Introduction to OpenMP GPU-offloading

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Overview

- OpenMP is an API for multithreading that was first developed in 1997.
- Originally it only supported Shared-Memory parallel computing on multicore architectures.
- Since OpenMP 4.0, it added support for "target offloading" on heterogenous architectures, such as CPU+GPU.
- Version 5.2 was released in November 2021. See https://www.openmp.org/wp-content/uploads/OpenMP-API-Specification-5-2.pdf
- OpenMP uses a set of compiler directives and API function calls.

```
{
 #pragma omp parallel
 {
   printf("Hello from process: %d\n",
   omp_get_thread_num());
 }
}
```

Loop-Level Parallelism with OpenMP

OpenMP directives are expressed in pragmas. In C/C++, they begin with #pragma omp

If OpenMP is not supported or enabled, the #pragma's will be ignored by the compiler.

The most useful OpenMP pragma may be the one for loop-level parallelism:

- #pragma omp parallel for
- Which needs to be followed immediately with a for loop

The compiler takes the directive and parallelizes the loop for you.

- You can set the number of parallel threads through the OMP_NUM_THREADS environment variable at runtime
- Or you can set it in the code through omp_set_num_threads()

Other commonly used constructs: reduction, private, task, simd

CPU+GPU Heterogeneous Computing

- At present, GPUs are used as accelerators to the host CPUs.
- The CPU launches the program and dispatches the work to either the CPU or the GPU.
- Data will usually first be loaded to the CPU memory from storage.
- To perform GPU computation, you need to make sure data is available on the GPU memory. Two ways to do this:
  - Explicit data management
    - map clause
    - omp_target_alloc()
  - Unified shared memory/managed memory

OpenMP for GPU Computing

- To enable GPU computing, OpenMP uses the “target offloading” model.
- When the target region is encountered, the main thread will attempt to initiate the computation on the target device, e.g., the GPU in this case.
- Data will be moved to/from the GPU as needed/specified by the user.
- OpenMP is a specification; actual support and implementations for different GPU architectures depend on the compilers. See https://www.openmp.org/resources/openmp-compilers-tools/

Example: axpy

```
void axpy(double a, double *x, double *y, int sz)
{
#pragma omp target teams distribute parallel for \
                   map(to:x[0:sz]) \
                   map(tofrom:y[0:sz])
  for (int i = 0; i < sz; i++)
  {
    y[i] = a * x[i] + y[i];
  }
}
```

LLVM: clang++ -fopenmp -fopenmp-targets=nvptx64-nvidia -Xopenmp-target -march=<gpu_arch>
GNU: g++ -fopenmp `-foffload=<gpu_arch>`
NVIDIA: nvc++ -mp=gpu

target – indicates the code block below will be executed on the target device.
teams distribute – indicates there will be a league of teams doing the work
parallel for – the work will be shared by parallel threads
How teams distribute/parallel map to the GPU architectures depends on the compiler
map – copy the data associated with the variables to or from the target memory, or just allocate target memory
Different from Python: data[st:sz] instead of data[st:ed]

Optimizing Data Transfers 1: Explicit map

- If map clauses are not added to target constructs, presence checks determine if data is already available in the device data environment.
- If not, a map(tofrom:…) is added for that data item.
- If data is a pointer to the first element of the array, need to specify the size.

```
   double x[sz];
   double y[sz];
#pragma omp target teams distribute parallel for
   for (int i = 0; i < sz; i++)
   {
      y[i] = a * x[i] + y[i];
   }
```

```
   double x[sz];
   double y[sz];
#pragma omp target teams distribute parallel for \
                              map(to:x[0:sz]) \
                              map(tofrom:y[0:sz])
   for (int i = 0; i < sz; i++)
   {
      y[i] = a * x[i] + y[i];
   }
```

Optimizing Data Transfers 2: Data environment

```
{
    double *x = …
    double *y = …
    axpy(a, x, y, sz);
    axpy(a, x, y, sz);
}
```

- The above code copy x from host to device twice
- Use data environment to remove the unnecessary data copy

```
{
    double *x = …
    double *y = …
#pragma omp target enter data map(to:x[0:sz])
    axpy(a, x, y, sz);
    axpy(a, x, y, sz);
#pragma omp target exit data map(delete:x[0:sz])
}
```

With careful data environment setup (enter data/ exit data), we can remove map clause inside axpy to remove the unnecessary data copy

target_alloc()

```
{
  int h = omp_get_initial_device();  //host id
  int t = omp_get_default_device();  //device id
  double * x_d = (double *)omp_target_alloc( sizeof(double) * N, t);
#pragma omp target is_device_ptr(x_d) device(t)
#pragma omp teams distribute parallel for
  for(int i=0;i<N;i++)
    x_d[i] = sqrt(double(i));
  omp_target_free(x_d, t);
}
```

- Don't need to allocate memory on host
- Usage more similar to CUDA
- Can still use omp_target_memcpy() to do memory transfer between host/device and device/device

Atomic operation and scattering add

- One important kernel in wire-cell is scattering add:

  res[idx[i]] += data[i]

- Use atomic construct to implement this for parallel execution

```
#pragma omp target teams distribute parallel for simd
   for(int i=0; i<N; i++)
   {
#pragma omp atomic update
     res[pos[i]] += data[i];
   }
```

- Or we can use use_device_ptr with a wrapper of cuda/hip atomicAdd API

Atomic operation and scattering add

N = 1024 * 1024 * 32 res.size() = 1024 * 128 Use float as data type	clang 15, NVIDIA V100 (BNL lambda), no -O3	clang 15, NVIDIA V100 (BNL lambda), with -O3	nvc++ 21.9, NVIDIA V100 (Cori nersc)	clang 13, AMD gfx906
Openmp with atomic	1.28145	0.016413	0.00908089	0.0454831
Cuda/hip	0.00890096	0.00889986	0.00764084	0.0453169
Openmp with use_device_ptr	0.00870609	0.0101511[BUG!]	0.00758791	NULL

- Must turn on -O3 with clang compiler to get good performance
- Performance is still a factor of two lower than cuda
- Some strange bug appears, see

https://github.com/GKNB/test-benchmark-OpenMP-atomic/tree/main/test_use_device_ptr_atomic

Use vendor library

- OpenMP does not provide libraries like BLAS, FFT, random number
- Currently, one way to do that is to call those functions in vendor library using "use_device_ptr" clause
- The use_device_ptr map type allows OpenMP device arrays to be passed to accelerated libraries.
- Don't confuse that with is_device_ptr, which does the opposite.

```
   float *x = (float*)malloc(sizeof(float) * sz)
   float *y = (float*)malloc(sizeof(float) * sz)
   float a = 2.0
#pragma omp target data map(to:x[0:sz]) map(tofrom:y[0:sz])
   {
   #pragma omp target data use_device_ptr(x,y)
      {
         cublasSaxpy(handle, sz, &a, x, 1, y, 1);
      }
   }
```

```
cudaMalloc((void**)&x_d,  sz * sizeof(float));
cudaMalloc((void**)&y_d,  sz * sizeof(float));
saxpy(n, a, x_d, y_d);
cudaMemcpy(y,y_d, …);
//==================================================
void saxpy(int n, float a, float *x_d, float *y_d)
{
#pragma omp target teams distribute parallel for \
                  is_device_ptr(x_d, y_d)
   for(int i=0; i<n; i++)  y_d[i] += a*x_d[i]
}
```

Random number generator

- We build our own library for generating random numbers, which is basically a wrapper for curand/rocrand/std::random/random123
- https://github.com/GKNB/test-benchmark-OpenMP-RNG
- Various architectures support: NVIDIA GPU, AMD GPU, CPU running in serial, CPU running in parallel
- Currently support uniform/normal distribution of float/double
- Various engine used (not for all architectures): philox, xorwow, mt19937, ...
- Simple usage for GPU:

1).

```
double* data_d = (double*)omp_target_alloc(sizeof(double) * sz, device_id);
omp_get_rng_normal_double(data_d, sz, 0.0, 10.0, 1234ull, generator_enum::philox);
```

2).

```
#pragma omp target data map(alloc:data[0:sz]) use_device_ptr(data)
  omp_get_rng_normal_double(data, sz, 0.0, 10.0, 1234ull, generator_enum::philox);
```

- Currently trying to add more features into the library and still under testing

Shared memory

OpenMP also allows explicit use of shared memory

```
#pragma omp target teams distribute
 for(int ib=0; ib<N/BLOCK_SIZE; ib++)
 {
   int temp[BLOCK_SIZE + 2 * RADIUS];
#pragma omp allocate(temp) allocator(omp_pteam_mem_alloc)
#pragma omp parallel for num_threads(BLOCK_SIZE)
   for(int it=0; it<BLOCK_SIZE; it++)
   {
    int gindex = it + ib * BLOCK_SIZE;
    int lindex = it + RADIUS;
    temp[lindex] = in[gindex + RADIUS];
    if(it < RADIUS)
    {
      temp[lindex - RADIUS] = in[gindex - RADIUS + RADIUS];
      temp[lindex + BLOCK_SIZE] = in[gindex + BLOCK_SIZE + RADIUS];
    }
   }
#pragma omp parallel for num_threads(BLOCK_SIZE)
   for(int it=0; it<BLOCK_SIZE; it++)
   {
    int gindex = it + ib * BLOCK_SIZE;
    int lindex = it + RADIUS;
    int result = 0;
    for (int offset = -RADIUS; offset <= RADIUS; offset++)
      result += temp[lindex + offset];
    out[gindex + RADIUS] = result;
   }
 }
```

Example of 1D stencil,
use omp_pteam_mem_alloc to indicate the type of memory (shared memory) we allocate

Split the inner for loop into two to perform synchronization

- Can observe the usage of shared memory with nsight-compute.
- If allocate too much shared memory, a compile-time error would occur

Asynchronous Offloads

OpenMP target constructs are synchronous by default

- The encountering host thread awaits the end of the target region before continuing
- The nowait clause makes the target constructs asynchronous
- We can have asynchronous behavior between different kernels and data movement

Example of Asynchronous Offloads

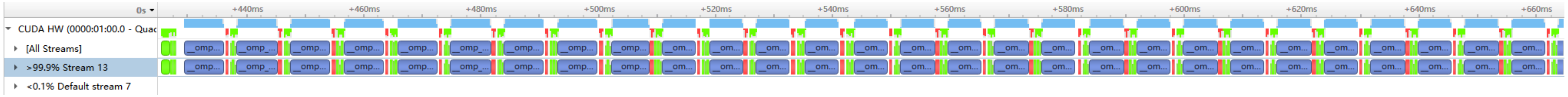
```
 for(int batch = 0; batch<nb; batch++)
 {
   int st = N / nb * batch;
   int sz = N / nb;
   int *anext = a + st;
   int *bnext = b + st;
   int *cnext = c + st;
#pragma omp target enter data map(to:anext[0:sz],bnext[0:sz],cnext[0:sz])  nowait depend(out:anext[0:sz],bnext[0:sz],cnext[0:sz])
#pragma omp target teams distribute parallel for nowait depend(inout:anext[0:sz],bnext[0:sz],cnext[0:sz])
   for(int i=0; i<sz; i++)
   {
     compute_c_from_a_and_b();
   }
#pragma omp target exit data map(release:anext[0:sz],bnext[0:sz])  nowait depend(in:anext[0:sz],bnext[0:sz])
#pragma omp target exit data map(from:cnext[0:sz])  nowait depend(in:cnext[0:sz])
 }   //batch
#pragma omp taskwait
```

depend (in/out/inout): determine the data dependency graph

nowait: remove the synchronization at the end of the loop

taskwait: an explicit barrier

Example of Asynchronous Offloads



clang++ results

For nvc++, the earlier code will not output Asynchronous behavior

Future

- Testing and apply other syntax
  - unroll
  - tile
  - Loop
  - managed memory
- OpenMP side
  - Support for target scan (prefix sum)
  - General wrapper for vendor library
  - Bug fixing