

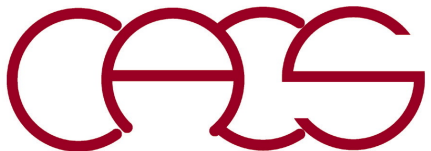
Hybrid MPI+OpenMP+CUDA Programming

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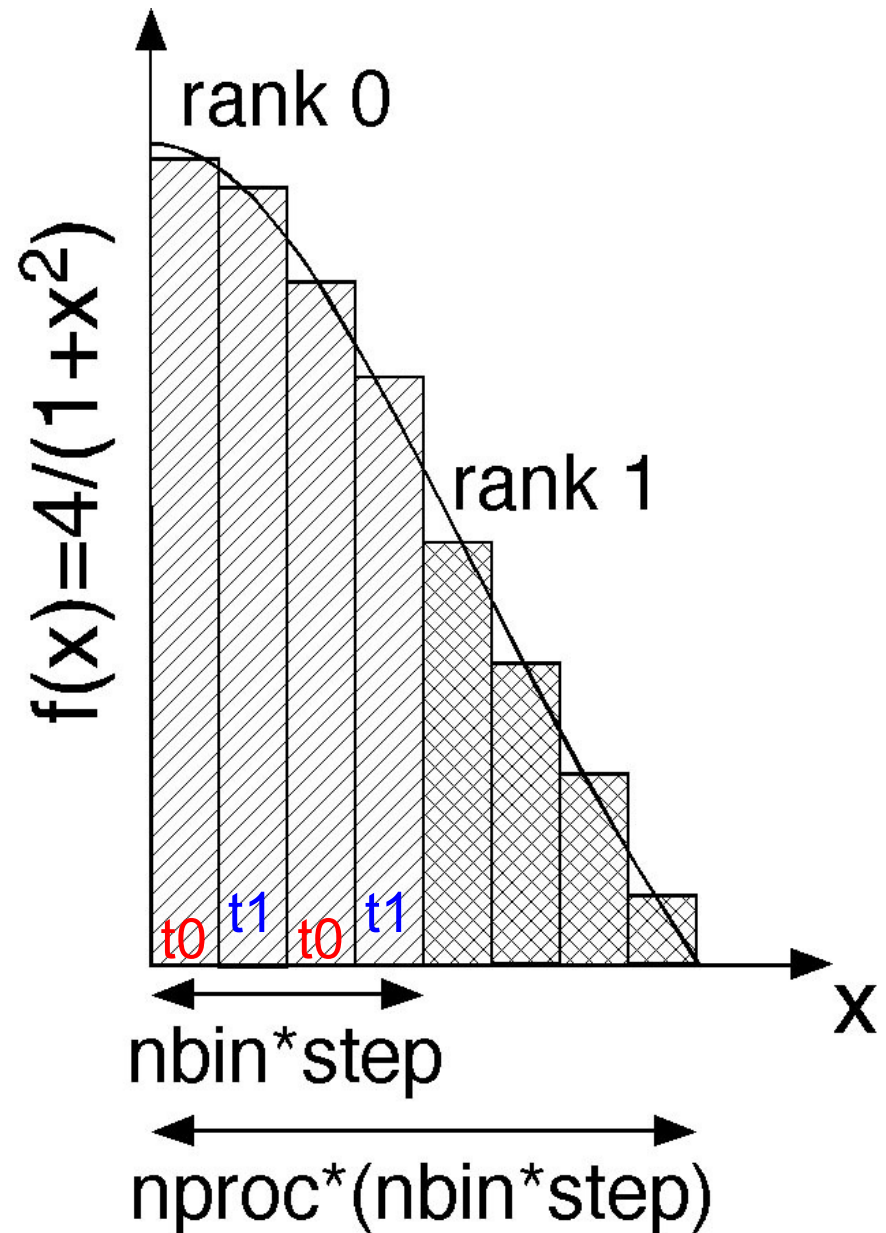
Objective: Hands-on experience in MPI+OpenMP+CUDA programming for hybrid parallel computing on a cluster of GPU-accelerated multicore computing nodes



MPI+CUDA Calculation of π

- **Spatial decomposition by offset:** Each MPI process integrates over a range of width $1/\text{nproc}$, as a discrete sum of nbin bins each of width step
- **Interleaving by skipping indices:** Within each MPI process, $\text{NUM_BLOCK} \times \text{NUM_THREAD}$ CUDA threads perform part of the sum

$$\pi = \int_0^1 \frac{4}{1+x^2} dx \cong \Delta \sum_{i=0}^{N-1} \frac{4}{1+x_i^2}$$



Calculate Pi with MPI+CUDA: hypi.cu (1)

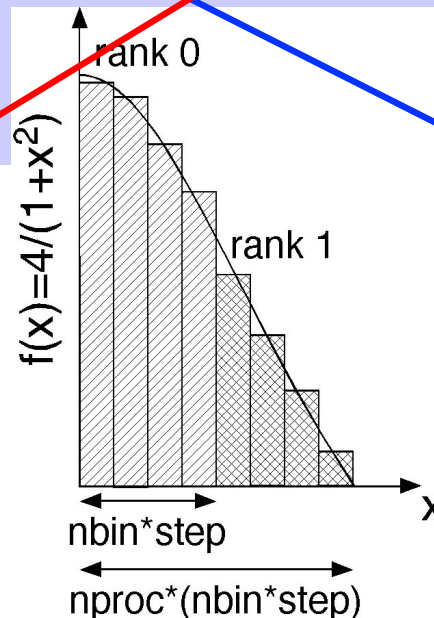
```
#include <stdio.h>
#include <mpi.h>
#include <cuda.h>

#define NBIN 10000000 // Number of bins
#define NUM_BLOCK 13 // Number of thread blocks
#define NUM_THREAD 192 // Number of threads per block

// Kernel that executes on the CUDA device
__global__ void cal_pi(float *sum, int nbin, float step, float offset, int nthreads, int nblocks)
{
    int i;
    float x;
    int idx = blockIdx.x*blockDim.x+threadIdx.x; // Sequential thread index across blocks
    for (i=idx; i< nbin; i+=nthreads*nblocks) { // Interleaved bin assignment to threads
        x = offset+(i+0.5)*step;
        sum[idx] += 4.0/(1.0+x*x);
    }
}
```

Difference from base pi.cu program in red

**MPI spatial decomposition
via offset (how many bins
have been computed before
me?)**



**CUDA thread interleaving
(give way bins to the other
threads)**

cf. Kernel in <https://aiichironakano.github.io/cs653/src/parallel/pi.cu>

Calculate Pi with MPI+CUDA: hypi.cu (2)

```
int main(int argc, char **argv) {
    int myid, nproc, nbin, tid;
    float step, offset, pi=0.0, pig;
    dim3 dimGrid(NUM_BLOCK, 1, 1); // Grid dimensions (only use 1D)
    dim3 dimBlock(NUM_THREAD, 1, 1); // Block dimensions (only use 1D)
    float *sumHost, *sumDev; // Pointers to host & device arrays
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &myid); // My MPI rank
    MPI_Comm_size(MPI_COMM_WORLD, &nproc); // Number of MPI processes
    nbin = NBIN/nproc; // Number of bins per MPI process
    step = 1.0/(float)(nbin*nproc); // Step size with redefined number of bins
    offset = myid*step*nbin; // Quadrature-point offset
    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
    cudaMemset(sumDev, 0, size); // Reset array in device to 0
    // Calculate on device (call CUDA kernel)
    cal_pi <<<dimGrid, dimBlock>>> (sumDev, nbin, step, offset, NUM_THREAD, NUM_BLOCK);
    // Retrieve result from device and store it in host array
    cudaMemcpy(sumHost, sumDev, size, cudaMemcpyDeviceToHost);
    // Reduction over CUDA threads
    for(tid=0; tid<NUM_THREAD*NUM_BLOCK; tid++) pi += sumHost[tid];
    pi *= step;
    // CUDA cleanup
    free(sumHost);
    cudaFree(sumDev);
    printf("myid = %d: partial pi = %f\n", myid, pi);
    // Reduction over MPI processes
    MPI_Allreduce(&pi, &pig, 1, MPI_FLOAT, MPI_SUM, MPI_COMM_WORLD);
    if (myid==0) printf("PI = %f\n", pig);
    MPI_Finalize();
    return 0;}
```

Difference from base pi.cu program in red

nbin per MPI rank instead of total NBIN in pi.cu

Compiling MPI+CUDA on Discovery

- **Set an environment (add the following lines in your .bashrc)**
module purge
module load usc
module load cuda
- **Compilation (this also works for MPI+OpenMP+CUDA programs) — this should be typed all in one line:**

```
nvcc -Xcompiler -fopenmp hypi.cu -o hypi -  
I${OPENMPI_ROOT}/include -L${OPENMPI_ROOT}/lib -lmpi -lgomp
```



This should be all in one line

Running MPI+CUDA on Discovery

- **Submit the following Slurm script using the sbatch command**

```
#!/bin/bash
#SBATCH --partition=gpu
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=1
#SBATCH --gpus-per-task=1
#SBATCH --time=00:00:59
#SBATCH --output=hypi.out
#SBATCH -A anakano_429
mpirun -n 2 ./hypi
```

- **Output**

```
myid = 1: partial pi = 1.287001
myid = 0: partial pi = 1.854596
PI = 3.141597
```

Variation: Using 2 GPUs per Node (1)

- Run multiple MPI processes on each node, and assign different GPUs to different processes

`hypi_setdevice.cu`

```
int main(int argc, char **argv) {
    int dev_used;
    ...
    MPI_Comm_rank(MPI_COMM_WORLD, &myid); // My MPI rank
    cudaSetDevice(myid%2); // Pick one of the 2 GPUs (0 or 1)
    ...
    cudaGetDevice(&dev_used); // Find which GPU is being used
    printf("myid = %d: device used = %d; partial pi = %f\n", myid, dev_used, pi);
    ...
}
```

https://aiichironakano.github.io/cs653/src/parallel/hypi_setdevice.cu

Variation: Using 2 GPUs per Node (2)

- **Submit the following Slurm script using the sbatch command**

```
#!/bin/bash
#SBATCH --partition=gpu
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=2
#SBATCH --cpus-per-task=1
#SBATCH --gpus-per-task=2
#SBATCH --time=00:00:59
#SBATCH --output=hypi_setdevice.out
#SBATCH -A anakano_429
mpirun -n 4 ./hypi_setdevice
```

- **Output**

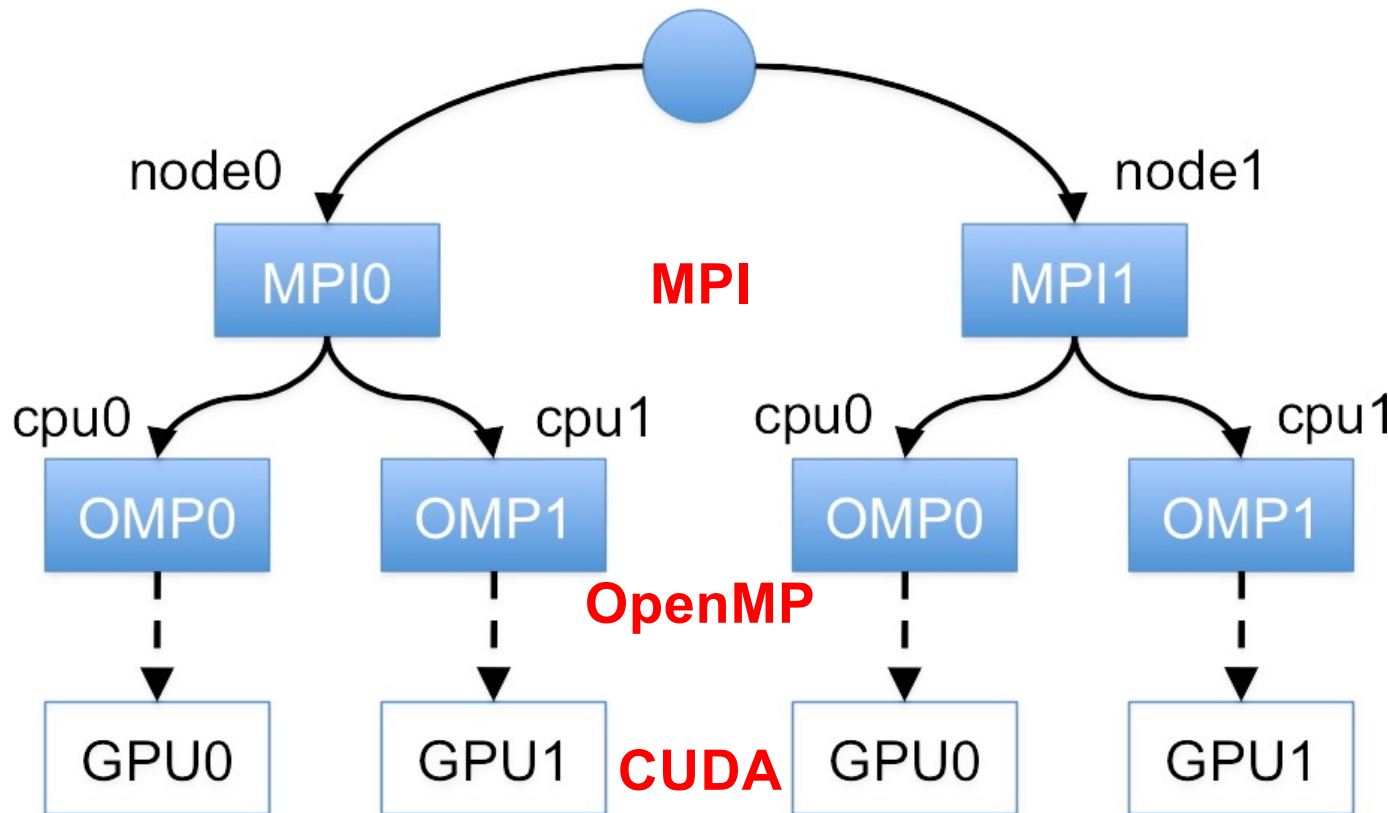
```
myid = 0: device used = 0; partial pi = 0.979926
myid = 1: device used = 1; partial pi = 0.874671
myid = 2: device used = 0; partial pi = 0.719409
myid = 3: device used = 1; partial pi = 0.567582
PI = 3.141588
```

Problem: What if ranks 0 & 2 are assigned to the same node → recommended to MPI+OpenMP+CUDA instead

<https://www.carc.usc.edu/user-guides/hpc-systems/using-our-hpc-systems/running-jobs>
<https://www.carc.usc.edu/user-guides/hpc-systems/using-our-hpc-systems/slurm-templates>

MPI+OpenMP+CUDA Computation of π

- Write a triple-decker MPI+OpenMP+CUDA program, `pi3.cu`, by inserting an OpenMP layer to the double-decker MPI+CUDA program, `hypi_setdevice.cu`
- Launch one MPI rank per node, where each rank spawns two OpenMP threads that run on different CPU cores & use different GPU devices



https://aiichironakano.github.io/cs653/src/parallel/hypi_setdevice.cu

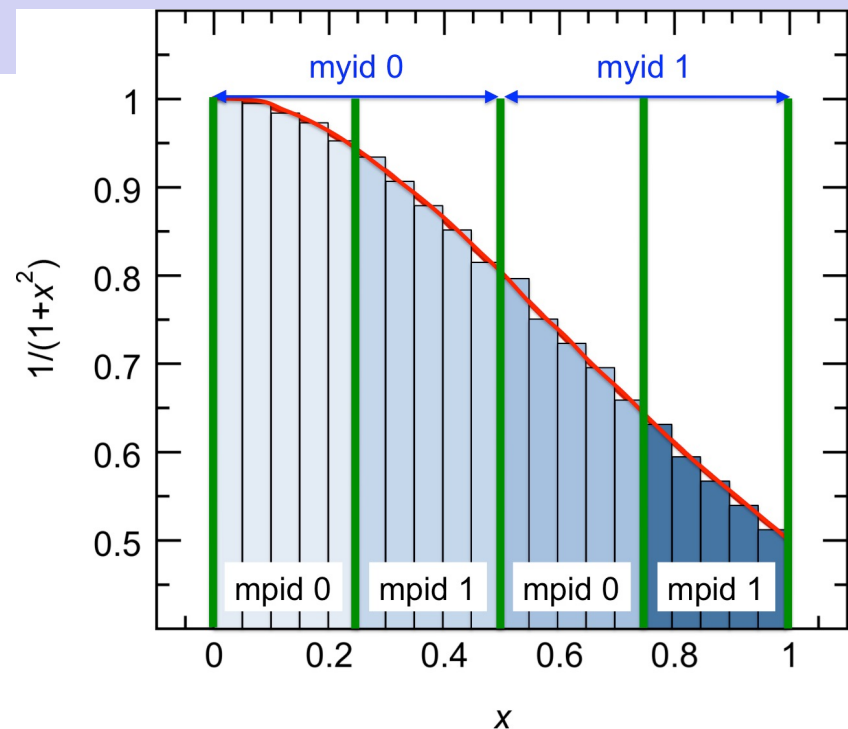
MPI+OpenMP Spatial Decompositions

```
#include <omp.h>
#define NUM_DEVICE 2 // # of GPU devices = # of OpenMP threads
...
// In main()
MPI_Comm_rank(MPI_COMM_WORLD, &myid); // My MPI rank
MPI_Comm_size(MPI_COMM_WORLD, &nproc); // # of MPI processes
omp_set_num_threads(NUM_DEVICE); // One OpenMP thread per GPU device
nbin = NBIN/(nproc*NUM_DEVICE); // # of bins per OpenMP thread
step = 1.0/(float)(nbin*nproc*NUM_DEVICE);
#pragma omp parallel private(list the variables that need private copies)
{
    int mpid = omp_get_thread_num();
    offset = (NUM_DEVICE*myid+mpid)*step*nbin; // Quadrature-point offset
    cudaSetDevice(mpid%2);
    ...
}
```

$$\text{offset} = \left(\underbrace{\underbrace{\underbrace{\text{how many threads before this rank}}_{\text{omp threads/rank}} \times \underbrace{\text{my rank}}_{\text{myid}}}_{\text{integration range per omp thread}} + \underbrace{\text{my thread ID in this rank}}_{\text{mpid}} \right) \times \underbrace{\underbrace{\text{per omp thread}}_{\text{nbin}} \times \underbrace{\text{bin width}}_{\text{step}}}$$

- For the CUDA layer, leave the interleaved assignment of quadrature points to CUDA threads in `hypi_setdevice.cu` as it is

Hierarchical MPI+OpenMP spatial decomposition



Data Privatization

- Circumvent the race condition for variable `pi`, by defining a private accumulator per OpenMP thread (or GPU device):

```
float pid[NUM_DEVICE];
```
- Use the array elements as dedicated accumulators for the OpenMP threads
- Upon exiting from the OpenMP parallel section, perform reduction over the elements of `pid[]` to obtain the partial sum, `pi`, per MPI rank

- Alternatively use (recall false sharing)

```
#pragma omp parallel reduction(+:pi)
```

Output

- To report which of the two GPUs has been used for the run, insert the following lines within the OpenMP parallel block:

```
cudaGetDevice(&dev_used);  
printf("myid = %d; mpid = %d: device used = %d; partial pi =  
%f\n", myid, mpid, dev_used, pi);
```

MPI rank

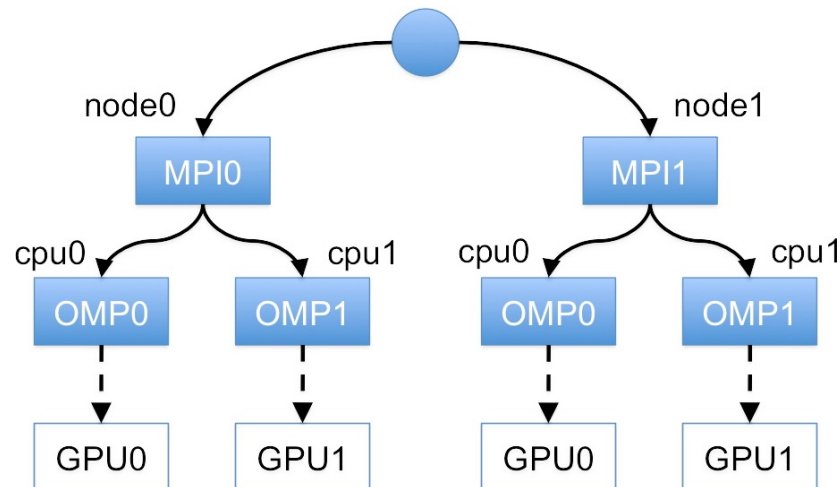
OpenMP
thread ID

ID of the GPU device
(0 or 1) that was used

Partial sum per OpenMP
thread or `pid[mpid]` if
data privatized manually

- Output

```
myid = 0; mpid = 0: device used = 0; partial pi = 0.979926  
myid = 0; mpid = 1: device used = 1; partial pi = 0.874671  
myid = 1; mpid = 0: device used = 0; partial pi = 0.719409  
myid = 1; mpid = 1: device used = 1; partial pi = 0.567582  
PI = 3.141588
```



Compiling MPI+OpenMP+CUDA

- Set an environment (add the following lines in your `.bashrc`)

```
module purge  
module load usc  
module load cuda
```

- **Compilation**  **nvcc option to pass the following option (-fopenmp) to gcc**

```
nvcc -Xcompiler -fopenmp pi3.cu -o pi3 -I${OPENMPI_ROOT}/include  
-L${OPENMPI_ROOT}/lib -lmpi -lgomp
```



This should be all in one line, and no space between - sign & next letter

Running MPI+OpenMP+CUDA

- **Submit the following Slurm script using the sbatch command**

```
#!/bin/bash
#SBATCH --partition=gpu
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=2
#SBATCH --gpus-per-task=2
#SBATCH --time=00:00:59
#SBATCH --output=pi3.out
#SBATCH -A anakano_429
mpirun -bind-to none -n 2 ./pi3
```

- **Output**

```
myid = 1; mpid = 1: device used = 1; partial pi = 0.567582
myid = 1; mpid = 0: device used = 0; partial pi = 0.719409
myid = 0; mpid = 0: device used = 0; partial pi = 0.979926
myid = 0; mpid = 1: device used = 1; partial pi = 0.874671
PI = 3.141588
```

Q: Why MPI+OpenMP+CUDA?

A: All US supercomputers will be GPU-accelerated

Q: Why calculus (quantum dynamics) on GPU?

A: Differentiable machine learning for all
(Example) Natural language processing (NLP)

DP (dynamic programming) → **DL** (deep learning) → **DiffL** (differentiable learning)

Take-home lessons:

- **GPU-offload basics:** host2device → kernel → device2host
- **Multiple GPUs per node (4 on Frontier and 6 on Aurora):**
`cudaSetDevice(OMP thread ID%NUM_DEVICE)`

`cudaGetDeviceCount(int *)`

Where to go from here = make it orders-of-magnitude faster:

- **Overlap CPU+GPU computations: Persistent & asynchronous kernels**
- **Minimize CPU-GPU communication**

