Hybrid MPI+OpenMP+CUDA Programming

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https://hpcc.usc.edu/support/documentation/gpucluster/
MPI+CUDA Calculation of $\pi$

- **Spatial decomposition:** Each MPI process integrates over a range of width $1/n_{\text{proc}}$, as a discrete sum of $n_{\text{bin}}$ bins each of width $\text{step}$.

- **Interleaving:** Within each MPI process, $\text{NUM\_BLOCK}*\text{NUM\_THREAD}$ CUDA threads perform part of the sum.

$$\pi = \int_0^1 \frac{4}{1 + x^2} \, dx \approx \Delta \sum_{i=0}^{N-1} \frac{4}{1 + x_i^2} \text{ with } n_{\text{bin}} \times \text{step} \leq n_{\text{proc}} \times (n_{\text{bin}} \times \text{step})$$

![Graph showing the calculation of $\pi$ using spatial decomposition and interleaving.](image-url)
Calculate Pi with MPI+CUDA: hypi.cu (1)

```c
#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);
    }
}
```

MPI spatial decomposition

CUDA thread interleaving
int main(int argc, char **argv) {
    int myid, nproc, nbin, tid;
    float step, offset, pi, 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 = %.15f\n", myid, pi);
    // Reduction over MPI processes
    MPI_Allreduce(&pi, &pig, 1, MPI_FLOAT, MPI_SUM, MPI_COMM_WORLD);
    if (myid==0) printf("PI = %.15f\n", pig);
    MPI_Finalize();
    return 0;
}
Compiling MPI+CUDA on HPC

- **Set an environment on the front-end (ssh to hpc-login3.usc.edu)**
  
  source /usr/usc/openmpi/default/setup.csh (if tcsh)
  
  source /usr/usc/cuda/default/setup.csh
  
  or
  
  source /usr/usc/openmpi/default/setup.sh (if bash)
  
  source /usr/usc/cuda/default/setup.csh

- **Compilation (this is for MPI+OpenMP+CUDA)**
  
  nvcc -Xcompiler -fopenmp hypi.cu -o hypi
  
  -I/usr/usc/openmpi/default/include
  
  -L/usr/usc/openmpi/default/lib -lmpi -lgomp
Interactive Run on HPC

Here, we assume that you have included the source commands (in the previous slide) to set up interoperable OpenMPI & CUDA environments within your .cshrc or .bashrc in your home directory.

```
[anakano@hpc-login3 ~]$ salloc --nodes=2 --ntasks-per-node=1 --cpus-per-task=1 --gres=gpu:1 -t 29
salloc: Pending job allocation 2140476
salloc: job 2140476 queued and waiting for resources
salloc: job 2140476 has been allocated resources
salloc: Granted job allocation 2140476
salloc: Waiting for resource configuration
salloc: Nodes hpc[3820,3823] are ready for job
[anakano@hpc3820 anakano]$ srun -n 2 ./hypi
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

```c
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);
  ...
}
```
Variation: Using 2 GPUs per Node (2)

```
[anakano@hpc-login3 ~/work596]$ salloc --nodes=2 --ntasks-per-node=2 --cpus-per-task=1 --gres=gpu:2 -t 29
salloc: Pending job allocation 2140495
salloc: job 2140495 queued and waiting for resources
salloc: job 2140495 has been allocated resources
salloc: Granted job allocation 2140495
salloc: Waiting for resource configuration
salloc: Nodes hpc[3820-3821] are ready for job
[anakano@hpc3820 anakano]$ srun -n 4 ./hypi_setdevice
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
```
**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.
• For the CUDA layer, leave the interleaved assignment of quadrature points to CUDA threads in `hypi_setdevice.cu` as it is
Data Privatization

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

  ```c
  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 $\text{pid}[\ ]$ to obtain the partial sum, $\pi$, per MPI rank

- Alternatively use (recall false sharing)

  ```c
  #pragma omp parallel reduction(+:pi)
  ```
• To report which of the two GPUs has been used for the run, insert the following lines within the OpenMP parallel block:

```c
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
```
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  source /usr/usc/cuda/default/setup.csh

  or

  source /usr/usc/openmpi/default/setup.sh (if bash)

  source /usr/usc/cuda/default/setup.sh

- Compilation

  `nvcc` option to pass the following option (\texttt{-fopenmp}) to `gcc`

  `nvcc -Xcompiler -fopenmp pi3.cu -o pi3`

  -I/usr/usc/openmpi/default/include

  -L/usr/usc/openmpi/default/lib -lmpi -lgomp`
Running MPI+OpenMP+CUDA on HPC

• Submit the following Slurm script using the sbatch command
  ```bash
  #!/bin/bash
  #SBATCH --nodes=2
  #SBATCH --ntasks-per-node=1
  #SBATCH --cpus-per-task=2
  #SBATCH --gres=gpu:2
  #SBATCH --time=00:00:59
  #SBATCH --output=pi3.out
  #SBATCH -A lc_an2
  source /usr/usc/openmpi/default/setup.sh
  source /usr/usc/cuda/default/setup.sh
  WORK_HOME=/home/rcf-proj/an2/YourID
  cd $WORK_HOME
  srun -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
  ```
  No need if in .bashrc