

Pair Distribution Computation on GPU

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Goal: Using multidimensional Grid & Block

See B. G. Levine et al., *J. Comput. Phys.* **230**, 3556 (2011)
<https://aiichironakano.github.io/cs596/Levin-RDFonGPU-JCP11.pdf>



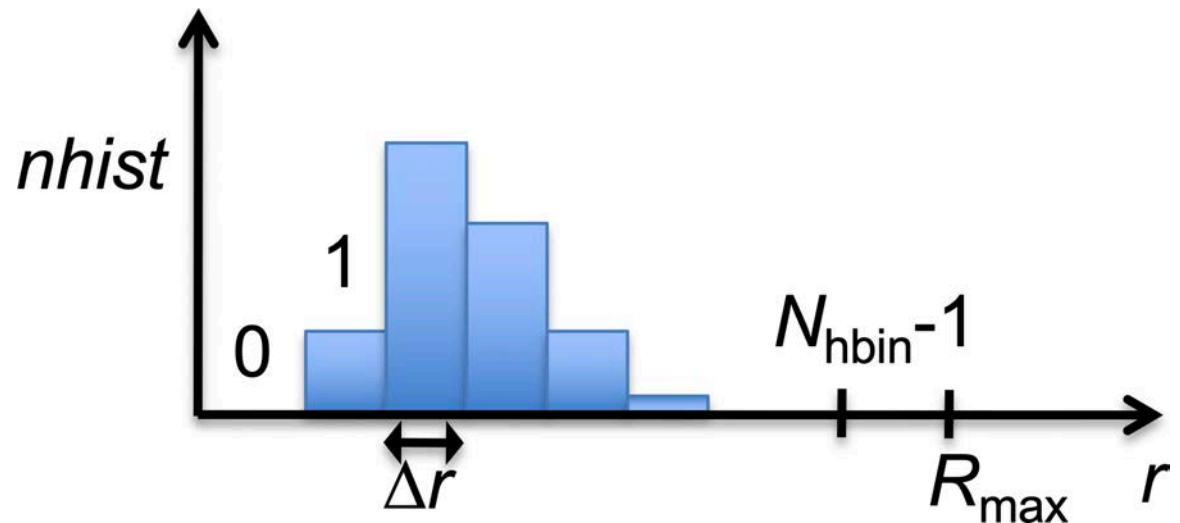
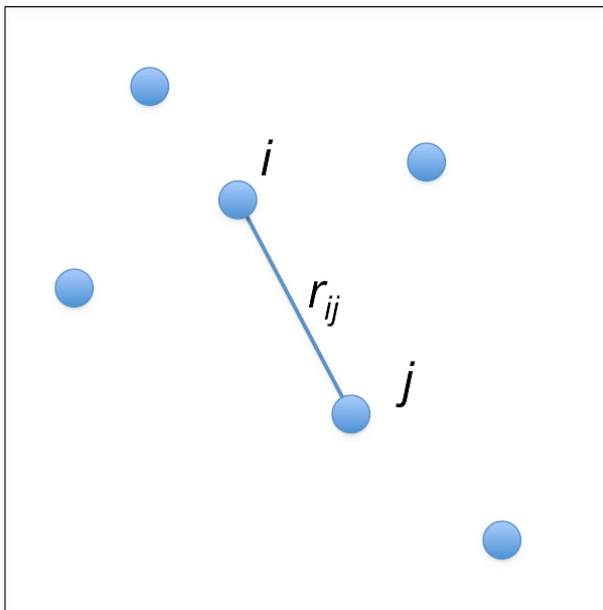
Pair Distribution

- **Pair-distance histogram**, `nhist[Nhbin]`

```
for all histogram bins i
  nhist[i] = 0
for all atomic pairs (i,j)
  ++nhist[ $\lfloor |\vec{r}_{ij}| / \Delta r \rfloor$ ]
```

reset

count



Pair Distribution Function

- Pair-distribution function, $g(r)$**

$$g(r_i) = \frac{nhist(i)}{2\pi r_i^2 \Delta r \rho N}$$

N : # of atoms
 ρ : # density

$g(r)$: For each atom, how many other atoms are distance r apart, normalized by # of atoms expected from average density; deviation from 1 signifies correlation with an atom at $r = 0$

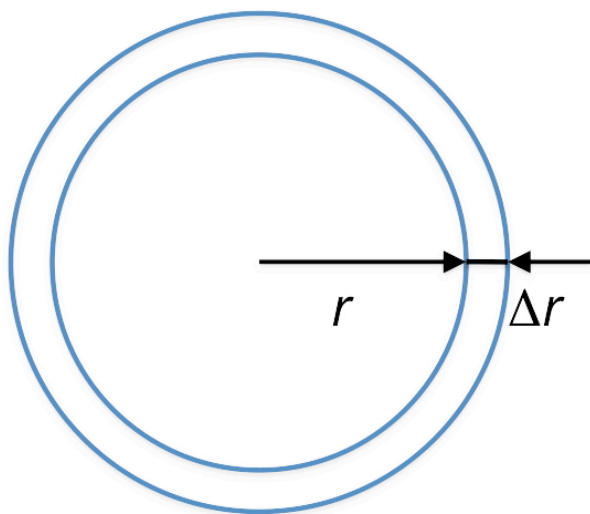
With minimum-image convention,

$$R_{\max} = \sqrt{\sum_{\alpha=x,y,z} \left(\frac{al[\alpha]}{2} \right)^2}$$

r_{\max}

$$\Delta r = R_{\max} / N_{\text{hbin}}; r_i = (i+1/2)\Delta r$$

drh

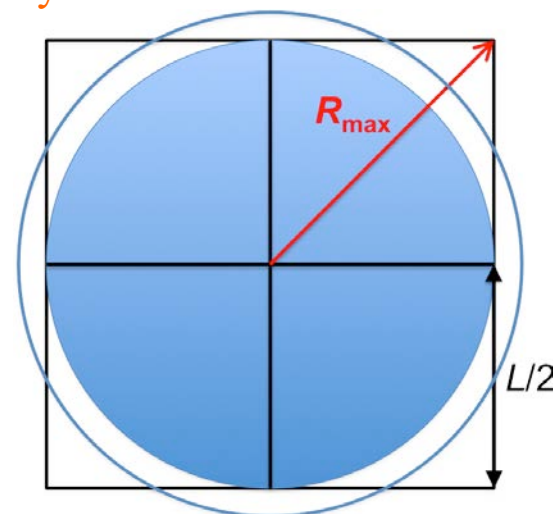


$$\therefore g(r_i) = \frac{2 \times nhist(i)}{N} \times \frac{1}{4\pi r_i^2 \Delta r \times \rho}$$

of other atoms j in a concentric shell with thickness Δr at distance r_i from atom i ; factor 2, since each pair is computed only once

Volume of the shell

Average number density



Big Loops over Atomic Pairs

input: $r[]$, n **Program:** pdf0.c (atomic positions in pos.d)

```
for (i=0; i<n-1; i++) {  
    for (j=i+1; j<n; j++) {  
        rij = 0.0;  
        for (a=0; a<3; a++) {  
            dr = r[3*i+a]-r[3*j+a];  
            /* Periodic boundary condition */  
            dr = dr-SignR(alth[a],dr-alth[a])-SignR(alth[a],dr+alth[a]);  
            rij += dr*dr; Minimum-image convention (cf. MD lecture)  
        } https://aiichironakano.github.io/cs596/01MD.pdf  
        rij = sqrt(rij); /* Pair distance */  
        ih = rij/drh;  
        nhis[ih] += 1.0; /* Entry to the histogram */  
    } // End for j  
} // Endo for i
```

output: $nhis[]$

- n : **Number of atoms**
- $r[3*n]$: $r[3*i | 3*i+1 | 3*i+2]$ is the x|y|z coordinate of the i -th atom
- $alth[a] = al[a]/2$: **Half the simulation box lengths**

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

<https://aiichironakano.github.io/cs596/src/md/md.h>

Variables in Device Memory

```
__constant__ float DALTH[3];
__constant__ int DN;
__constant__ float DDRH;
float* dev_r;      // Atomic positions
float* dev_nhis;   // 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);

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

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

cudaFree(dev_r);
cudaFree(dev_nhis);
```

- **cudaMemcpyToSymbol:**

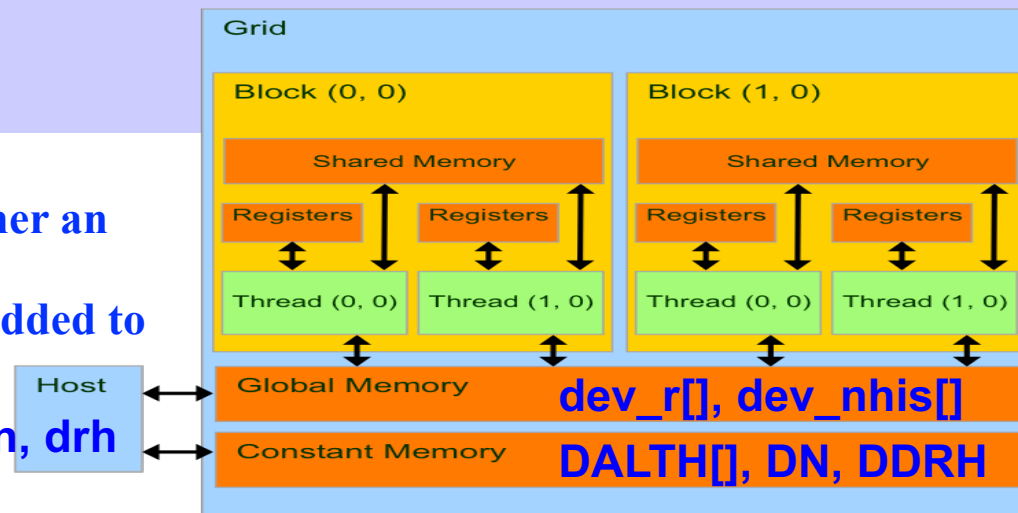
Destination (in device) is either an address or variable name

Memory offset (in bytes) is added to destination

r[], nhis[], alth[], n, drh

In read-only constant memory

memory offset

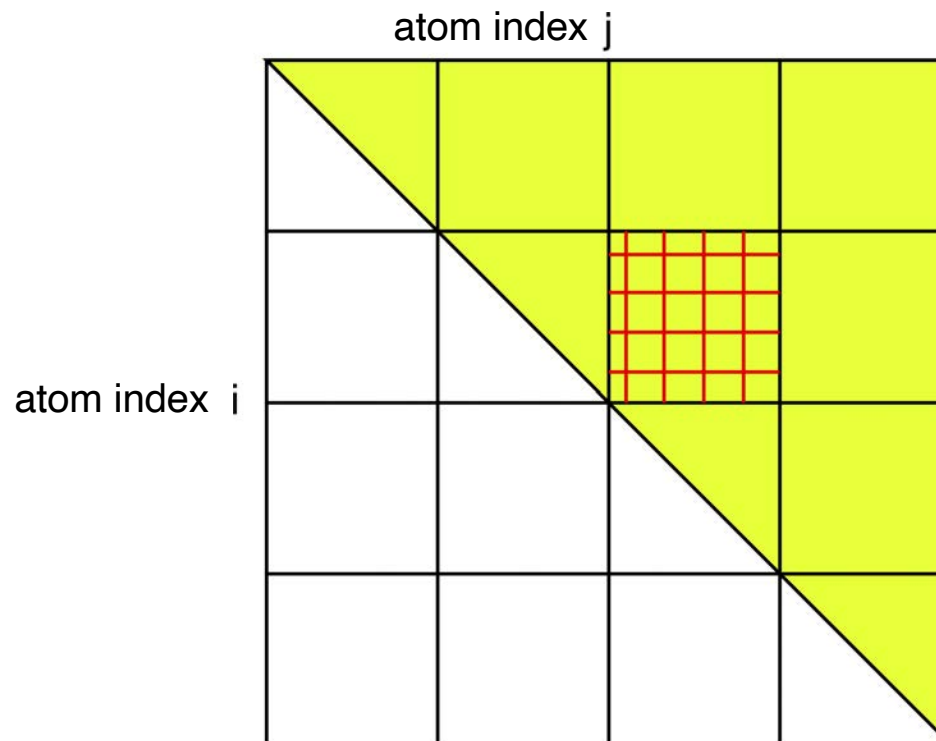


Who Does What: Nested Decompositions

- Nested block & thread decompositions
 - > Spatial decomposition among blocks
 - > Loop-index interleaving among threads within each block

In host program:

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



- Use a large enough number of blocks to reduce load imbalance among streaming multiprocessors (SMs)

Device Program for Histogram

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

This is only called from the device program

```
__global__ void gpu_histogram_kernel(float *r,float *nhis) {
```

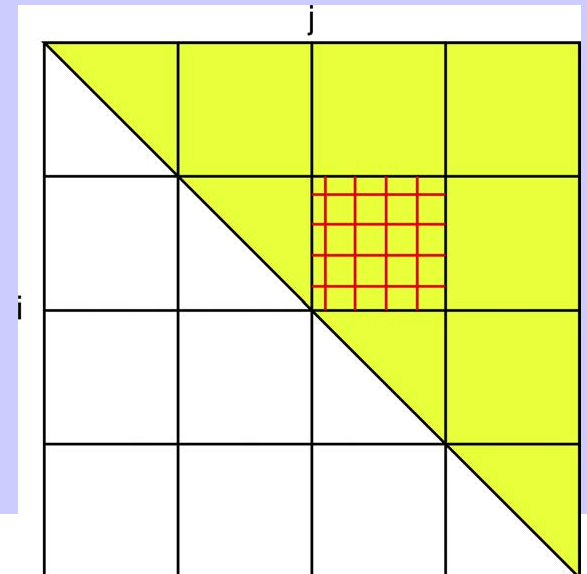
```
    int iBlockBegin = (DN/gridDim.x)*blockIdx.x;  
    int iBlockEnd = (DN/gridDim.x)*(blockIdx.x+1);  
    if (blockIdx.x == gridDim.x-1) iBlockEnd = DN;
```

```
    int jBlockBegin = (DN/gridDim.y)*blockIdx.y;  
    int jBlockEnd = (DN/gridDim.y)*(blockIdx.y+1);  
    if (blockIdx.y == gridDim.y-1) jBlockEnd = DN;
```

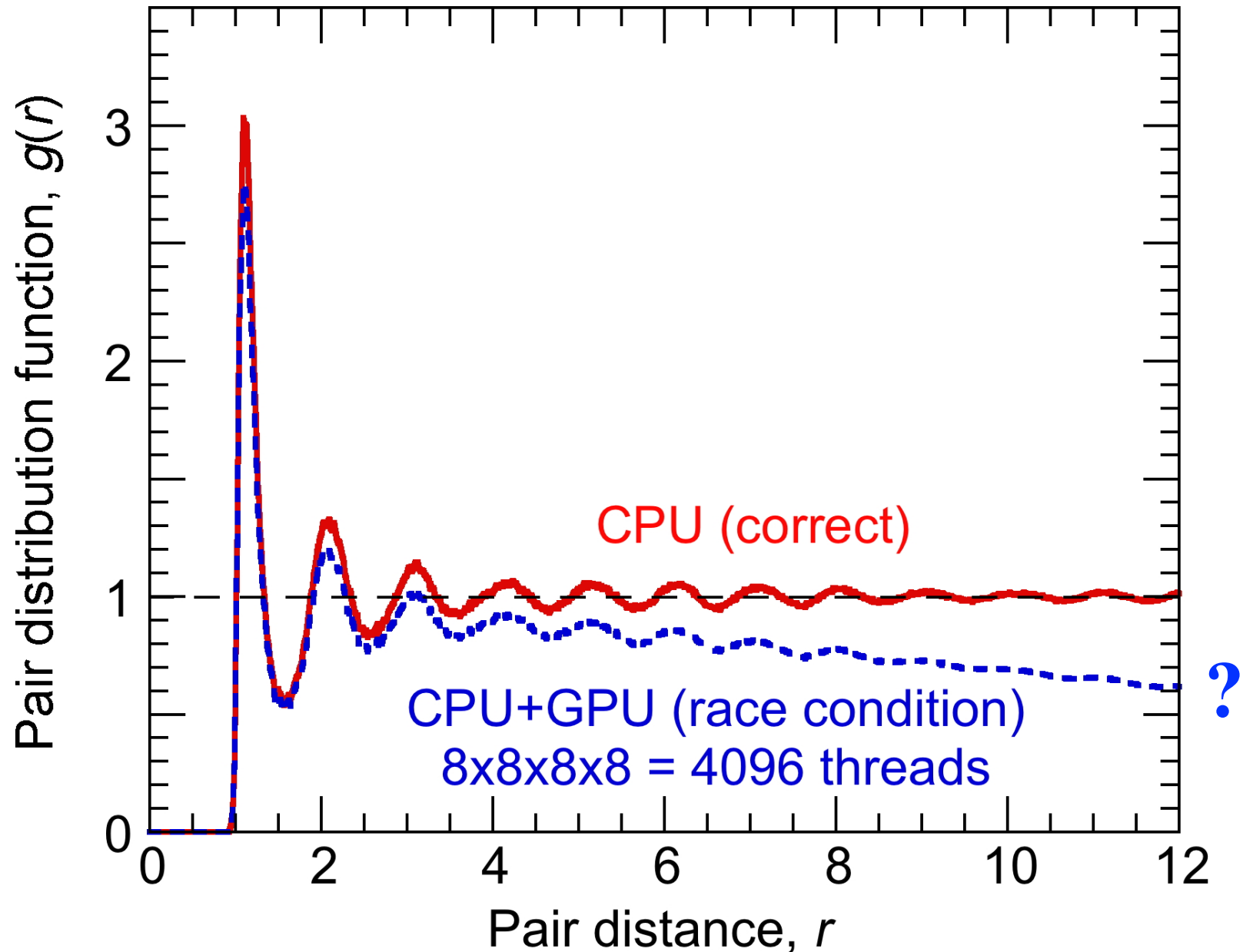
```
    for (i=iBlockBegin+threadIdx.x; i<iBlockEnd; i+=blockDim.x) {  
        for (j=jBlockBegin+threadIdx.y; j<jBlockEnd; j+=blockDim.y) {  
            if (i<j) {  
                // Process (i,j) atom pair  
                rij = 0.0;  
                ...  
                nhis[ih] += 1.0;  
            } // end if i<j  
        } // end for j  
    } // end for i  
}
```

**Thread interleaving
by skipping indices**

**Block spatial decomposition
via index offset**



Numerical Results



Race Condition

We just “saw” race condition in action!

```
for (i=iBlockBegin+threadIdx.x; i<iBlockEnd; i+=blockDim.x) {
    for (j=jBlockBegin+threadIdx.y; j<jBlockEnd; j+=blockDim.y) {
        if (i<j) {
            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; /* Entry to the histogram */
        } // end if i<j
    } // end for j
} // end for i
```

- In newer versions of CUDA, use atomic update
atomicAdd(&nhis[ih],1.0);

Running CPU & GPU Versions at HPC

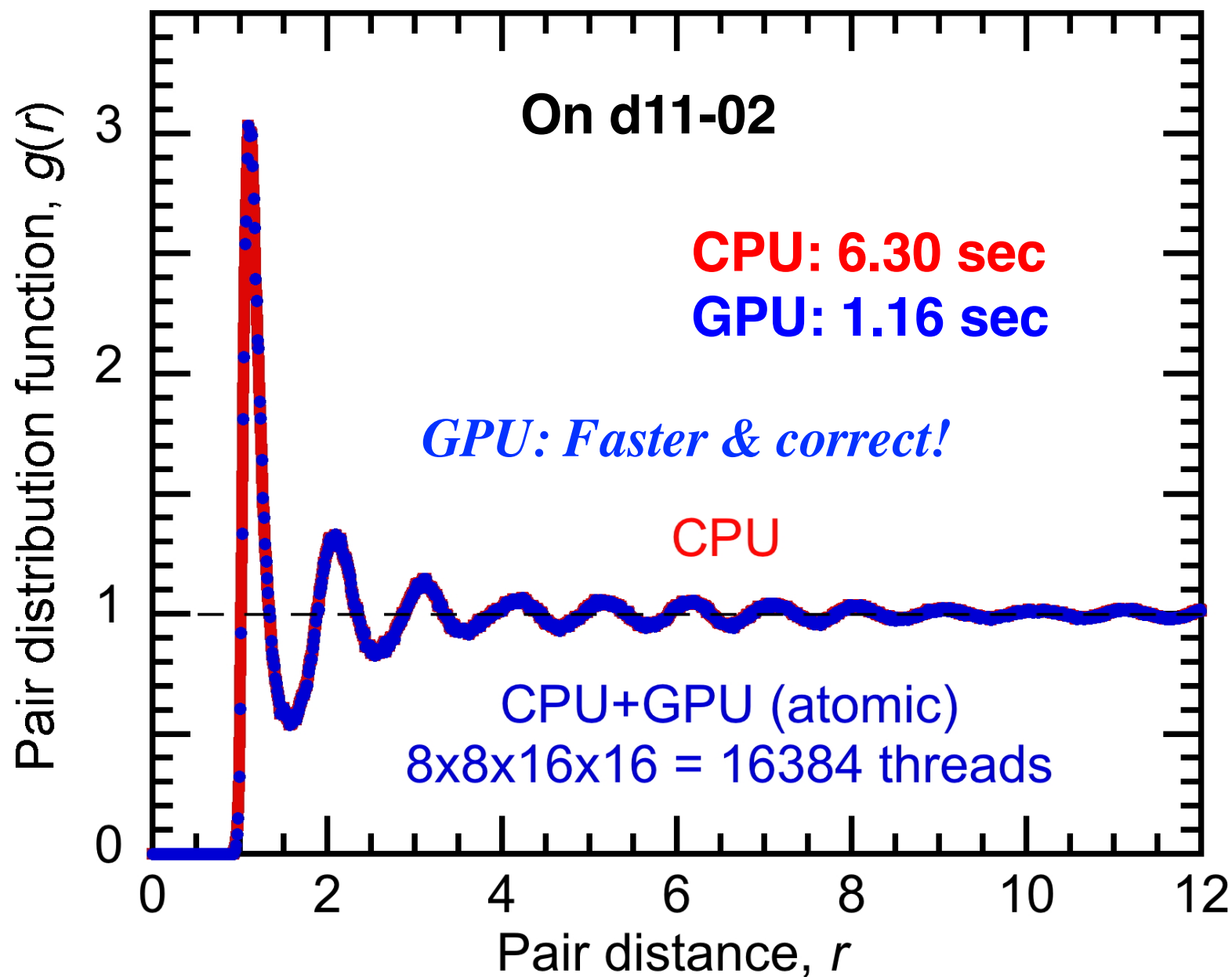
Script

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --gres=gpu:1
#SBATCH --time=00:00:59
#SBATCH --output=pdf.out
#SBATCH -A anakano_429
echo '##### CPU: gcc -o pdf0 pdf0.c -lm #####'
./pdf0
echo '##### GPU: nvcc -o pdf pdf.cu #####'
./pdf
```

Output

```
##### CPU: gcc -o pdf0 pdf0.c -lm #####
Execution time (s) = 6.300000e+00
##### GPU: nvcc -o pdf pdf.cu #####
Execution time (s) = 1.160000e+00
```

Numerical Results



Summary: CUDA Pair-Distribution Computing

copy: host  **device**

input: $r[]$
constants: $alth[], n, drh$

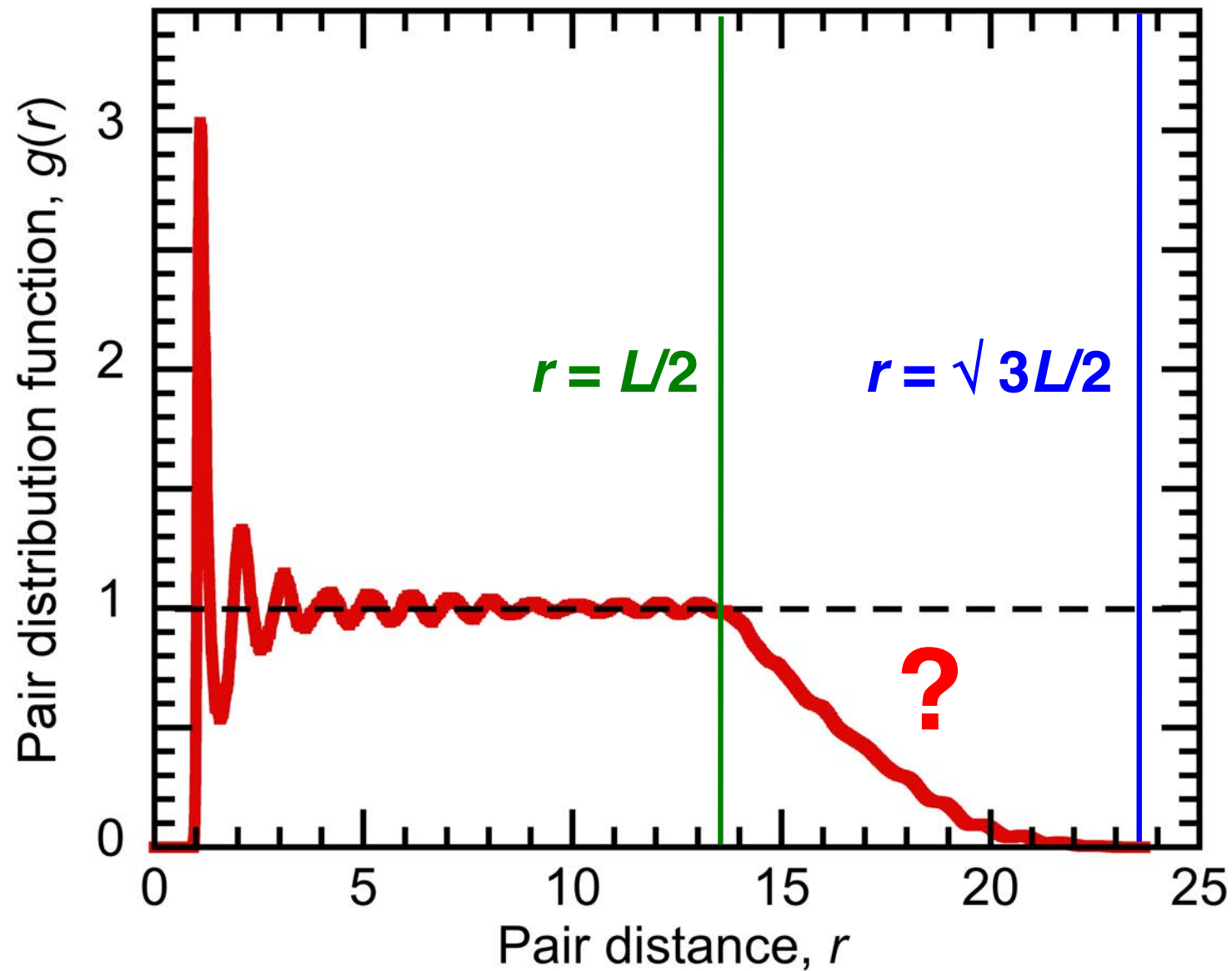
**Multithreading
(SPMD):**

big (i, j) loop —
hybrid block
(SM) spatial
decomposition
& thread (SP)
interleaving

copy: host  **device**

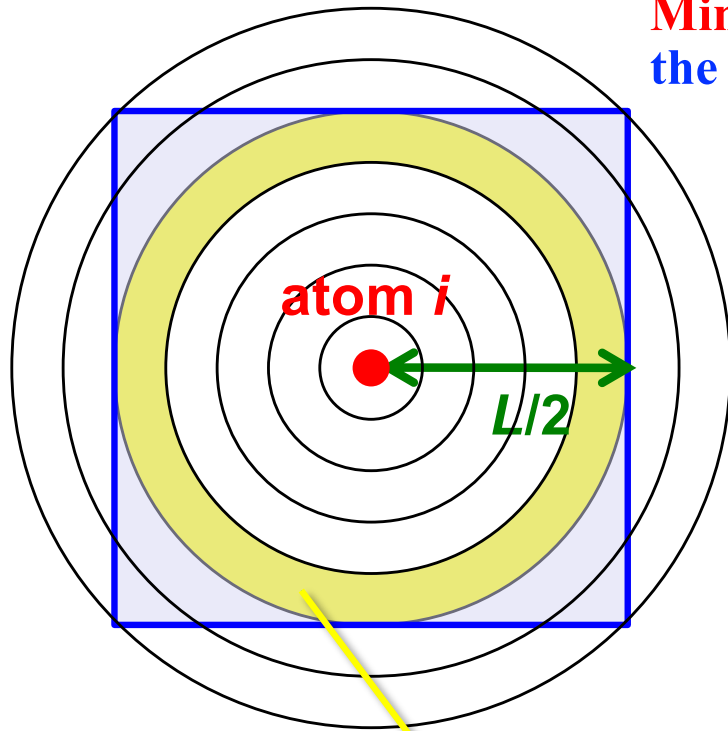
output: $nhis[]$

Finite-Size Effect on $g(r)$



Geometric Factor in $g(r)$

Minimum-image convention: For atom i , pick the closest periodic image of neighbor atom j

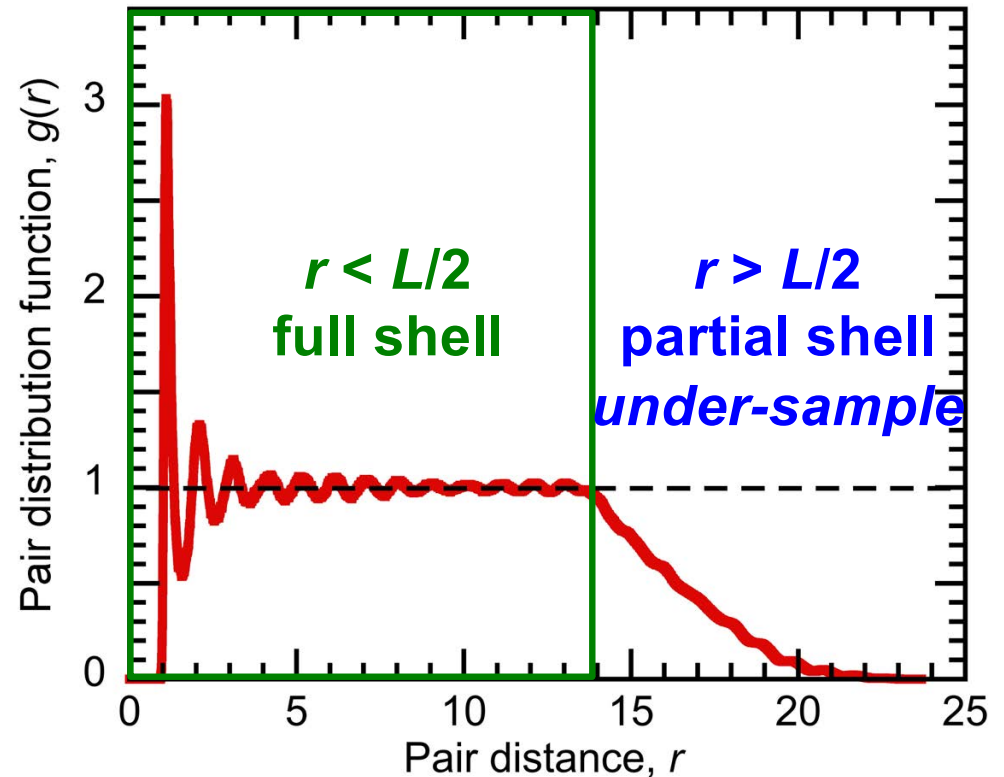


$$g(r) = \frac{2 \times nhist(i)}{N} \times \frac{1}{4\pi r^2 \Delta r} \times (N/V)$$

of other atoms j in a concentric shell with thickness Δr at distance r from atom i

Volume of the shell

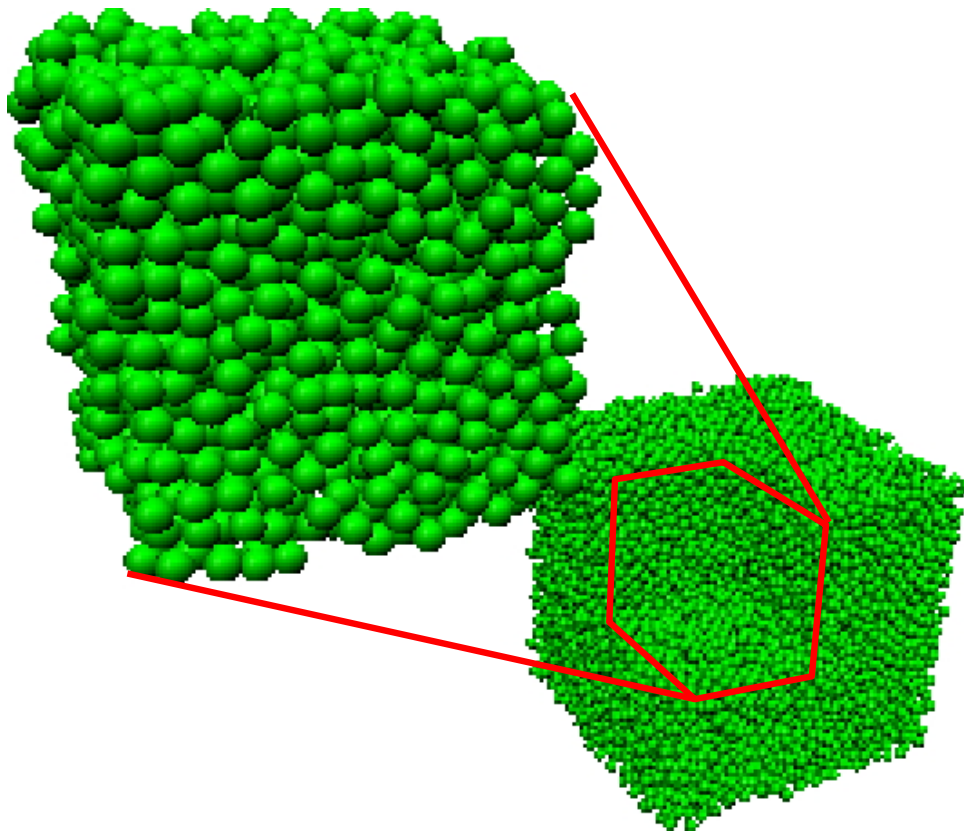
Average density



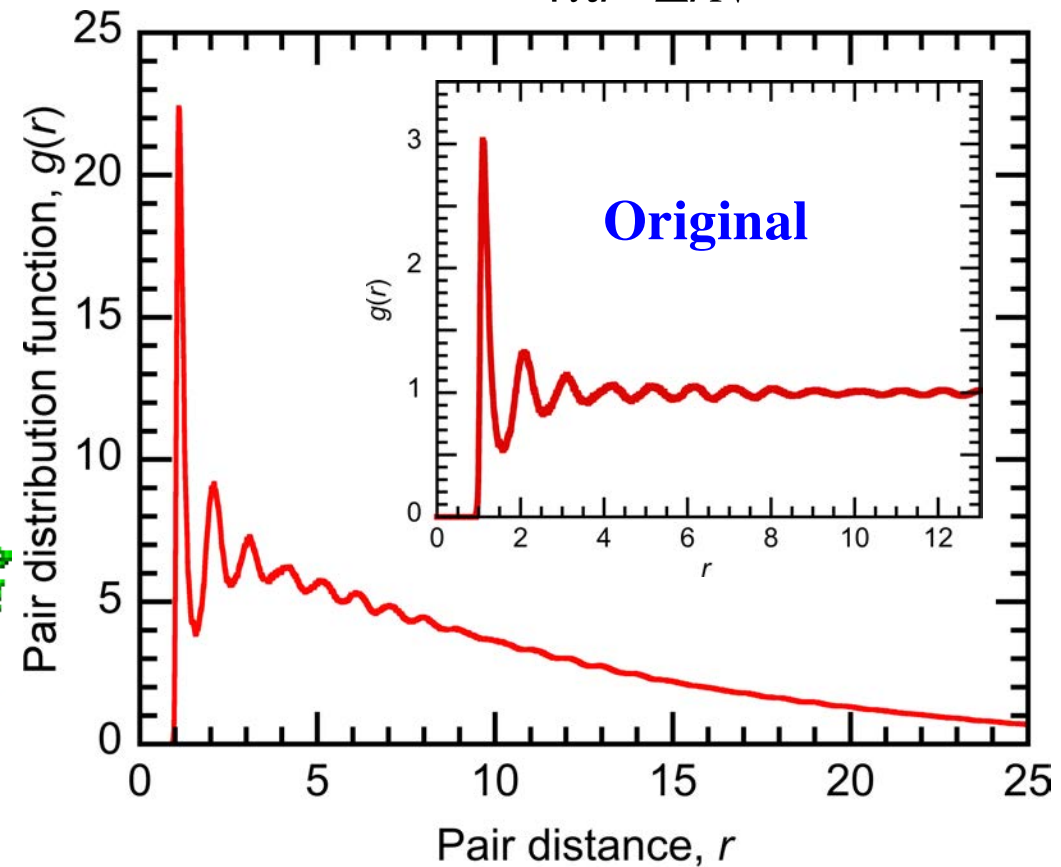
Physically meaningful result

Large-scale Correlation in $g(r)$

One octant of the system
cut-out & displaced



$$g(r) = \frac{V \times nhist(i)}{4\pi r^2 \Delta r N^2}$$

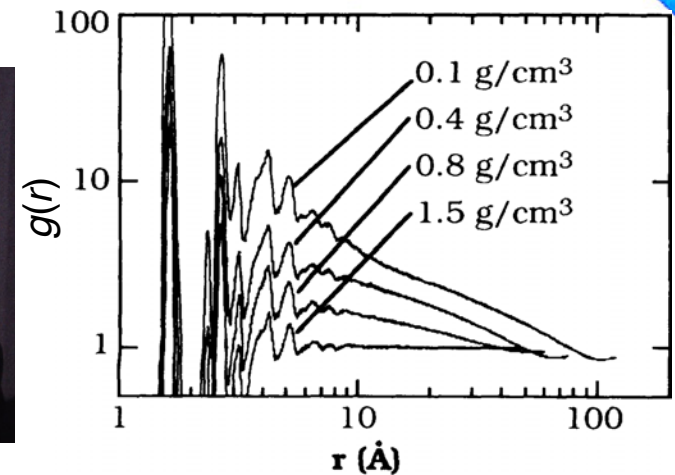
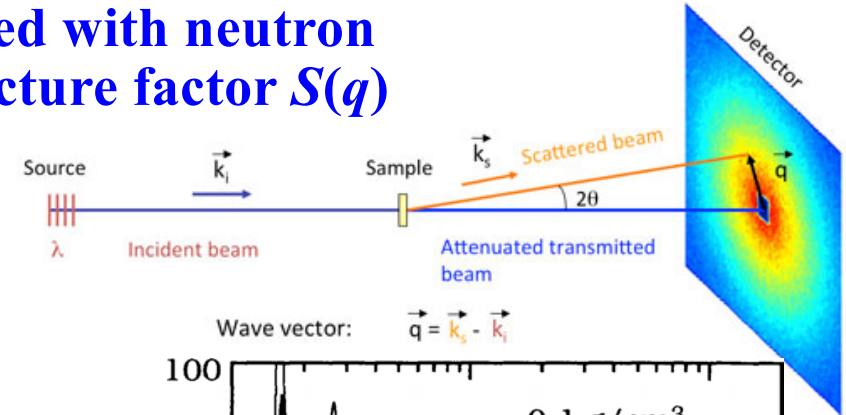
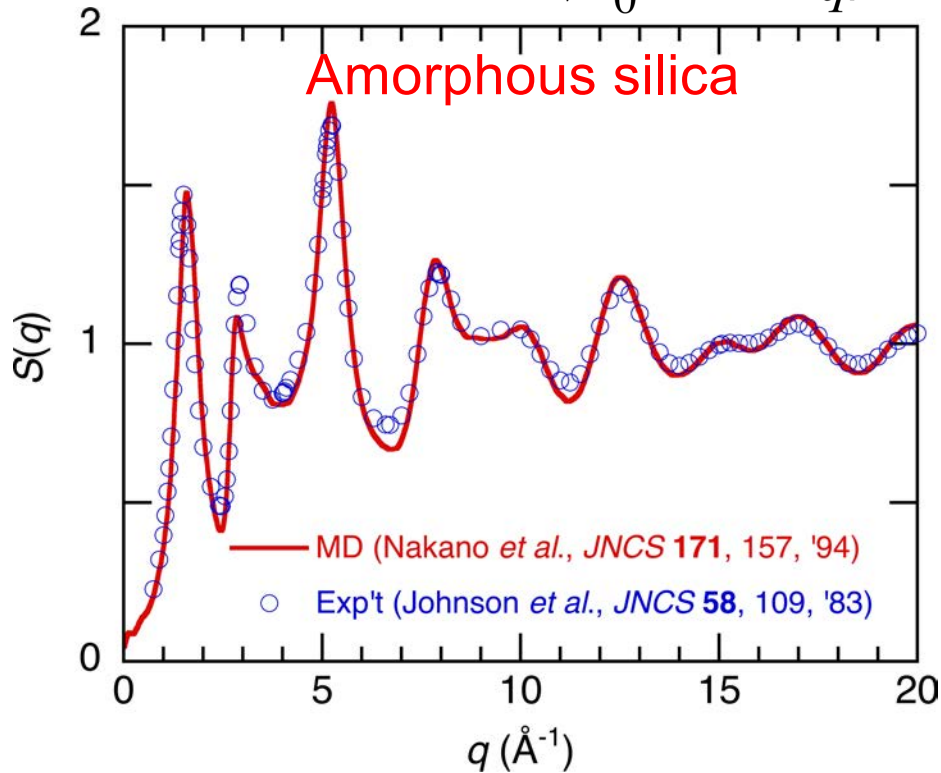


- Short-range correlation (*i.e.* peak positions) unchanged, just magnified by the lower average density, N/V_{expanded}
- Superimposed with larger length-scale geometric factors

Experimental Connection

- Short-range correlations are directly compared with neutron or X-ray scattering measurements of the structure factor $S(q)$

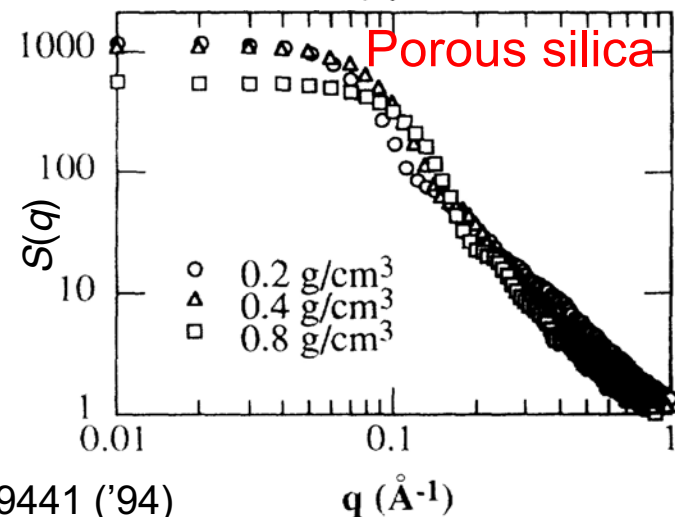
$$S(q) = 1 + 4\pi \frac{N}{V} \int_0^\infty dr r^2 \frac{\sin(qr)}{qr} [g(r) - 1]$$



- Long-range correlations are measured by small-angle neutron or X-ray scattering structure factors (SANS or SAXS)

$$S(q) \propto q^{-d_f}$$

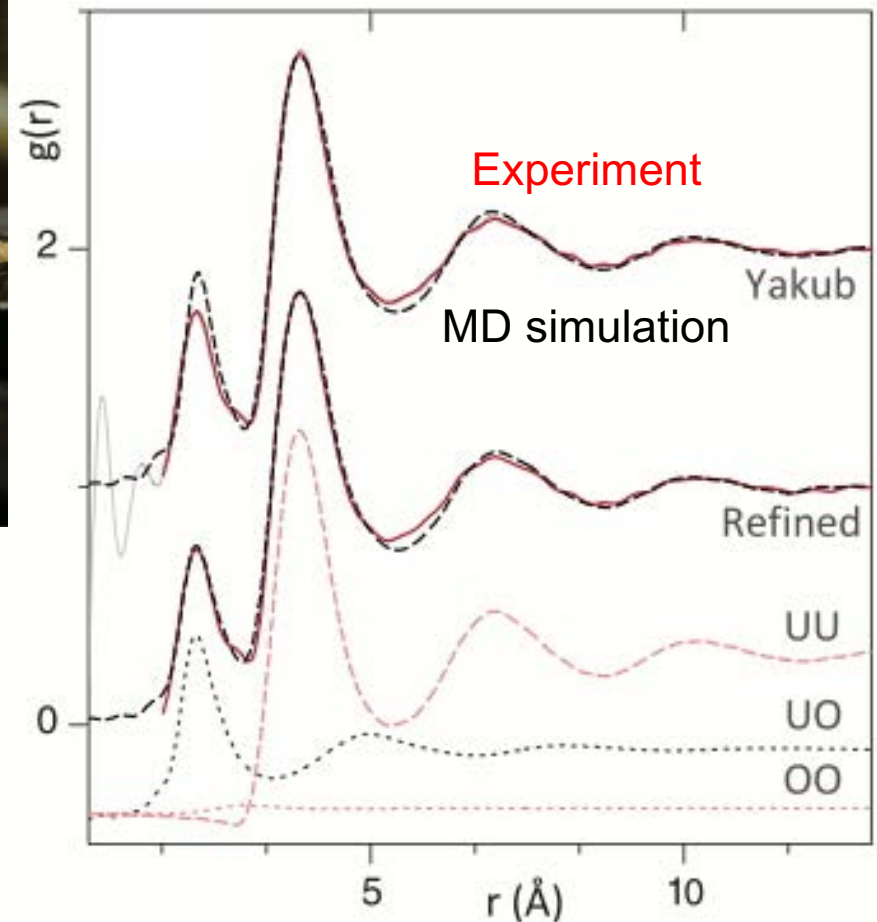
d_f : Fractal dimension



Nakano *et al.*, PRL 71, 85 ('93); PRB 49, 9441 ('94)

$g(r)$ of Molten UO_2

- X-ray scattering measurement using synchrotron radiation from 7 GeV electrons at the Advanced Photon Source of the Argonne National Lab.



Skinner *et al.*, *Science* **346**, 984 ('14)

More Pair-Distribution Computation

Use the force! Reduced variance estimators for densities, radial distribution functions, and local mobilities in molecular simulations 

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Submitted: 9 September 2020 • Accepted: 29 September 2020 •

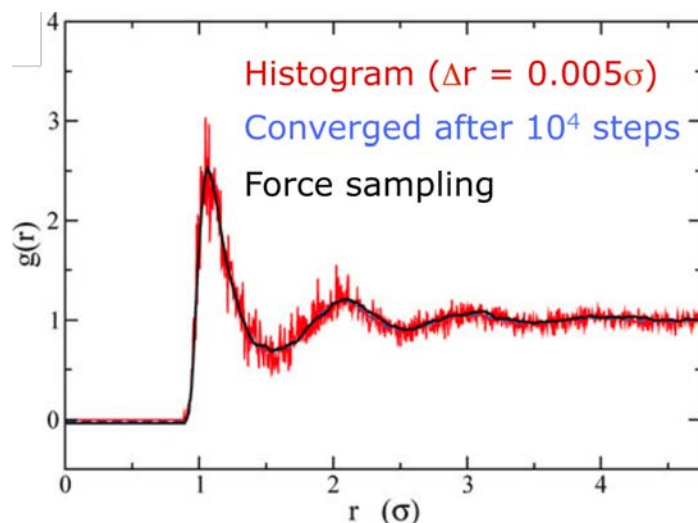
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<https://aiichironakano.github.io/cs596/Rotenberg-UseTheForce-JCP20.pdf>