

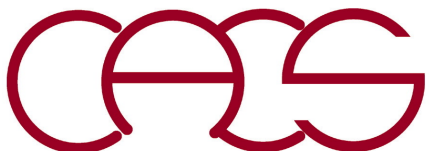
OpenMP Target Offload for Heterogeneous Architectures

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

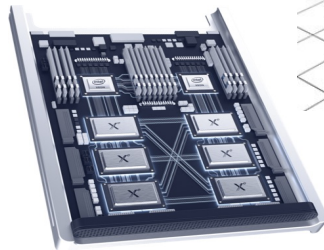


Exaflop/s Supercomputing

- Diverse exaflop/s supercomputing platforms



Summit (0.2 Exaflop/s)
IBM CPU/NVIDIA GPU



GPU Architecture

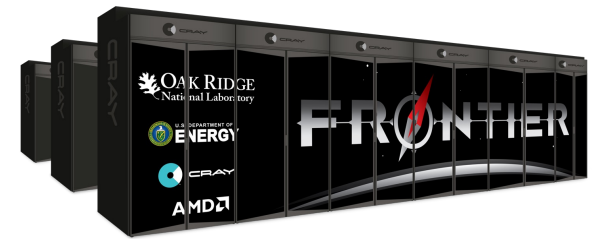
X^e arch-based “Ponte Vecchio”
GPUS tile-based, chiplets, HBM
stack, Foveros 3D integration, 7nm

On-Node Interconnect

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



Aurora (2.0 Exaflop/s)
Intel CPU/Intel GPU



Frontier (2.1 Exaflop/s)
AMD CPU/AMD GPU



El Capitan (2.7 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 <https://extremecomputingtraining.anl.gov/agenda-2025/>

Frontier (AMD) Programming

Frontier Programming Environment

- Compilers
 - Cray CCE
 - C/C++ LLVM-based
 - Cray Fortran
 - AMD ROCm
 - C/C++ LLVM-based
 - GCC
 - oneAPI DPC++
 - LLVM-based
 - user-managed
- Programming Models & Abstraction Layers
 - OpenMP
 - HIP
 - Kokkos
 - RAJA
 - SYCL
 - via user-managed DPC++
 - OpenACC
 - C/C++ via user-managed clacc
 - OpenCL
 - UPC++

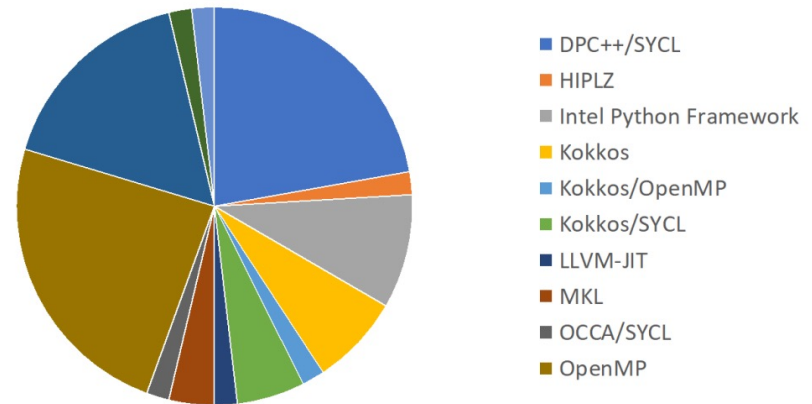
Aurora (Intel) Programming

Aurora Programming Models

- Aurora applications may use
 - DPC++/SYCL
 - OpenMP
 - Kokkos
 - Raja
 - OpenCL
- Experimental
 - HIP
- Not available on Aurora
 - CUDA
 - OpenACC



Early Science Application Programming Model Distribution



Open Programming Models

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

<https://www.openacc.org/>

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

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



[https://www.amazon.com/Using-OpenMP The-Next-Step-Accelerators/dp/0262534789](https://www.amazon.com/Using-OpenMP-The-Next-Step-Accelerators/dp/0262534789)

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 device*), *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

See “OpenMP 4.5 Target Offload” (NASA Ames)

https://aiichironakano.github.io/cs653/OpenMP4.5_3-20-19.pdf

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;  
    }  
    ...  
}
```

- 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

int main() {
    float step, sum=0.0, pi;
    step = 1.0/(float)NBIN;
    #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);
        }
    }

    pi = sum*step;
    printf("PI = %f\n", pi);
    return 0;
}
```

The only addition for GPU offload

Thread reduction of sum

Specify # of GPU threads

This line is identical for CPU & GPU

1. Black: original serial code
2. Green: one-line multithreading
3. Red: another line for GPU offload

GPU: Easy & Hard Ways

Serial: 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;
}
```

OpenMP: omp_target_pi.c

```
#include <omp.h>
#include <stdio.h>
#define NBIN 1000000
int main() {
    float step, sum=0.0, pi;
    step = 1.0/(float)NBIN;
    #pragma omp target map(step, sum)
    {
        #pragma omp parallel for reduction(+:sum)
        for (long long i=0; i<NBIN; i++) {
            float x = (i+0.5)*step;
            sum += 4.0/(1.0+x*x);
        }
    }
    pi = sum*step;
    printf("PI = %f\n", pi);
    return 0;
}
```

↘

↗

SYCL: 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

int main()
{
    float step = 1.0f/NBIN;
    std::array<float, NTRD> sum;
    for (int i=0; i<NTRD; ++i) sum[i] = 0.0f;

    queue q(gpu_selector{});

    std::cout << "Running on: " <<
    q.get_device().get_info<info::device::name>() << std::endl;

    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=0; 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 += sum[i];
    pi *= step; // Multiply bin width to complete integration

    std::cout << "Pi = " << pi << std::endl;

    return 0;
}
```

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 nbins, 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< nbins; 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

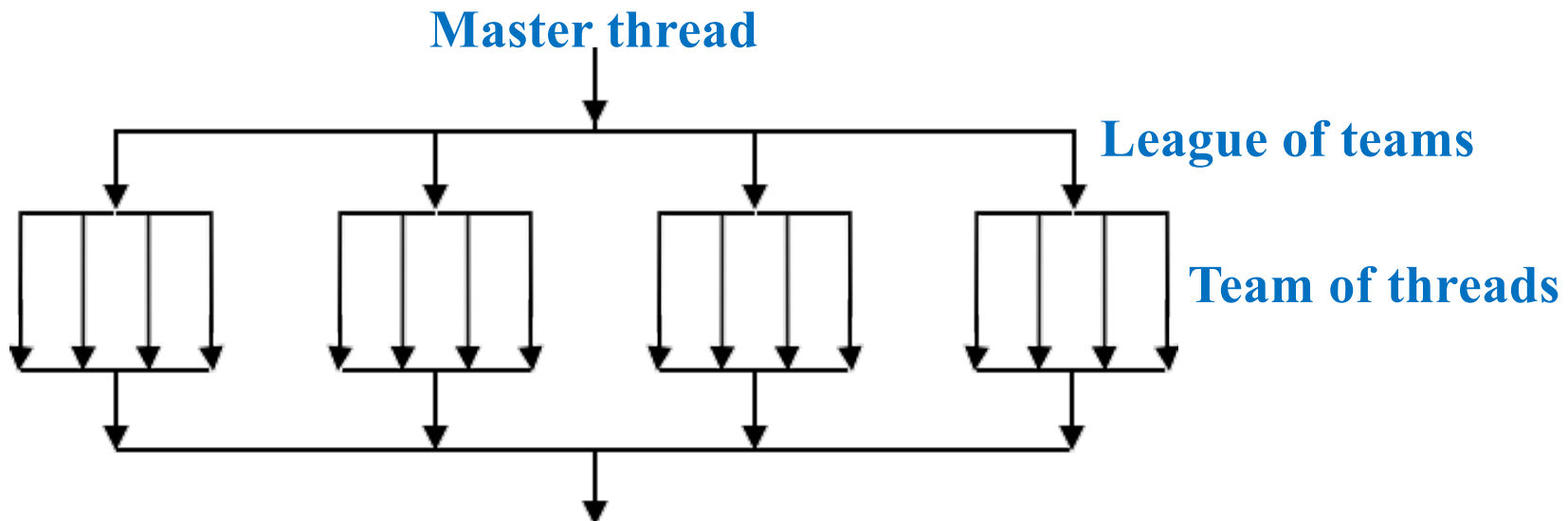
- `#pragma omp teams`

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

Remember NVIDIA SM/SP
& Intel slice/stack?

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;
...
#pragma omp target teams map(step,sum_teams) num_teams(NTMS)
{
    #pragma omp distribute
    for (int j=0; j<NTMS; j++) {
        long long ibgn = NBIN/NTMS*j;
        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=ibgn; i<iend; i++) {
            float x = (i+0.5)*step;
            sum_teams[j] += 4.0/(1.0+x*x);
        }
    }
}

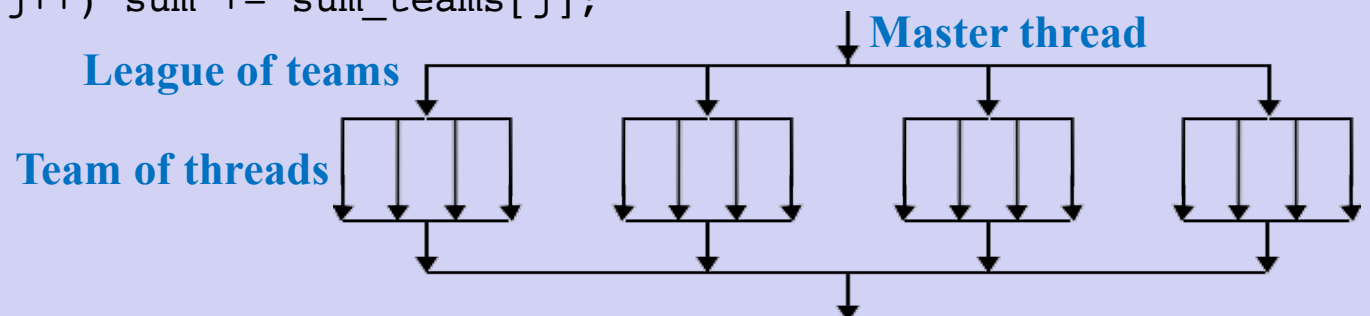
for (int j=0; j<NTMS; j++) sum += sum_teams[j];
```

Data privatization among teams

New: teams & distribute constructs

NBIN/NTMS × NTMS could be less than NBIN

Modified: offset & private accumulator



Using OpenMP Target on Discovery

- **Necessary module**

```
module purge  
module load nvhpc
```

- **Compilation**

```
nvc -o omp_target_pi omp_target_pi.c
```

— NVIDIA C compiler supports newer C constructs

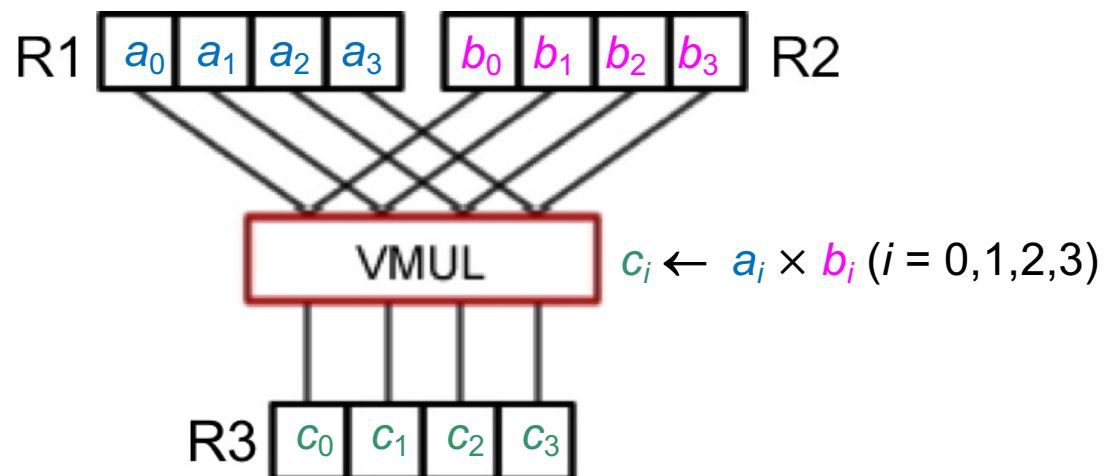
- **Execute on a GPU-accelerated node**

```
[anakano@discovery]$ salloc --partition=gpu --ntasks=1 --gpus-per-task=1 --  
time=00:30:00  
salloc: Nodes e16-03 are ready for job  
[anakano@e16-03]$ ./omp_target_pi  
PI = 3.141593
```

Single Instruction Multiple Data

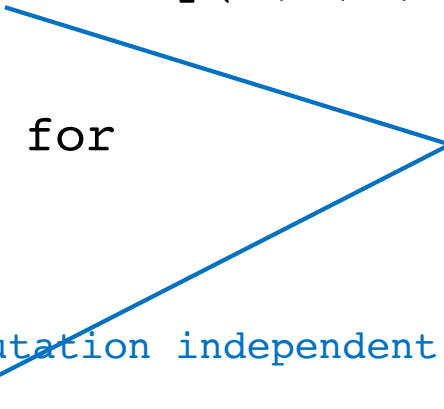
- OpenMP 4.5 & later supports several other new features
- **Single-instruction multiple-data (SIMD) parallelism:** An arithmetic operation is operated on multiple operand-pairs stored in vector registers (each of which can hold multiple operands) using vector instructions
- OpenMP `simd` construct instructs the compiler to vectorize the loop

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



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  
}
```



cf. MPI_Irecv() & MPI_Wait()

- 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

*cf. 3-phase (host-to-device copy→kernel execution→device-to-host copy)
performance bottleneck*

```
// Pre-allocate GPU array
#pragma omp target enter data map(alloc:psi[0:Nmax])

...
// make the device data environment consistent with the host
#pragma omp target update to(psi[0:Nmax]) to: host-to-device

...
// Keep operating on 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];

...
// De-allocate GPU array
#pragma omp target exit data map(delete:psi[0:Nmax])
```

Stand-alone directive to map variables to device memory

to: host-to-device
from: device-to-host

Runtime system keeps track of CPU & GPU memory access
& avoids unnecessary CPU-GPU data transfer

Stand-alone directive to unmap variables from device memory

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 // Spawn multiple CPU threads
{
    #pragma omp target
    { // Different GPU threads perform computation or data transfer }
}
```

See [OpenMP Offload Optimization](#) (Ye Luo, Argonne National Lab.) &
[Porting LFD Mini-app to GPU via OpenMP Offload](#) (Pankaj Rajak, USC/ANL)

See also [Accelerating quantum light-matter dynamics on graphics processing units](#),
T. Razach *et al.*, *Proc. IEEE IPDPSW/PDSEC* ('24)

and

[Multiscale light-matter dynamics in quantum materials: from electrons to topological superlattices](#), T. Razach *et al.*, *Proc. ACM/IEEE SC* ('25)