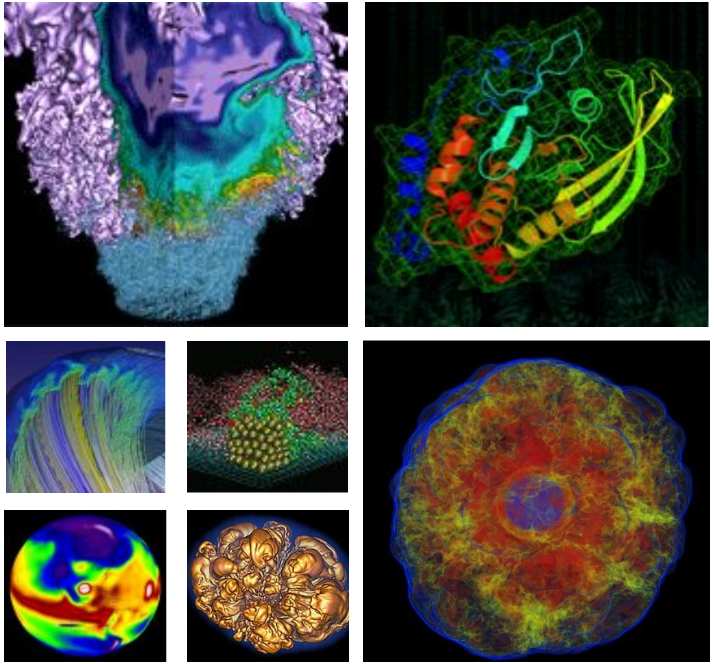
Best Practices for OpenMP



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GPU Best Practices Overview

1. Use the right combination of OpenMP directives to use *all* GPU parallelism
2. Make sure your loops are large enough to benefit from GPUs
3. Minimize the separation between “teams” and “parallel” directives
4. Use the family of “target data” directives to minimize data movement
5. Don’t map scalar variables (unnecessarily)
6. Avoid Fortran array operations and array sections (:) in target regions
7. Take advantage of compiler diagnostics and runtime tracing

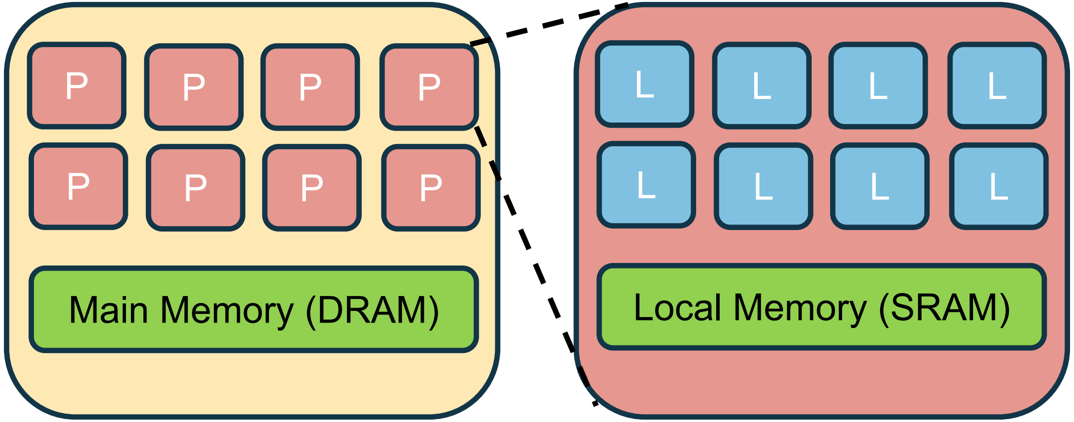
Best Practice #1

Use the right combination of OpenMP directives to use *all* GPU parallelism

GPUs and OpenMP directives

A GPU consists of many SIMD processors (P)

A SIMD processor consists of many physical SIMD lanes (L)



P: Also known as a “Streaming Multiprocessor (SM)” or “Compute Unit (CU)”

L: Also known as a “CUDA core”, “Stream core” or “Shader core”

OpenMP-5.2

#pragma omp teams
Needed to use more than 1 SIMD processor

#pragma omp parallel*
Needed to use more than 1 SIMD lane per SIMD processor

*Cray Fortran compiler sometimes needs “simd” directive. Tip: Always use ”parallel” and “simd”

Use the right combination of OpenMP directives to use *all* GPU parallelism

```
#pragma omp target parallel for
for (int i=0; i<N; ++i)
```
✗

Missing "teams" directive: will only use 1 SIMD processor (1/108th of an A100 GPU)

OpenMP-4.5 and 5

```
#pragma omp target teams distribute \
            parallel for [simd]
for (int i=0; i<N; ++i)
```
✓

"teams" and "parallel" directives needed to use all GPU parallelism

OpenMP-5

```
#pragma omp target teams loop
for (int i=0; i<N; ++i)
```
✓

"parallel" directive not needed
"loop" is a worksharing directive that can also generate parallelism

Use the right combination of OpenMP directives to use *all* GPU parallelism

```
#pragma omp target parallel for
for (int i=0; i<N; ++i)
```

✗

Missing “teams” directive: will only use 1 SIMD processor (1/108th of an A100 GPU)

OpenMP-4.5 and 5

```
#pragma omp target teams distribute \
           parallel for [simd]
for (int i=0; i<N; ++i)
```

✓

OpenMP-5

```
#pragma omp target teams loop
for (int i=0; i<N; ++i)
```

✓

“loop” directive has minimal support in the clang compilers

“teams” and “parallel” di
use all GPU parallelism

ıot needed
ring directive that can
also generate parallelism

Best Practice #2

Make sure your loops are large enough to benefit from GPUs

Reminder: You need a lot of software parallelism to benefit from GPUs

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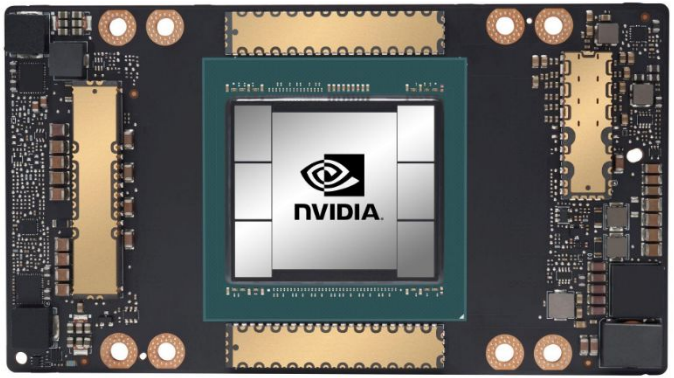
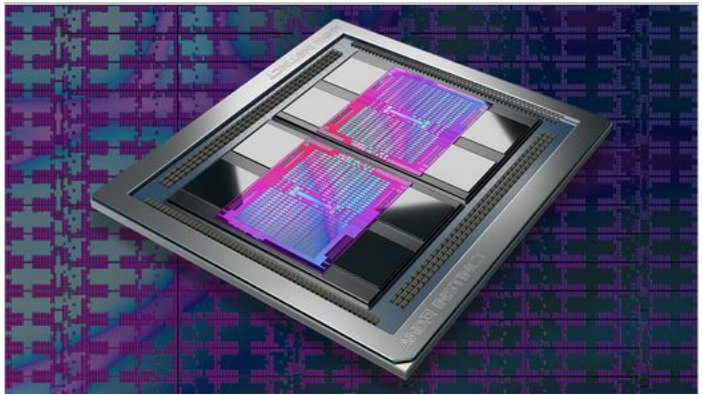
Perlmutter's NVIDIA A100



108 Streaming Multiprocessors (SM) *
64 warps per SM *
32 work items per warp =
Up to 221,184 active "threads"

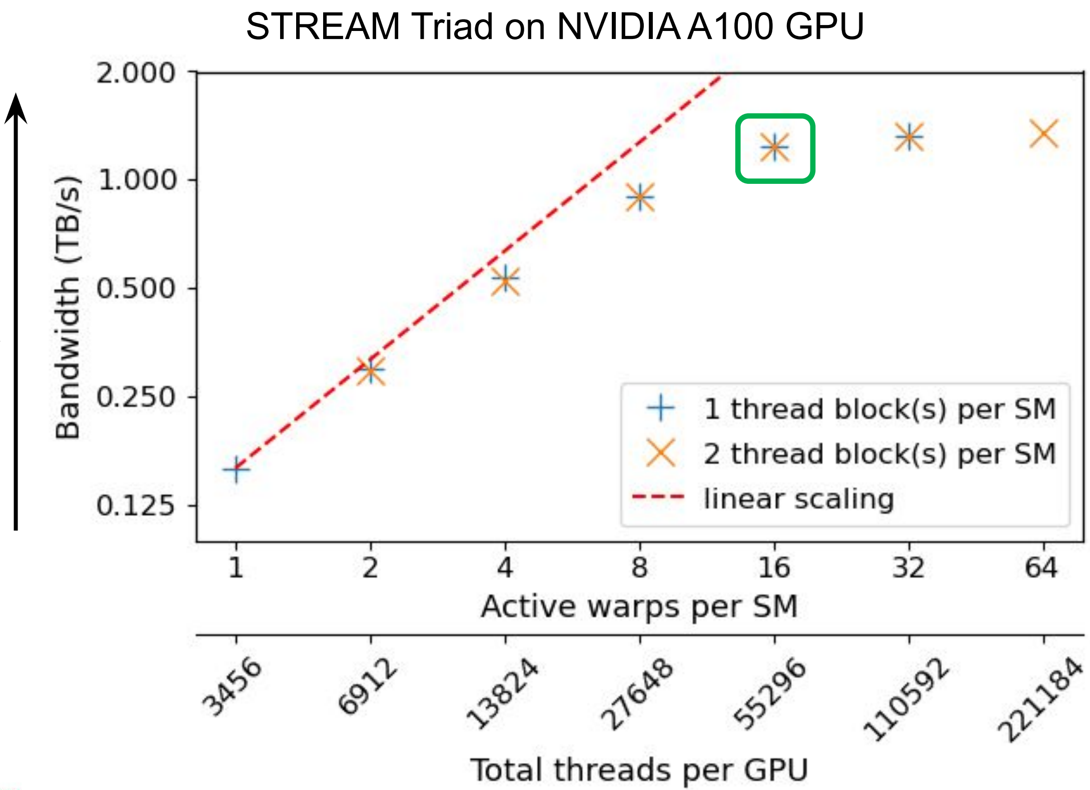
Frontier's AMD MI-250X



110 Compute Units (CU) *
40 wavefronts per CU *
64 work items per wavefront =
Up to 281,600 active "threads"
for each Graphical Compute Die (GCD)

Loops should have at least O(10K) iterations

Higher is better



The plot shows that 55K GPU threads are needed to get ~90% of NVIDIA A100 memory bandwidth

Although not shown, there is a similar performance characteristic for AMD MI-250X

The Collapse clause enables you to create larger parallel loops

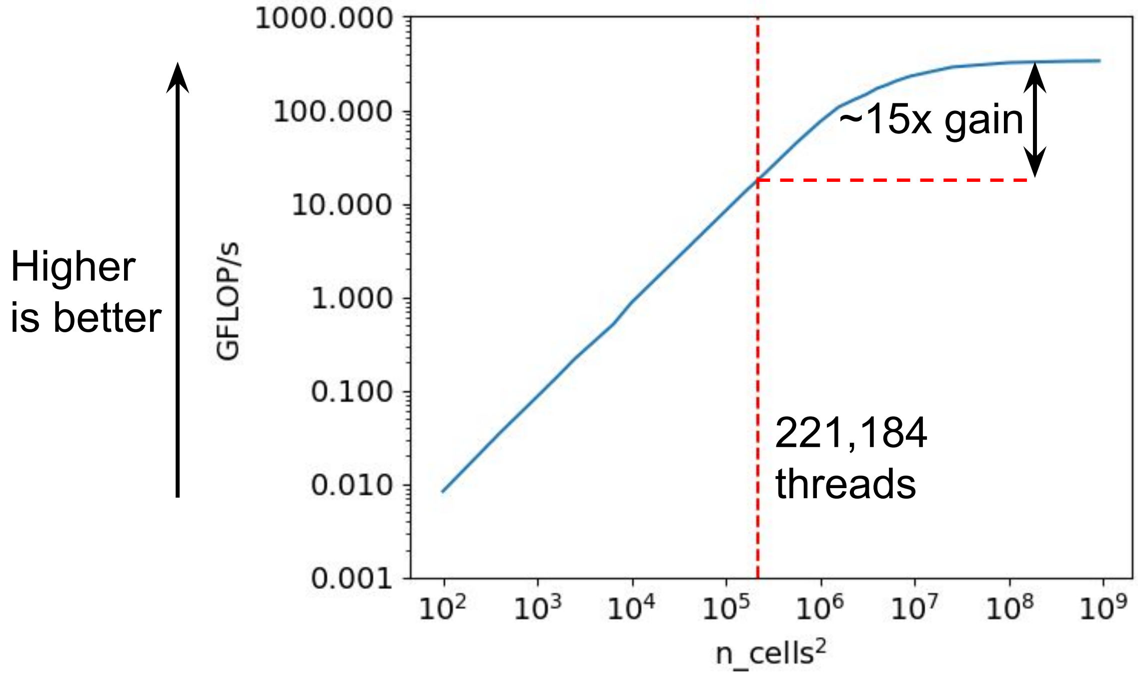
- The OpenMP collapse clause specifies the number of loops to collapse
- In the Day 1 exercise, we **collapsed two loops** to enable parallelization of **n_cells^2** iterations (critical for good utilization of GPUs):

```
// Tuned Jacobi exercise. First target region: only 4 FLOP per loop iteration
#pragma omp target teams loop collapse(2)
for (unsigned i = 1; i <= n_cells; i++)
  for (unsigned j = 1; j <= n_cells; j++)
    T_new(i, j) = 0.25 * (T(i + 1, j) + T(i - 1, j) + T(i, j + 1) + T(i, j - 1));
```

https://github.com/olcf/openmp-offload/tree/master/C/7-loop-combined

Note: Kernel launch overhead can be significant when there is minimal work

Tuned Jacobi. Performance of first target region on NVIDIA A100 GPU using "target teams loop"



The time to execute an OpenMP target region can be dominated by kernel launch time

Mitigate launch overhead with more loop iterations

Highly beneficial for our Jacobi kernel which has only 4 FLOP per loop iteration

Best Practice #3

Minimize the separation between “teams” and “parallel” directives

Minimize the separation between “teams” and “parallel” directives

- A single combined directive often gives the best performance, e.g.

```
#pragma omp target teams distribute parallel for [simd]
```

  - All GPU threads are active inside the target region (SPMD execution)

- If you stray from a single combined directive you are more likely to run into compiler correctness or performance issues
  - Sometimes OK: “teams” and “parallel” directives in the same function
  - Problematic: “teams” and “parallel” directives in different functions but in the same compilation unit
  - Very problematic: “teams” and “parallel” directives in different compilation units

Performance may be poor when splitting “teams” and “parallel” directives

The current NVIDIA and Clang compilers don’t always deliver high performance with this code organization:

```
#pragma omp target teams distribute
for (int i=0; i<N; ++i) {
#pragma omp parallel for
  for (int j=0; j<N; ++j) {
    x[i][j] += 1.0;
  }
}
```

Tip for NVIDIA compiler: use the “loop” directive to get the highest performance:

```
#pragma omp target teams loop
for (int i=0; i<N; ++i) {
#pragma omp loop
  for (int j=0; j<N; ++j) {
    x[i][j] += 1.0;
  }
}
```

Best Practice #4

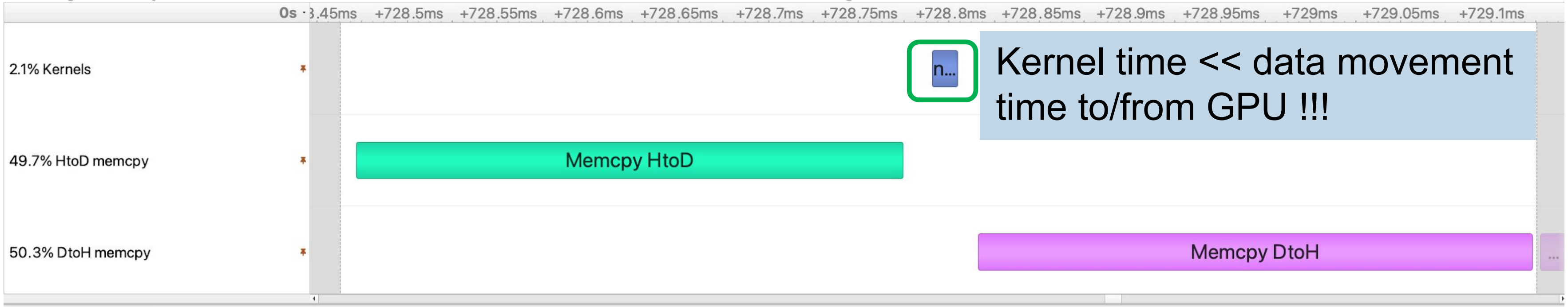
Use the family of “target data” directives to minimize data movement

Warning: Data movement can dominate runtime

Original Jacobi exercise: T and T_new are copied each time the kernel executes

```
#pragma omp target teams distribute parallel for simd collapse(2) \
        map(T[:SIZE], T_new[:SIZE])
```

Nsight Systems profile on NVIDIA A100 GPU using n_cells=1000



Kernel time << data movement time to/from GPU !!!

Events View

Name

#	Name	Start	Duration	GPU	Context
1	Memcpy HtoD	0.728472s	302.558 µs	GPU 0	Stream 13
2	nvkernel_kernel_gpu_teams_parallel_F1L81_2	0.728791s	13.312 µs	GPU 0	Stream 13
3	Memcpy DtoH	0.728816s	306.270 µs	GPU 0	Stream 13

Description:
nvkernel_kernel_gpu_teams_parallel_F1L81_2
Begins: 0.728791s
Ends: 0.728804s (+13.312 µs)

“target data” directives enable us to minimize data movement

Original:

```
while (residual > MAX_RESIDUAL && iteration <= max_iterations) {
#pragma omp target teams distribute parallel for simd collapse(2) \
            map(T[:SIZE], T_new[:SIZE])
```

Tuned:

```
#pragma omp target enter data map(to : T[:SIZE]) map(alloc : T_new[:SIZE])
while (residual > MAX_RESIDUAL && iteration <= max_iterations) {
#pragma omp target teams distribute parallel for simd collapse(2)
```

Use runtime tracing to identify excess data movement (Cray compiler)

CRAY_ACC_DEBUG=2

```
ACC: Start transfer 2 items from jacobi.c:84
ACC:       allocate, copy to acc 'T_new[:SIZE]' (8032032 bytes)
ACC:       allocate, copy to acc 'T[:SIZE]' (8032032 bytes)
ACC: End transfer (to acc 16064064 bytes, to host 0 bytes)
ACC: Execute kernel __omp_offloading_93_282c1f03_kernel_gpu_teams_parallel_l84_cce$noloop$form blocks:7813 threads:128 from jacobi.c:84
ACC: Start transfer 2 items from jacobi.c:84
ACC:       copy to host, free 'T[:SIZE]' (8032032 bytes)
ACC:       copy to host, free 'T_new[:SIZE]' (8032032 bytes)
ACC: End transfer (to acc 0 bytes, to host 16064064 bytes)
```

Use runtime tracing to identify excess data movement (NVIDIA compiler)

NVCOMPILER_ACC_NOTIFY=3

```
upload CUDA data  file=jacobi.c function=kernel_gpu_teams_parallel line=81 device=0 threadid=1
variable=T bytes=8032032
upload CUDA data  file=jacobi.c function=kernel_gpu_teams_parallel line=81 device=0 threadid=1
variable=T_new bytes=8032032
launch CUDA kernel file=jacobi.c function=kernel_gpu_teams_parallel line=81 device=0 host-threadid=0
num_teams=0 thread_limit=0 kernelname=nvkernel_kernel_gpu_teams_parallel_F1L81_2
grid=<<<7813,1,1>>> block=<<<128,1,1>>> shmem=0b
download CUDA data  file=jacobi.c function=kernel_gpu_teams_parallel line=88 device=0 threadid=1
variable=T_new bytes=8032032
download CUDA data  file=jacobi.c function=kernel_gpu_teams_parallel line=88 device=0 threadid=1
variable=T bytes=8032032
```

Best Practice #5

Don't map scalar variables (unnecessarily)

Specifying the variable as firstprivate is the most optimal

NOTE: Scalar variables are firstprivate by default on a target construct

```
void scale_array(int scalar, double *x) {
// Assume "x" already present on the GPU
// #pragma omp target teams loop map(to:scalar)
#pragma omp target teams loop firstprivate(scalar)
  for (int i=0; i<N; ++i) x[i] *= scalar;
}
```

The scalar is copied to GPU main memory using e.g. cudaMemcpy (slow ☹)

The scalar is passed as a kernel argument (fast ☺)

Best Practice #6

Avoid Fortran array operations and array sections (:) in target regions

Issues with Fortran array operations in target regions

```
!$omp target teams distribute parallel do
do i = 1, N
  x(:) = y(:) ! Error: Redundant execution by each GPU thread
  call mysub(x(i:1)) ! Performance issue: Array descriptor created by each GPU thread
end do

!$omp target teams
!$omp parallel
!$omp workshare
x(:) = y(:) ! Error: Workshared over threads only -- not teams
!$omp end workshare
!$omp end parallel
!$omp end target teams
```

Best Practice #7

Take advantage of compiler diagnostics and runtime tracing

All OpenMP compilers provide some compile-time diagnostics and/or tracing

Compiler	Diagnostics	Runtime tracing *
NVIDIA	-Minfo=mp,accel	NVCOMPILER_ACC_NOTIFY=3
Cray		CRAY_ACC_DEBUG=3
Clang	-Rpass=openmp-opt	LIBOMPTARGET_INFO=-1
GNU		GOMP_DEBUG=1

Tells you how the compiler is parallelizing loops over teams and threads

Shows you a timeline of data movement and kernel execution. This allows you to check that program flow matches your expectations

* Generally multiple trace values – see documentation

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Thank You

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