize the loops, just *which* loops to parallelize.

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
- nvc -fast -acc=gpu -Minfo=all <source_code.c> -o <executable>
  - -acc=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 NVIDIA GPU code”
  - Proof that your code generated GPU code

NVC

```
$ nvc -fast -acc=gpu -Minfo=all -o jacobi-acc-loop jacobi.c
initialize:
     41, Generated vector simd code for the loop
calcNext:
     49, Generating copy(A[:n*m]) [if not already present]
         Generating NVIDIA GPU code
         51, #pragma acc loop gang /* blockIdx.x */
             Generating implicit reduction(max:error)
         53, #pragma acc loop vector(128) /* threadIdx.x */
     49, Generating implicit copy(error) [if not already present]
         Generating copy(Anew[:n*m]) [if not already present]
     53, Loop is parallelizable
swap:
     64, Generating copy(A[:n*m],Anew[:n*m]) [if not already present]
         Generating NVIDIA GPU code
         66, #pragma acc loop gang /* blockIdx.x */
         68, #pragma acc loop vector(128) /* threadIdx.x */
     68, Loop is parallelizable
main:
    111, 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
    119, Loop not vectorized/parallelized: potential early exits
    134, deallocate inlined, size=2 (inline) file jacobi.c (76)
```

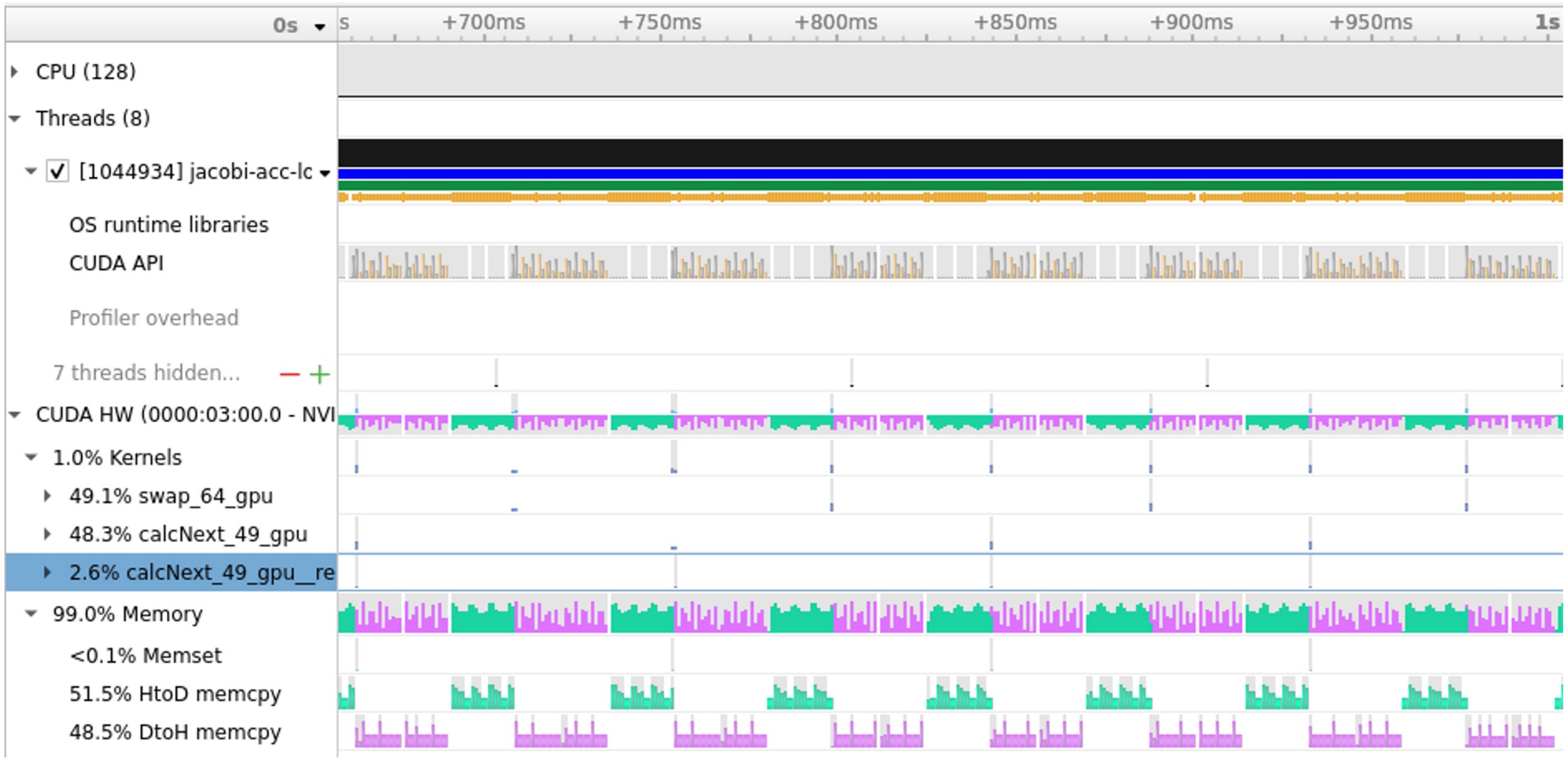
```
Jacobi relaxation
Calculation: 4096 x 4096
mesh
    0, 0.250000
  100, 0.002397
  200, 0.001204
  300, 0.000804
  400, 0.000603
  500, 0.000483
  600, 0.000403
  700, 0.000345
  800, 0.000302
  900, 0.000269
 total: 84.040213 s
```

Accelerated code using parallel and no data clauses takes 84.04 on GPUs
about 4 times slower than serial

Using NSight System

- nsys profile --gpu-metrics-device=all -o prof-${FILE}-nvc ./${FILE}
- FILE=<your file name>
- Download https://developer.nvidia.com/nsight-systems
- View your files

- Note the memory usage bars
- Not an optimized code
- Data being copied to and from GPU to and from the CPU all the time – hurts performance



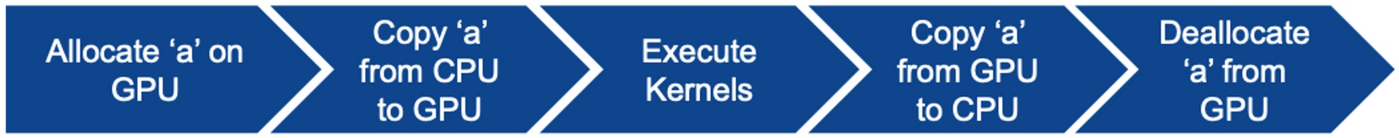
```
$ nvidia-smi
Fri Jun 23 06:46:07 2023
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 525.105.17   Driver Version: 525.105.17   CUDA Version: 12.0     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-SXM...  On   | 00000000:03:00.0 Off |                    0 |
| N/A   26C    P0    50W / 400W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-SXM...  On   | 00000000:41:00.0 Off |                    0 |
| N/A   25C    P0    49W / 400W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   2  NVIDIA A100-SXM...  On   | 00000000:82:00.0 Off |                    0 |
| N/A   26C    P0    53W / 400W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   3  NVIDIA A100-SXM...  On   | 00000000:C1:00.0 Off |                    0 |
| N/A   25C    P0    52W / 400W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+


+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

What was missing in the previous code?

Do data clauses to copy data from CPUs to GPUs

Let’s see how to add data clauses to our code



OpenACC Data Clauses

- **copyin(list)** - Allocates memory on GPU and copies data from host to GPU when entering region.
- **copyout(list)** - Allocates memory on GPU and copies data to the host when exiting region.
- **copy(list)** - Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.
- **create(list)** - Allocates memory on GPU but does not copy.
- **delete(list)** - Deallocate memory on the GPU without copying. (Unstructured Only)
- **present(list)** - Data is already present on GPU from another containing data region.

```
#pragma acc data copyout(a[0:N]), copyin(b[0:N])
{
 #pragma acc parallel loop present(a,b)
 for (int i=0; i<N; i++)
     a[i] = b[i] + 1;
}
```

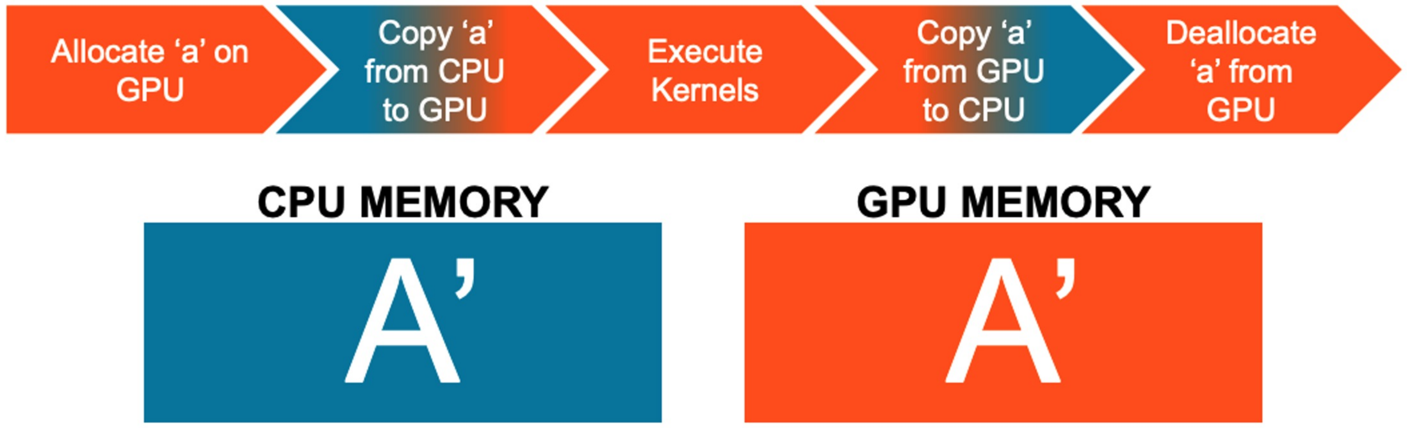
```
const int N=100;
#pragma acc data copy(a[0:N])
{
 #pragma acc parallel loop present(a)
 for (int i=0; i<N; i++)
     a[i] = a[i] + 1;
}
```

```
#pragma acc data copyout(a[0:N]), create(b[0:N])
{
 #pragma acc parallel loop
 for (int i=0; i<N; i++)
     b[i] = i * 2.0;
```

Table of content

copy(list) Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.

Principal use: For many important data structures in your code, this is a logical default to input, modify and return the data.



ARRAY SHAPING

- Sometimes the compiler needs help understanding the *shape* of an array
- The first number is the start index of the array
- In C/C++, the second number is how much data is to be transferred
- In Fortran, the second number is the ending index

```
copy(array[starting_index:length])
```

C/C++

```
copy(array(starting_index:ending_index))
```

Fortran

BASIC DATA MANAGEMENT

Multi-dimensional Array shaping

```
copy(array[0:N][0:M])
```

C/C++

```
copy(array(1:N, 1:M))
```

Fortran

```
#pragma acc data copy(A[:n*m]) create(Anew[:n*m])
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])
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])
for( int j = 1; j < n-1; j++)
{
  for( int i = 1; i < m-1; i++ )
  {
    A[j][i] = Anew[j][i];
  }
}
```

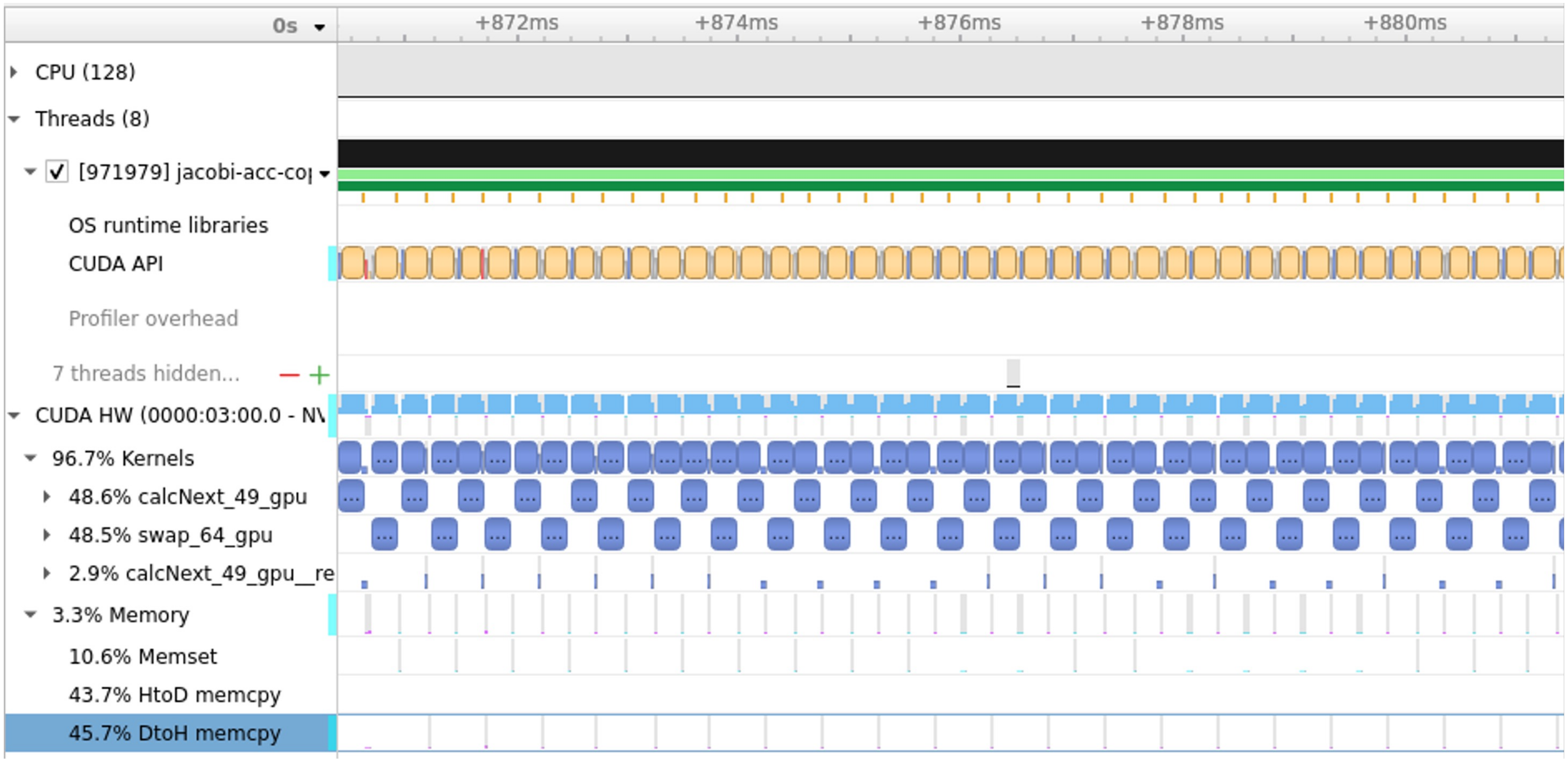
Parallelize second loop

```
$ nvc -fast -acc=gpu -Minfo=all -o jacobi-acc-copy jacobi.c
initialize:
     41, Generated vector simd code for the loop
calcNext:
     49, Generating copy(A[:n*m]) [if not already present]
         Generating NVIDIA GPU code
         51, #pragma acc loop gang /* blockIdx.x */
             Generating reduction(max:error)
         53, #pragma acc loop vector(128) /* threadIdx.x */
     49, Generating implicit copy(error) [if not already present]
         Generating copy(Anew[:n*m]) [if not already present]
     53, Loop is parallelizable
swap:
     64, Generating copy(A[:n*m],Anew[:n*m]) [if not already present]
         Generating NVIDIA GPU code
         66, #pragma acc loop gang /* blockIdx.x */
         68, #pragma acc loop vector(128) /* threadIdx.x */
     68, Loop is parallelizable
main:
    111, 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
    119, Generating create(Anew[:m*n]) [if not already present]
         Generating copy(A[:m*n]) [if not already present]
         Loop not vectorized/parallelized: potential early exits
    134, deallocate inlined, size=2 (inline) file jacobi.c (76)
```

```
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: 1.589625 s
```

Accelerated code using parallel and data clauses taking 1.58s on GPUs

Using Nsight System



We reduced data movement to/from GPU to host

Results

Serial Code takes **23.364053s** on GPUs

Accelerated code using parallel and NO data clauses on main loop takes **84.040213s** on GPUs

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

What to avoid?

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

#pragma acc parallel loop reduction(max:error) copy(A[0:n*m]) copy(Anew[0:n*m])

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(Anew[0:n*m]) copy(A[0:n*m])

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

Copying **to and from** GPU for every iteration

Add data copy to the main loop; this would avoid the copy on every iteration

Table of content

```
#pragma acc data copy(A[:n*m]) create(Anew[:n*m])
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])
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])
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

Use multicore flag

Set cores

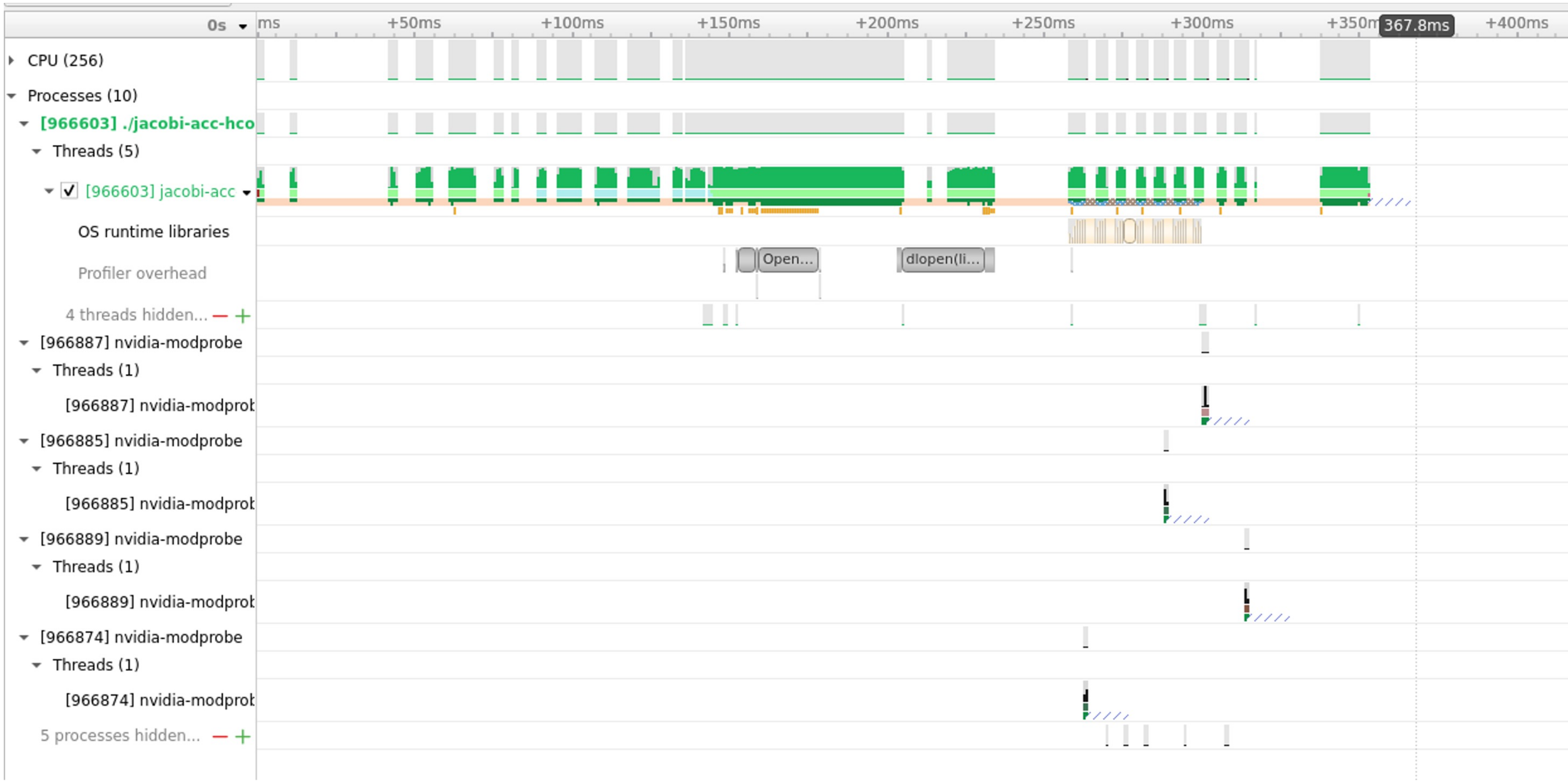
```
$ nvc -fast -acc=multicore -Minfo=all -o jacobi-acc-hcopy jacobi.c
initialize:
     41, Generated vector simd code for the loop
calcNext:
     49, Generating Multicore code
         51, #pragma acc loop gang
     51, Generating reduction(max:error)
     53, Loop is parallelizable
         Generated vector simd code for the loop containing
reductions
swap:
     64, Generating Multicore code
         66, #pragma acc loop gang
     68, Loop is parallelizable
         Memory copy idiom, loop replaced by call to __c_mcopy8
main:
    111, 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
    119, Loop not vectorized/parallelized: potential early exits
    134, deallocate inlined, size=2 (inline) file jacobi.c (76)
```

```
$ export ACC_NUM_CORES=64
$ ./jacobi-acc-hcopy
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: 0.852060 s
```

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

AMD EPYC 7763 64-Core Processor

Using Nsight System



Results

- Serial Code takes **23.364053s** on a single core CPU
- Accelerated code using parallel and no data clauses on main loop takes **84.040213s** on NVIDIA A100 GPUs
- Accelerated code using parallel and data clauses take **1.589625s** on NVIDIA A100 GPUs
- Parallelized code using parallel construct took **0.852060s** on 64 core AMD EPYC multicore CPUs

Is something looking odd?

Increasing the size of the mesh size

- Was the GPU fed with enough compute to do?
- Try nvidia-smi to determine GPU occupancy

4096 x 4096 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

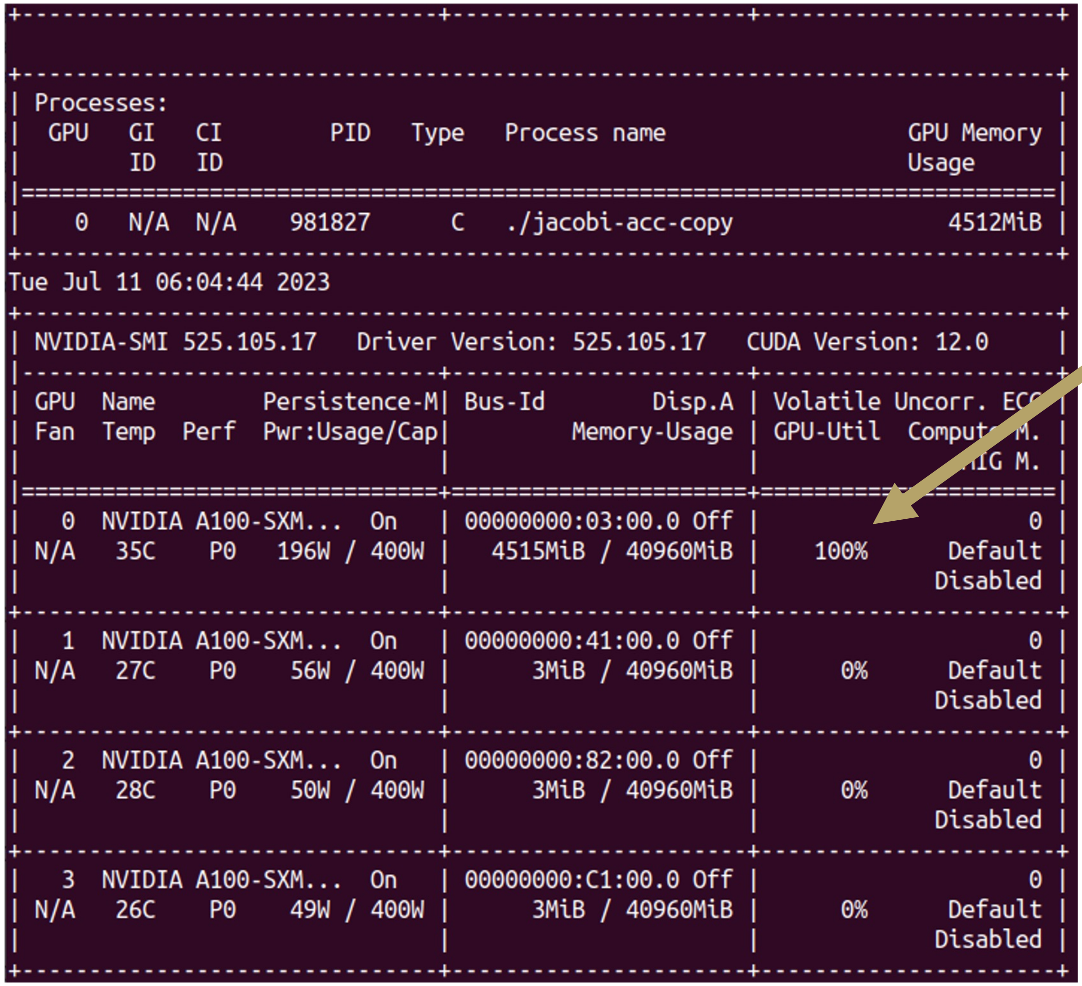
16384 x 16384 GRID

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

Increasing the size of the mesh size

For grid size 16384 x 16384



```
+-----------------------------------------------------------------------------+
+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|    0   N/A  N/A    981827      C   ./jacobi-acc-copy                4512MiB |
+-----------------------------------------------------------------------------+
Tue Jul 11 06:04:44 2023
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 525.105.17   Driver Version: 525.105.17   CUDA Version: 12.0     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-SXM...  On   | 00000000:03:00.0 Off |                    0 |
| N/A   35C    P0   196W / 400W |   4515MiB / 40960MiB |    100%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-SXM...  On   | 00000000:41:00.0 Off |                    0 |
| N/A   27C    P0    56W / 400W |      3MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   2  NVIDIA A100-SXM...  On   | 00000000:82:00.0 Off |                    0 |
| N/A   28C    P0    50W / 400W |      3MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   3  NVIDIA A100-SXM...  On   | 00000000:C1:00.0 Off |                    0 |
| N/A   26C    P0    49W / 400W |      3MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
```