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 \( 1/nproc \), as a discrete sum of \( nb \) bins each of width \( \text{step} \).

- **Interleaving:** Within each MPI process, \( \text{NUM BLOCK} \times \text{NUM THREAD} \) CUDA threads perform part of the sum.

\[
\pi = \int_0^1 \frac{4}{1 + x^2} \, dx \equiv \Delta \sum_{i=0}^{N-1} \frac{4}{1 + x_i^2}
\]
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=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
    cudaMemcpy(sumDev, 0, size, cudaMemcpyDeviceToHost);  // 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;}

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
  nvcc -Xcompiler -fopenmp hypi_setdevice.cu -o hypi_setdevice
    -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 second slide) to set up interoperable OpenMP & 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

```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)
    ...
    cudaMemcpy(&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
```
• 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
#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)
{
    mpid = omp_get_thread_num();
    offset = (NUMDEVICE*myid+mpid)*step*nbin; // Quadrature-point offset
cudaSetDevice(mpid%2);...
}

• 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):
  
  ```
  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
  
  ```
  #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);
```

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
```
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.sh

Compilation

nvcc option to pass the following option (-fopenmpi) 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
  #!/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