CSCI_596_HW6
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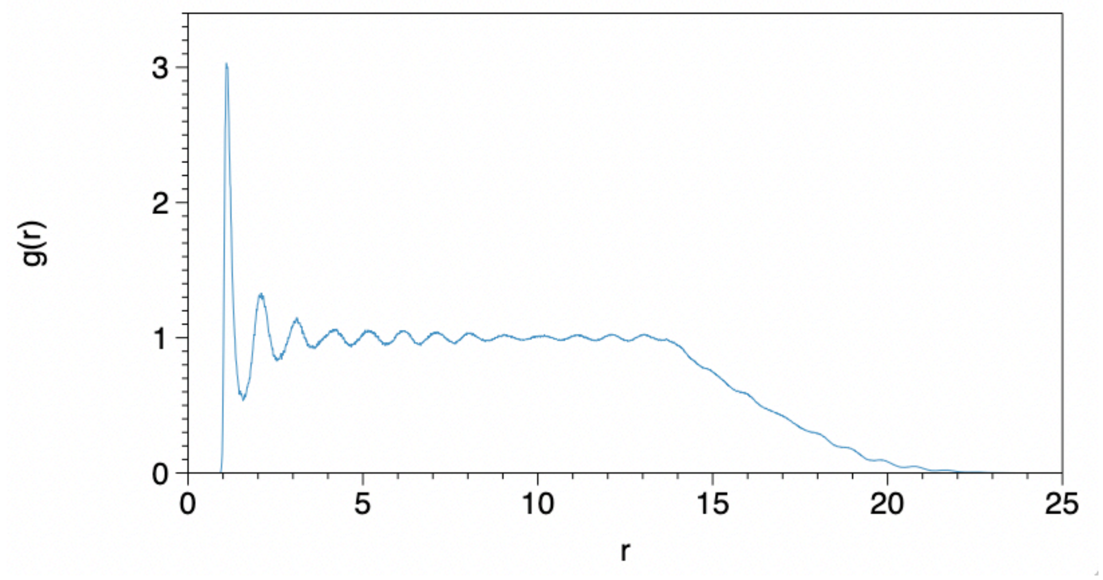
Part I: Pair-Distribution Computation with CUDA

Code of pdf.cu (modified from pdf0.c):

```
/*----------------------------------------------------------------------
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>
#include <cuda.h> // changed

#define NHBIN 2000 // Histogram size

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

/*  changed below */
__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 = (DN / gridDim.x) * (blockIdx.x + 1);
    if (blockIdx.x == gridDim.x - 1)
        iBlockEnd = DN;
    int jBlockBegin = (DN / gridDim.y) * blockIdx.y;
    int jBlockEnd = (DN / gridDim.y) * (blockIdx.y + 1);
    if (blockIdx.y == gridDim.y - 1)
        jBlockEnd = 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
}
/* changed above */

/*--------------------------------------------------------------------*/
void histogram()
{
    /*----------------------------------------------------------------------
Constructs a histogram NHIS for atomic-pair distribution.
----------------------------------------------------------------------*/
    float alth[3];
    float *nhis; // Histogram array
    float rhmax, drh, dr, rij, density, gr;
    int a, ih, i, j;

    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

    /* changed below */
    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);

    // Compute dev_nhis on GPU: dev_r[] -> dev_nhis[]

    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;
}
```

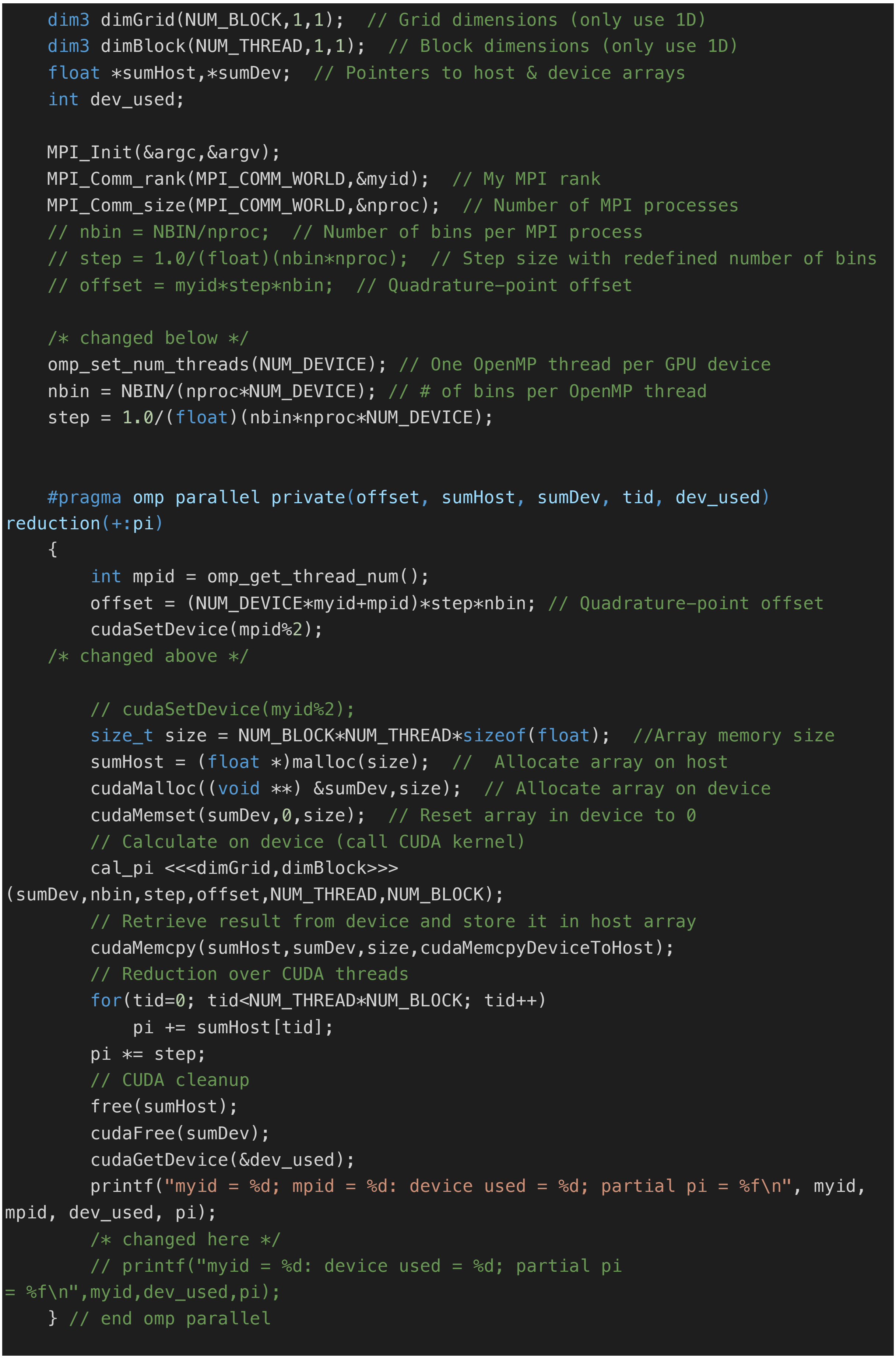
Plot of the resulting pair distribution function:



Part II: MPI+OpenMP+CUDA Computation of Pi

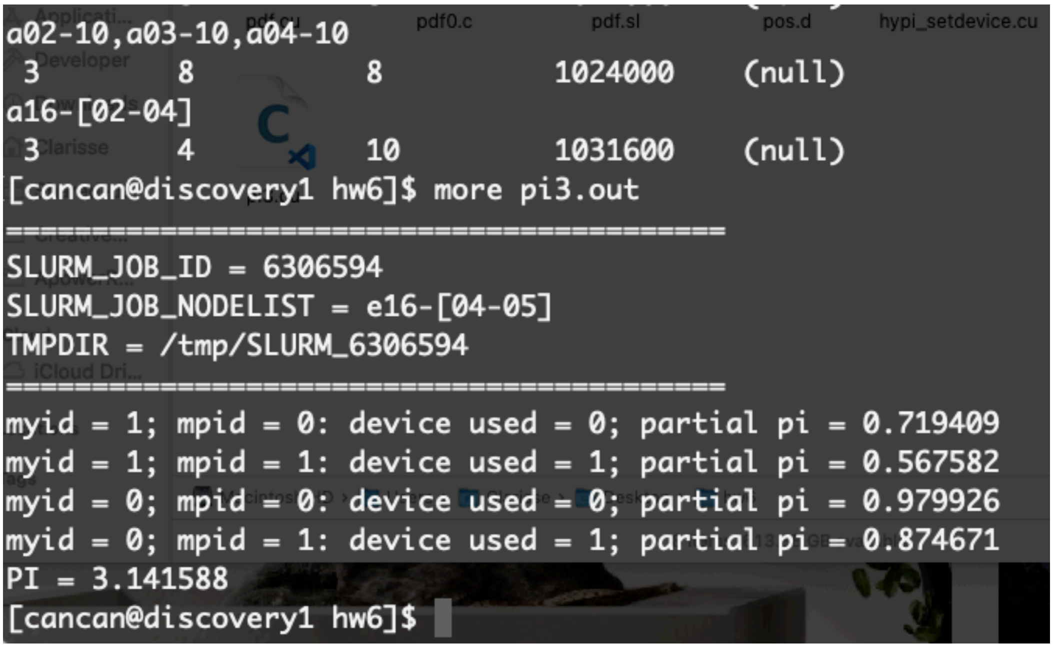
MPI+OpenMP+CUDA code (pi3.cu):

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

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

    /* changed below */
    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(offset, sumHost, sumDev, tid, dev_used)
reduction(+:pi)
    {
        int mpid = omp_get_thread_num();
        offset = (NUM_DEVICE*myid+mpid)*step*nbin; // Quadrature-point offset
        cudaSetDevice(mpid%2);
    /* changed above */

        // 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; mpid = %d: device used = %d; partial pi = %f\n", myid,
mpid, dev_used, pi);
        /* changed here */
        // printf("myid = %d: device used = %d; partial pi
= %f\n",myid,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;
}
```

My output:



```
a02-10,a03-10,a04-10
 3      8       8       1024000    (null)
a16-[02-04]
 3      4       10      1031600    (null)
[cancan@discovery1 hw6]$ more pi3.out
=========================================
SLURM_JOB_ID = 6306594
SLURM_JOB_NODELIST = e16-[04-05]
TMPDIR = /tmp/SLURM_6306594
=========================================
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
[cancan@discovery1 hw6]$
```