OpenMP Target Offload for Heterogeneous Architectures

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Quantitative & Computational Biology
University of Southern California

Email: anakano@usc.edu

Goal: Unified open high-level programming of both CPU & GPU





Exaflop/s Supercomputing

• Diverse exaflop/s supercomputing platforms



Summit (0.2 Exaflop/s, current)

IBM CPU/NVIDIA GPU



X^e arch-based "Ponte Vecchio" GPUTile-based, chiplets, HBM stack, Foveros 3D integration, 7nm

On-Node Interconnect

CPU-GPU: PCle GPU-GPU: X^e Link



Aurora (Exaflop/s)
Intel CPU/Intel GPU



1 HPC and Al Optimized
AMD EPYC CPU
4 Purpose Built AMD
Radeon Instinct GPU



Frontier (1.5 Exaflop/s)

AMD CPU/AMD GPU

• Need an *open* programming model for *heterogeneous* (e.g. GPU-accelerated) clusters (note CUDA is a proprietary language by NVIDIA)

See http://press3.mcs.anl.gov/atpesc/files/2021/08/ATPESC-2021-Track-1-Talk-8-Muralidharan-Aurora.pdf

Open Programming Models

OpenACC (Open Computing Language)
 Open standard for directive-based programming of heterogeneous devices

USING OPENMP -

THE NEXT STEP

Affinity, Accelerators, Tasking, and SIMD

Ruud van der Pas, Eric Stotzer,

https://www.openacc.org/

OpenMP 4.5/5
 Starting specification version 4.5,
 OpenMP allows offloading the execution of the code & data to heterogeneous devices

https://www.openmp.org/specifications/

OpenMP Offload

- Latest version of OpenMP allows one to maintain one version of a code, which can run on either a general-purpose central processing unit (CPU) or an accelerator (e.g. graphics processing unit, GPU; tensor processing unit, TPU; digital signal processor, DSP; field-programmable gate array, FPGA)
- Objective is to execute parts of the program on a heterogeneous accelerator device (or target deice), i.e., dedicated computer hardware outside CPU (which will be called host device) to execute certain functions faster than CPU
- In OpenMP, program execution begins on the host, which offloads the execution of parts of the code & data to accelerator

OpenMP Target Construct

Simple example

```
main() {
   float a[1000],b[1000],c,d;
   ...
   #pragma omp target map(a,b,c,d)
   {
      int i;
      #pragma omp parallel for
      for (i=0; i<N; i++)
        a[i] = b[i]*c+d;
   }
   ...
}</pre>
```

- When a host thread encounter the #pragma omp target directive, the target region specified by it will be executed by a new thread running on an accelerator, cf. CUDA GPU kernel
- Before the new thread starts executing the target region, the variable in the map() clause are mapped onto accelerator memory, which often is disjunct from the host memory, cf. cudaMemcpy()
- The offloaded code is usually a data-parallel structured block, which can be handled by multiple threads on accelerator using standard OpenMP constructs like #pragma omp parallel for

Computing the Value of π on GPU

omp_target_pi.c

```
#include <omp.h>
#include <stdio.h>
#define NBIN 1000000
#define NTRD 96
                                 The only addition for GPU offload
int main() {
  float step, sum=0.0, pi;
  step = 1.0/(float)NBIN;
                                          Thread reduction of sum
  #pragma omp target map(step,sum)
    # pragma omp parallel for reduction(+:sum) num threads(NTRD)
    for (long long i=0; i<NBIN; i++) {
      float x = (i+0.5)*step;
      sum += 4.0/(1.0+x*x);
                                            Specify # of GPU threads
                            This line is identical for CPU & GPU
  pi = sum*step;
  printf("PI = %f\n",pi);
                                             1. Black: original serial code
  return 0;
                                             2. Green: one-line multithreading
                                             3. Red: another line for GPU offload
```

GPU: Easy & Hard Ways

Serial: pi.c OpenMP: omp_target_pi.c

```
#include <stdio.h>
#define NBIN 100000000
int main() {
    double step, x, sum=0.0, pi;
    step = 1.0/NBIN;
    for (long long i=0; i<NBIN; i++) {
        x = (i+0.5)*step;
        sum += 4.0/(1.0+x*x);
    }
    pi = sum*step;
    printf("PI = %f\n",pi);
    return 0;
}</pre>
```

DPC++: pi.cpp

```
#include <CL/sycl.hpp>
#include <iostream>
#include <array>
using namespace cl::sycl;
#define NBIN 1000000 // # of bins for quadrature
#define NTRD 512 // # of threads
 float step = 1.0f/NBIN;
 std::array<float, NTRD> sum;
 for (int i=0; i<NTRD; ++i) sum[i] = 0.0f;
 queue q(qpu selector{});
 std::cout << "Running on: " <<
 q.get_device().get_info<info::device::name>() << std::endl;</pre>
 range<1> sizeBuf{NTRD};
   buffer<float, 1> sumBuf(sum.data(), sizeBuf);
   q.submit([&](handler &h){
     auto sumAccessor =
     sumBuf.get access<access::mode::read write>(h);
     h.parallel_for(sizeBuf, [=](id<1> tid) {
       for (int i=tid; i<NBIN; i+=NTRD) {
         float x = (i+0.5f)*step;
         sumAccessor[tid] += 4.0f/(1.0f+x*x);
     }); // End parallel for
   }); // End queue submit
 float pi=0.0f;
 for (int i=0; i<NTRD; i++) // Inter-thread reduction
 pi *= step; // Multiply bin width to complete integration
 std::cout << "Pi = " << pi << std::endl;
```

CUDA: pi.cu

```
// Using CUDA device to calculate pi
#include <stdio.h>
#include <cuda.h>
#define NBIN 10000000 // Number of bins
#define NUM BLOCK 13 // Number of thread blocks
#define NUM THREAD 192 // Number of threads per block
int tid:
float pi = 0;
// Kernel that executes on the CUDA device
__global__ void cal_pi(float *sum, int nbin, float step, int nthreads, int nblocks) {
  int i:
  float x:
  int idx = blockIdx.x*blockDim.x+threadIdx.x; // Sequential thread index across the blocks
  for (i=idx; i< nbin; i+=nthreads*nblocks) {
     x = (i+0.5)*step;
     sum[idx] += 4.0/(1.0+x*x);
// Main routine that executes on the host
int main(void) {
  dim3 dimGrid(NUM_BLOCK,1,1); // Grid dimensions
  dim3 dimBlock(NUM THREAD, 1, 1); // Block dimensions
  float *sumHost, *sumDev; // Pointer to host & device arrays
  float step = 1.0/NBIN; // Step size
  size_t size = NUM_BLOCK*NUM_THREAD*sizeof(float); //Array memory size
  sumHost = (float *)malloc(size); // Allocate array on host
  cudaMalloc((void **) &sumDev, size); // Allocate array on device
  // Initialize array in device to 0
  cudaMemset(sumDev, 0, size);
  // Do calculation on device
  cal_pi <<<dimGrid, dimBlock>>> (sumDev, NBIN, step, NUM_THREAD, NUM BLOCK); // call CUDA kernel
  // Retrieve result from device and store it in host array
  cudaMemcpy(sumHost, sumDev, size, cudaMemcpyDeviceToHost);
  for(tid=0; tid<NUM_THREAD*NUM_BLOCK; tid++)
     pi += sumHost[tid];
  pi *= step;
  // Print results
  printf("PI = %f\n",pi);
  // Cleanup
  free(sumHost):
  cudaFree(sumDev):
  return 0:
```

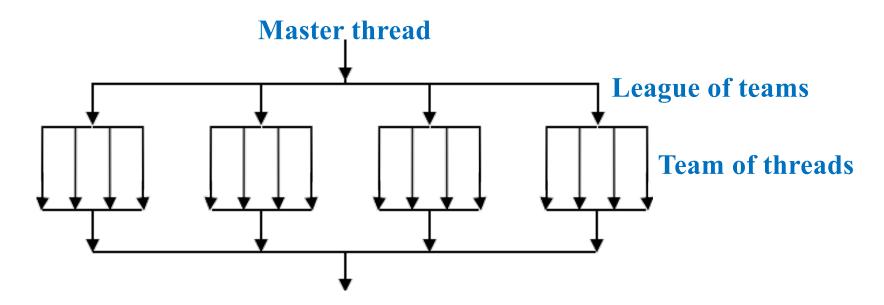
Hierarchical Parallelization

• #pragma omp teams

Starts a league of multiple thread teams; teams construct must be nested immediately inside a target construct, so they are commonly used as #pragma omp target teams; num_teams clause can be used to specify the number of teams

(Example) #pragma omp target teams num_teams(13)

#pragma omp distribute
 Distribute the work across the teams



cf. CUDA grid of blocks & block of threads

Teams for Computing π

Spatial decomposition via offset among teams & data privatization

```
#define NTMS 12
float sum_teams[NTMS];
for (int j=0; j<NTMS; j++) sum_teams[j] = 0.0;</pre>
                                                    - Data privatization among teams
#pragma omp target teams map(step,sum teams) num teams(NTMS)
  #pragma omp distribute _____
                                             New: teams & distribute constructs
  for (int j=0; j<NTMS; j++) {
    long long ibgn = NBIN/NTMS*j;
                                           L NBIN/NTMS_*NTMS could be less than NBIN
    long long iend = NBIN/NTMS*(j+1);
    if (j == NTMS-1) iend = NBIN;
    # pragma omp parallel for reduction(+:sum teams[j]) num threads(NTRD)
    for (long long i=ibqn; i<iend; i++) {
      float x = (i+0.5)*step;
      sum teams[j] += 4.0/(1.0+x*x);
                 Modified: offset & private accumulator
for (int j=0; j<NTMS; j++) sum += sum teams[j];</pre>
                                                              Master thread
                            League of teams
                        Team of threads
```

Using OpenMP Target on Discovery

• Necessary module

```
module purge
module load llvm // Use LLVM compiler
```

Compilation

```
clang -fopenmp -fopenmp-targets=nvptx64-nvidia-cuda -Xopenmp-target
-march=sm_70 --gcc-toolchain=/spack/apps/gcc/8.3.0 omp_target_pi.c
-o omp_target_pi
```

Type all in one line

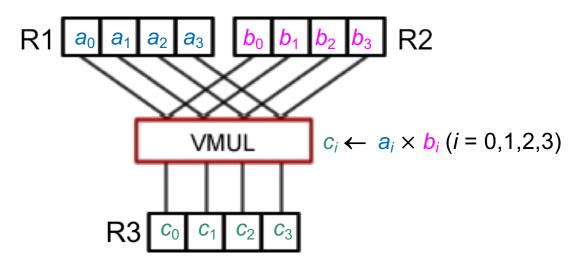
Execute on a GPU-accelerated node

```
[anakano@discovery]$ salloc --partition=gpu --gres=gpu:v100:1 --time=00:30:00
salloc: Nodes d11-02 are ready for job
[anakano@d11-02]$ ./omp_target_pi
PT = 3.141593
```

Single Instruction Multiple Data

- Single-instruction multiple-data (SIMD) parallelism: An arithmetic operation is operated on multiple operand-pairs stored in vector registers (each of which can hold multiple operands) using vector instructions
- OpenMP simd construct instructs the compiler to vectorize the loop

```
#pragma omp for simd
for (int i=0; i<n; i++)
    a[i] = b[i]+c[i];</pre>
```



Asynchronous Offload

```
main() {
  float a[1000],b[1000],c,d;
   ...
  #pragma omp target nowait map(a,b,c,d)
  {
    int i;
    #pragma omp parallel for
    for (i=0; i<N; i++)
        a[i] = b[i]*c+d;
  }
  func(b); // perform computation independent of device output
  #pragma omp taskwait
  func(a); // perform computation dependent on device output
}</pre>
```

- By default, the thread that encounters a device construct waits for the construct to complete before executing the next line
- When a nowait clause is added to the device construct, the encountering thread does not wait but instead continues executing the code passed the construct
- The taskwait constructs lets the original thread wait for the completion of the target task generated by it before continuing to the next line

Overlap CPU & GPU computations for high performance

Persistent GPU Memory Allocation

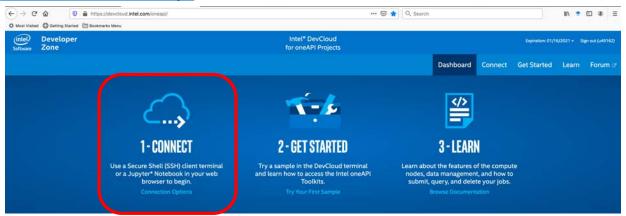
• Expensive CPU-GPU data transfer associated with the map clause can be minimized by making GPU memory allocation persistent

```
// Pre-allocate GPU array
#pragma omp target enter data map(alloc:psi[0:Nmax])
                       Stand-alone directive to map variables to device memory
// Keep accessing device array only from device
#pragma omp target parallel for \
map(tofrom:psi[0:Nmax]) map(to:u[0:Nmax])
for (int i=0; i< Nmax; i++) psi[i] *= u[i];</pre>
// De-allocate GPU array
#pragma omp target exit data map(delete:psi[0:Nmax])
                       Stand-alone directive to unmap variables from device memory
```

(Optional) Using Intel DevCloud (1)

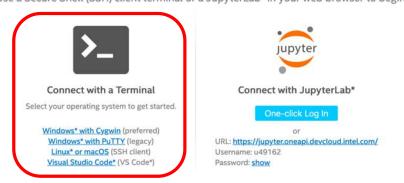
Sign up at the Intel developer's cloud (DevCloud) site:

https://devcloud.intel.com/oneapi



• Setup terminal connection to develoud server CONNECT TO INTEL® DEVCLOUD

Use a Secure Shell (SSH) client terminal or a JupyterLab* in your web browser to begin.



Log in to devcloud server
 macbook-pro:~ aiichironakano\$ ssh devcloud
 u49162@login-2:~\$

Using Intel DevCloud (2)

- Transfer omp_target_pi.c to devcloud server, e.g., using sftp
- Compile

```
u49162@login-2:~$ cc -o omp_target_pi omp_target_pi.c -fopenmp
```

• Interactive job on a GPU-accelerated computing node using PBS (portable batch system) job scheduler

```
u49162@login-2:~$ qsub -I -l nodes=1:gpu:ppn=2 qsub: waiting for job 694715.v-qsvr-1.aidevcloud to start qsub: job 694715.v-qsvr-1.aidevcloud ready u49162@s001-n177:~$
```

Run

```
u49162@s001-n177:~$ ./omp_target_pi
PI = 3.141593
```

• Start developing your own OpenMP target offload codes for GPU acceleration!

Where to Go from Here

- Start developing your own OpenMP target offload codes for GPU acceleration
- Plenty of room for performance optimization

 e.g., target region executed by different threads happens concurrently, used for , e.g., overlapping computation & data transfer

```
#pragma omp parallel
{
    #pragma omp target
    {// Different threads perform computation or data transfer }
}
```

See "OpenMP Offload Optimization" (Ye Luo, Argonne National Lab.)

https://aiichironakano.github.io/cs596/Luo-OpenMPoffload-SC20.pdf