CSCI596 Assignment 6—Hybrid MPI+OpenMP+CUDA Programming

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CSCI-596 assignment4
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Part 1:

pdf1.cu code:

```
/*----------------------------------------------------------------------
Program pdf0.c computes a pair distribution function for n atoms
given the 3D coordinates of the atoms.
----------------------------------------------------------------------*/
#include <stdio.h>
#include <math.h>
#include <time.h>
#include <stdlib.h>

#define NHBIN 2000    // Histogram size

float al[3];              // Simulation box lengths
int n;                    // Number of atoms
float *r;                 // Atomic position array
FILE *fp;

__constant__ float DALTH[3];
__constant__ int DN;
__constant__ float DDRH;

//float SignR(float v,float x) {if (x > 0) return v; else return -v;}
__device__ float d_SignR(float v,float x) {if (x > 0) return v; else return -v;}

__global__ void gpu_histogram_kernel(float *r,float *nhis) {
      int i,j,a,ih;
      float rij,dr;

      int iBlockBegin = (DN/gridDim.x)*blockIdx.x;
      int iBlockEnd = min((DN/gridDim.x)*(blockIdx.x+1),DN);

      int jBlockBegin = (DN/gridDim.y)*blockIdx.y;
      int jBlockEnd = min((DN/gridDim.y)*(blockIdx.y+1),DN);

      for (i=iBlockBegin+threadIdx.x; i<iBlockEnd; i+=blockDim.x) {
            for (j=jBlockBegin+threadIdx.y; j<jBlockEnd; j+=blockDim.y) {
```

```
                if (i<j) {
                // Process (i,j) atom pair
                    rij = 0.0;
                    for (a=0; a<3; a++) {
                        dr = r[3*i+a]-r[3*j+a];
                        /* Periodic boundary condition */
                        dr=dr-d_SignR(DALTH[a],dr-DALTH[a])-
d_SignR(DALTH[a],dr+DALTH[a]);
                        rij += dr*dr;
                    }
                    rij = sqrt(rij); /* Pair distance */
                    ih = rij/DDRH;
                    //nhis[ih] += 1.0;
                    atomicAdd(&nhis[ih],1.0);
                } // end if i<j
            } // end for j
        } // end for i
}
/*---------------------------------------------------------------------*/
void histogram() {
/*---------------------------------------------------------------------
Constructs a histogram NHIS for atomic-pair distribution.
---------------------------------------------------------------------*/
    float alth[3];
    float* nhis;    // Histogram array
    float rhmax,drh,density,gr;
    int a,ih;

    float* dev_r; // Atomic positions
    float* dev_nhis; // Histogram

    /* Half the simulation box size */
    for (a=0; a<3; a++) alth[a] = 0.5*al[a];
    /* Max. pair distance RHMAX & histogram bin size DRH */
    rhmax = sqrt(alth[0]*alth[0]+alth[1]*alth[1]+alth[2]*alth[2]);
    drh = rhmax/NHBIN;    // Histogram bin size

    nhis = (float*)malloc(sizeof(float)*NHBIN);
    //for (ih=0; ih<NHBIN; ih++) nhis[ih] = 0.0; // Reset the histogram

    cudaMalloc((void**)&dev_r,sizeof(float)*3*n);
    cudaMalloc((void**)&dev_nhis,sizeof(float)*NHBIN);

    cudaMemcpy(dev_r,r,3*n*sizeof(float),cudaMemcpyHostToDevice);
```

```
    cudaMemset(dev_nhis,0.0,NHBIN*sizeof(float));

    cudaMemcpyToSymbol(DALTH,alth,sizeof(float)*3,0,cudaMemcpyHostToDevice);
    cudaMemcpyToSymbol(DN,&n,sizeof(int),0,cudaMemcpyHostToDevice);
    cudaMemcpyToSymbol(DDRH,&drh,sizeof(float),0,cudaMemcpyHostToDevice);

    dim3 numBlocks(8,8,1);
    dim3 threads_per_block(16,16,1);
    gpu_histogram_kernel<<<numBlocks,threads_per_block>>>(dev_r,dev_nhis);

    cudaMemcpy(nhis,dev_nhis,NHBIN*sizeof(float),cudaMemcpyDeviceToHost);
    cudaFree(dev_r);
    cudaFree(dev_nhis);

    density = n/(al[0]*al[1]*al[2]);
    /* Print out the histogram */
    fp = fopen("pdf.d","w");
    for (ih=0; ih<NHBIN; ih++) {
       gr = nhis[ih]/(2*M_PI*pow((ih+0.5)*drh,2)*drh*density*n);
       fprintf(fp,"%e %e\n",(ih+0.5)*drh,gr);
    }
    fclose(fp);
    free(nhis);
}

/*---------------------------------------------------------------------*/
int main() {
/*---------------------------------------------------------------------*/
    int i;
    float cpu1,cpu2;

    /* Read the atomic position data */
    fp = fopen("pos.d","r");
    fscanf(fp,"%f %f %f",&(al[0]),&(al[1]),&(al[2]));
    fscanf(fp,"%d",&n);
    r = (float*)malloc(sizeof(float)*3*n);
    for (i=0; i<n; i++)
       fscanf(fp,"%f %f %f",&(r[3*i]),&(r[3*i+1]),&(r[3*i+2]));
    fclose(fp);

    /* Compute the histogram */
    cpu1 = ((float) clock())/CLOCKS_PER_SEC;
    histogram();
    cpu2 = ((float) clock())/CLOCKS_PER_SEC;
```

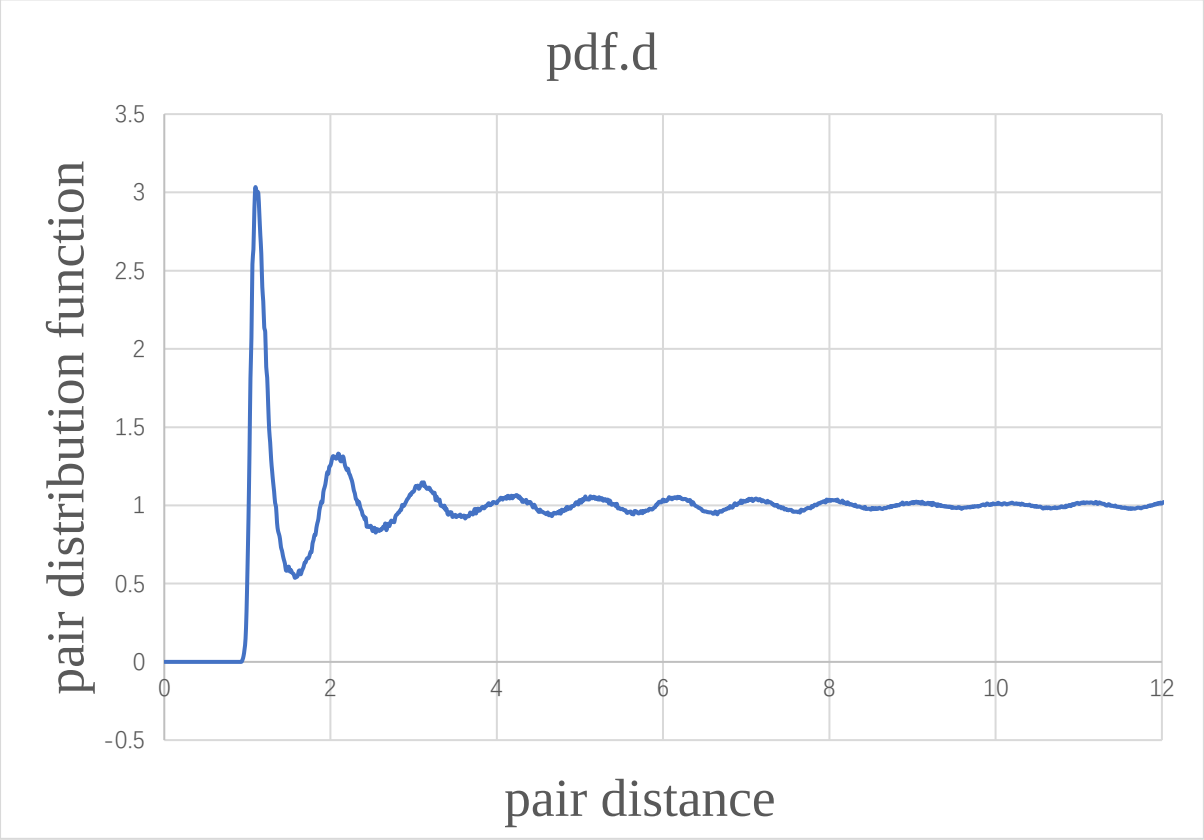
```
    printf("Execution time (s) = %le\n",cpu2-cpu1);

    free(r);
    return 0;
}
```

Output:

```
youzhiqu@hpc-login3:~/work596$ more pdf.out
---------- Begin SLURM Prolog ----------
Job ID:         2265101
Username:       youzhiqu
Accountname:    lc_an2
Name:           pdf.sl
Partition:      quick
Nodelist:       hpc3049
TasksPerNode:   1
CPUsPerTask:    Default[1]
TMPDIR:         /tmp/2265101.quick
SCRATCHDIR:     /staging/scratch/2265101
Cluster:        uschpc
HSDA Account:   false
---------- 2018-11-16 20:52:12 ----------
##### CPU: gcc -O -o pdf0 pdf0.c -lm #####
Execution time (s) = 2.660000e+00
##### GPU: nvcc -O -o pdf1 pdf1.cu #####
Execution time (s) = 2.300000e-01
```

2:



Part 2:

pi3.cu code:

```
// Hybrid MPI+OpenMP+CUDA computation of Pi
#include <stdio.h>
#include <mpi.h>
#include <omp.h>
#include <cuda.h>

#define NBIN    10000000    // Number of bins
#define NUM_DEVICE 2 // # of GPU devices = # of OpenMP threads
#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 the
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);
      }
}

int main(int argc,char **argv) {
      int myid,nproc,nbin,tid;
      int mpid;
      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
      int dev_used;

      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

      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(mpid,offset,SumHost,sumDev,tid,dev_used) reduction(+:pi)
    {
        mpid = omp_get_thread_num();
        offset = (NUM_DEVICE*myid+mpid)*step*nbin; // Quadrature-point offset
        cudaSetDevice(mpid%2);
        //cudaSetDevice(myid%2);
        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);
        cudaGetDevice(&dev_used);
        //printf("myid = %d: device used = %d; partial pi = %f\n",myid,dev_used,pi);
        printf("myid = %d; mpid = %d: device used = %d; partial pi = %f\n", myid, mpid, dev_used, pi);
    } // End omp parallel

    // 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;
}
```

2. output:

```
[youzhiqu@hpc-login3:~/work596$ salloc --nodes=2 --ntasks-per-node=2 --cpus-per-task=1 --gres=gpu:2 -t 29
 salloc: Granted job allocation 2265134
 salloc: Waiting for resource configuration
 salloc: Nodes hpc[3049,3052] are ready for job
 ---------- Begin SLURM Prolog ----------
 Job ID:        2265134
 Username:      youzhiqu
 Accountname:   lc_an2
 Name:          sh
 Partition:     quick
 Nodelist:      hpc[3049,3052]
 TasksPerNode:  2(x2)
 CPUsPerTask:   1
 TMPDIR:        /tmp/2265134.quick
 SCRATCHDIR:    /staging/scratch/2265134
 Cluster:       uschpc
 HSDA Account:  false
 ---------- 2018-11-16 21:10:29 ---------
 youzhiqu@hpc3049:/auto/dr-std/an2/youzhiqu$ source /usr/usc/openmpi/default/setup.sh
[youzhiqu@hpc3049:/auto/dr-std/an2/youzhiqu$ source /usr/usc/cuda/default/setup.sh
[youzhiqu@hpc3049:/auto/dr-std/an2/youzhiqu$ srun -n 2 ./pi3
 myid = 1; mpid = 0: device used = 0; partial pi = 0.719409
 myid = 1; mpid = 1: device used = 1; partial pi = 0.567582
 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
[youzhiqu@hpc-login3:~/work596$ salloc --nodes=2 --ntasks-per-node=2 --cpus-per-task=1 --gres=gpu:2 -t 29
 salloc: Granted job allocation 2265134
 salloc: Waiting for resource configuration
 salloc: Nodes hpc[3049,3052] are ready for job
 ---------- Begin SLURM Prolog ----------
 Job ID:        2265134
 Username:      youzhiqu
 Accountname:   lc_an2
 Name:          sh
 Partition:     quick
 Nodelist:      hpc[3049,3052]
 TasksPerNode:  2(x2)
 CPUsPerTask:   1
 TMPDIR:        /tmp/2265134.quick
 SCRATCHDIR:    /staging/scratch/2265134
 Cluster:       uschpc
 HSDA Account:  false
 ---------- 2018-11-16 21:10:29 ---------
 youzhiqu@hpc3049:/auto/dr-std/an2/youzhiqu$ source /usr/usc/openmpi/default/setup.sh
[youzhiqu@hpc3049:/auto/dr-std/an2/youzhiqu$ source /usr/usc/cuda/default/setup.sh
[youzhiqu@hpc3049:/auto/dr-std/an2/youzhiqu$ srun -n 2 ./pi3
 myid = 1; mpid = 0: device used = 0; partial pi = 0.719409
 myid = 1; mpid = 1: device used = 1; partial pi = 0.567582
 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
```