

Pair Distribution Computation on GPU

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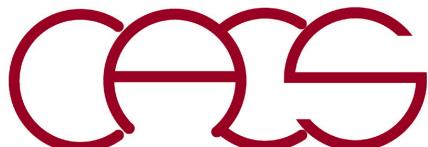
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Goal: Using multidimensional Grid & Block

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



cf. <https://aiichironakano.github.io/cs596/Grupcev-PairCorr-TKDE13.pdf>

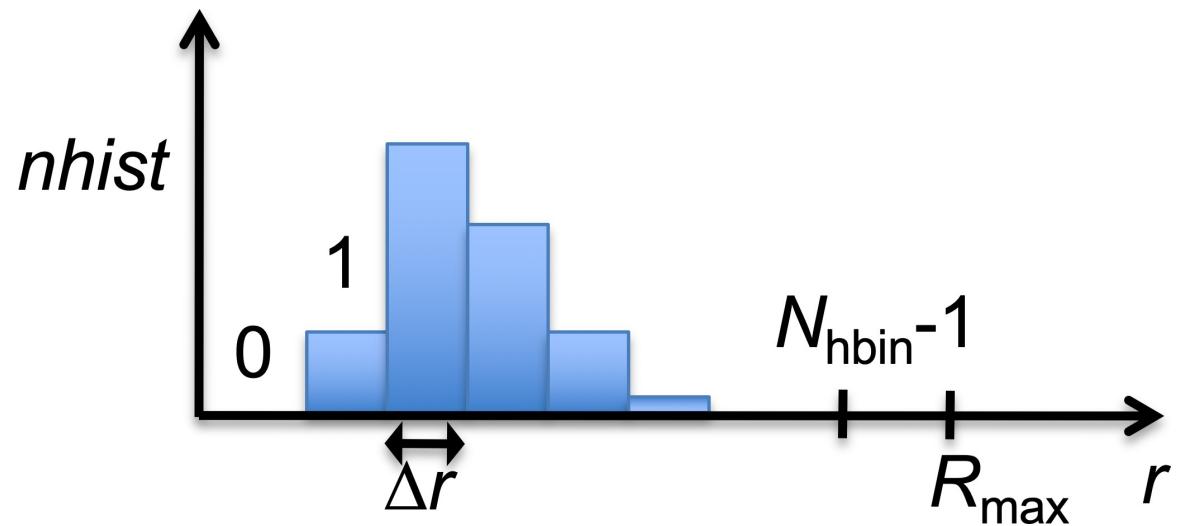
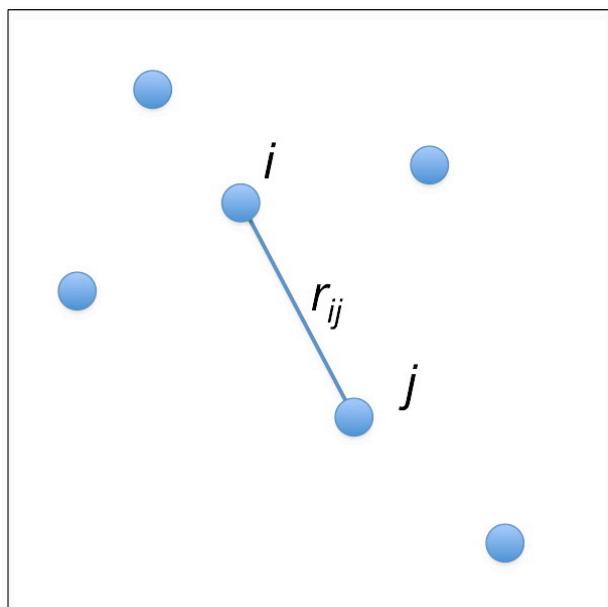


Pair Distribution

- 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, $g(r)$**

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

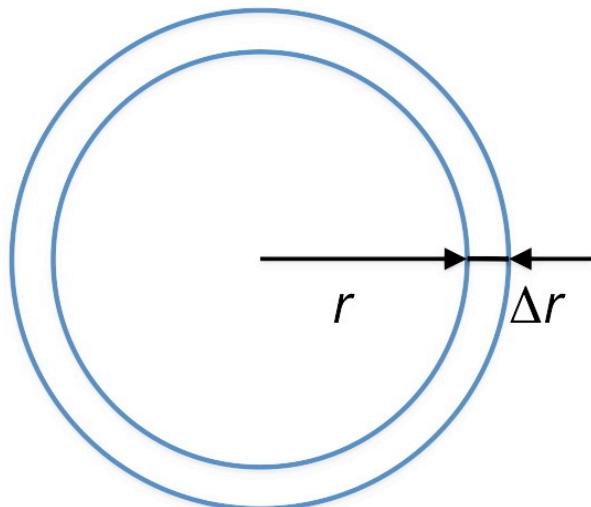
N: # of atoms ρ : # density

$g(r)$: 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,

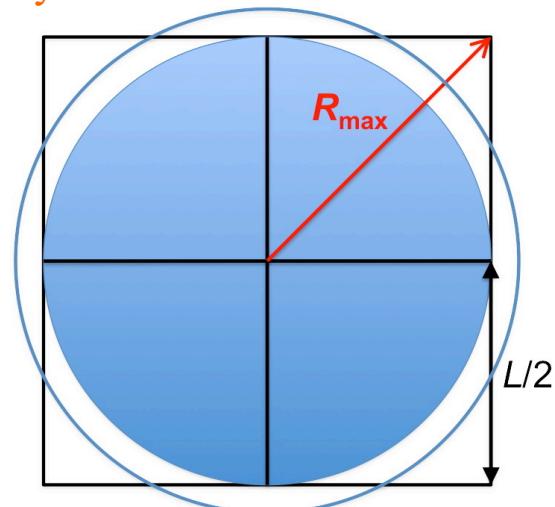
$$R_{\max} = \sqrt{\sum_{\alpha=x,y,z} \left(\frac{\text{al}[\alpha]}{2} \right)^2}$$

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



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

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)
        }
        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 $xlylz$ coordinate of the i -th atom
- $alh[a] = al[a]/2$: 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)); memory offset

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);

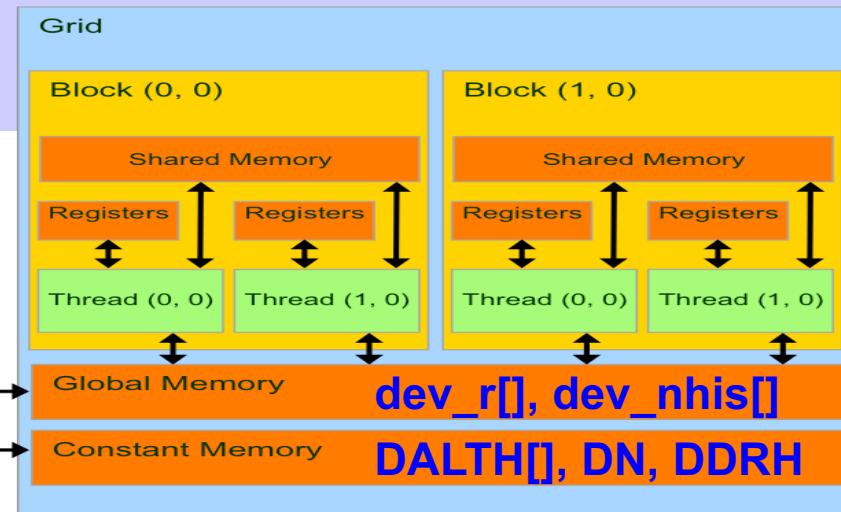
cudaFree(dev_r);
cudaFree(dev_nhis);
```

- **cudaMemcpyToSymbol:**

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

Memory offset (in bytes) is added to destination

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

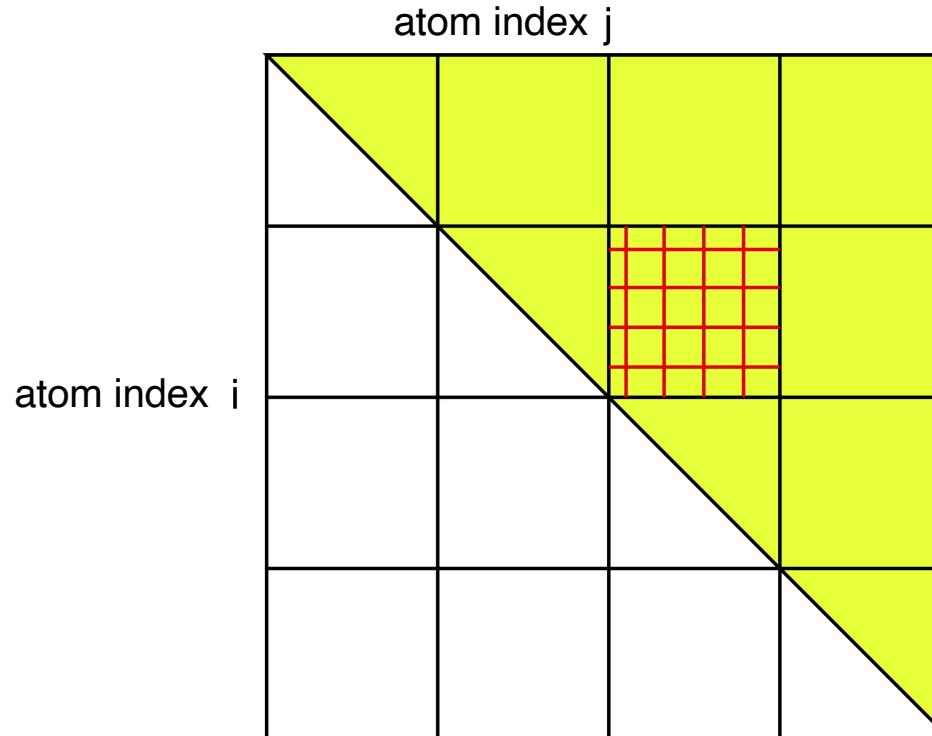


Who Does What: Nested Decompositions

- 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);           in      out
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) {

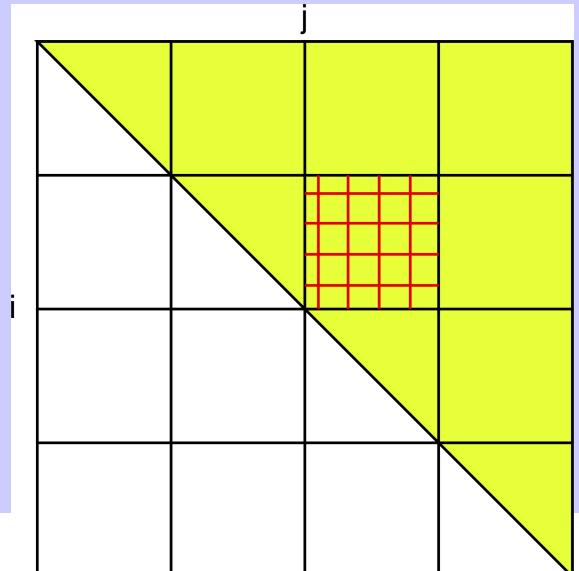
    int iBlockBegin = (DN/gridDim.x)*blockIdx.x;
    int iBlockEnd = (DN/gridDim.x)*(blockIdx.x+1);
    if (blockIdx.x == gridDim.x-1) iBlockEnd = DN;

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

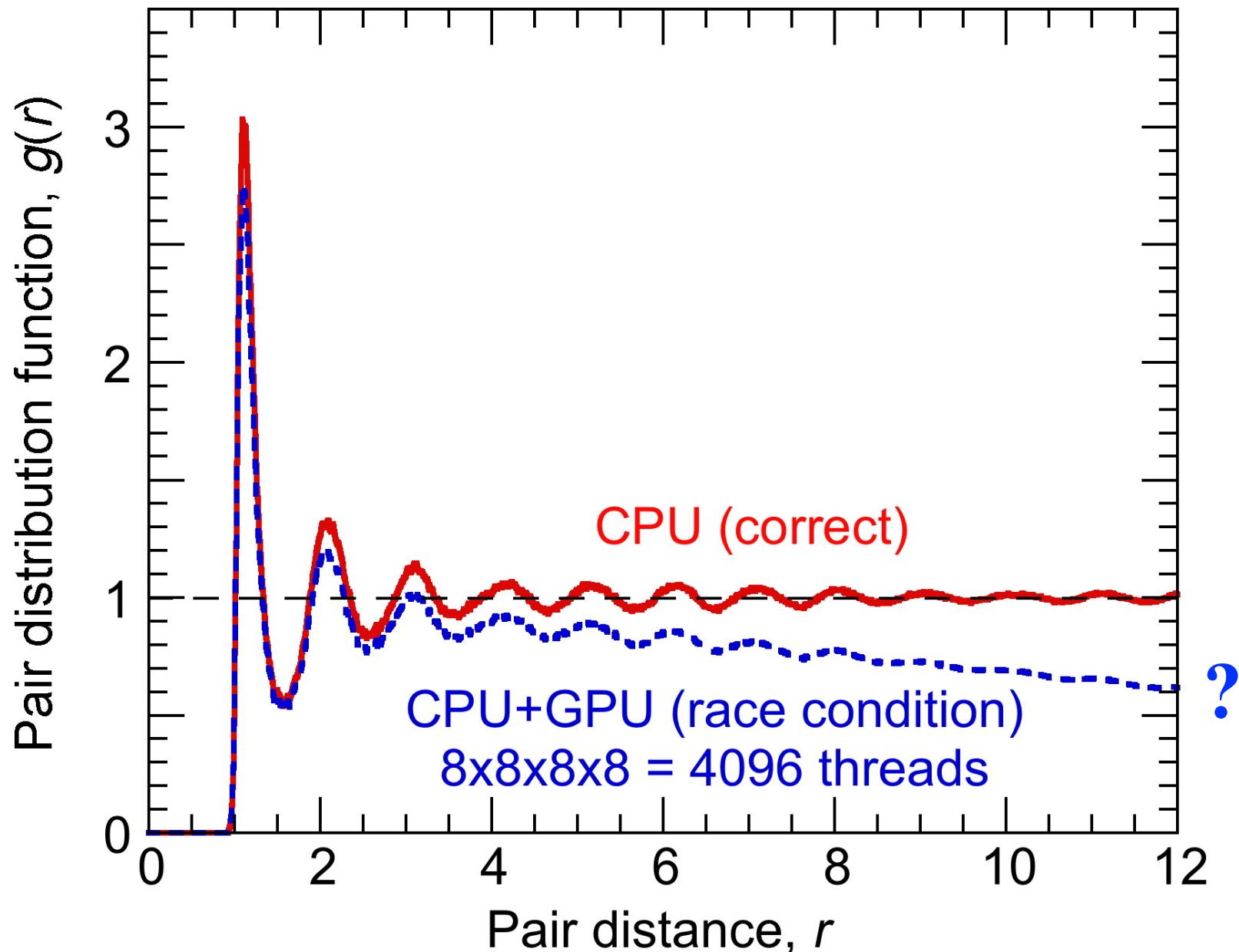
    for (int i=iBlockBegin+threadIdx.x; i<iBlockEnd; i+=blockDim.x) {
        for (int j=jBlockBegin+threadIdx.y; j<jBlockEnd; j+=blockDim.y) {
            if (i<j) {
                // Process (i,j) atom pair
                float rij = 0.0;
                ...
                nhis[ih] += 1.0;
            } // 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 (int i=iBlockBegin+threadIdx.x; i<iBlockEnd; i+=blockDim.x) {  
    for (int j=jBlockBegin+threadIdx.y; j<jBlockEnd; j+=blockDim.y) {  
        if (i<j) {  
            float rij = 0.0;  
            for (int a=0; a<3; a++) {  
                float 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  
            int 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);`

Compilation on Discovery

- **Load the necessary modules**

```
module purge
module load usc/8.3.0
module load cuda
```

- **Compilation of the CUDA program for GPU**

```
nvcc -o pdf pdf.cu
```

- **Compilation of the original serial program on CPU for comparison**

```
gcc -o pdf0 pdf0.c -lm
```

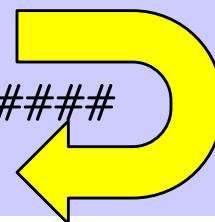
Running CPU & GPU Versions

Script: pdf.sl

```
#!/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

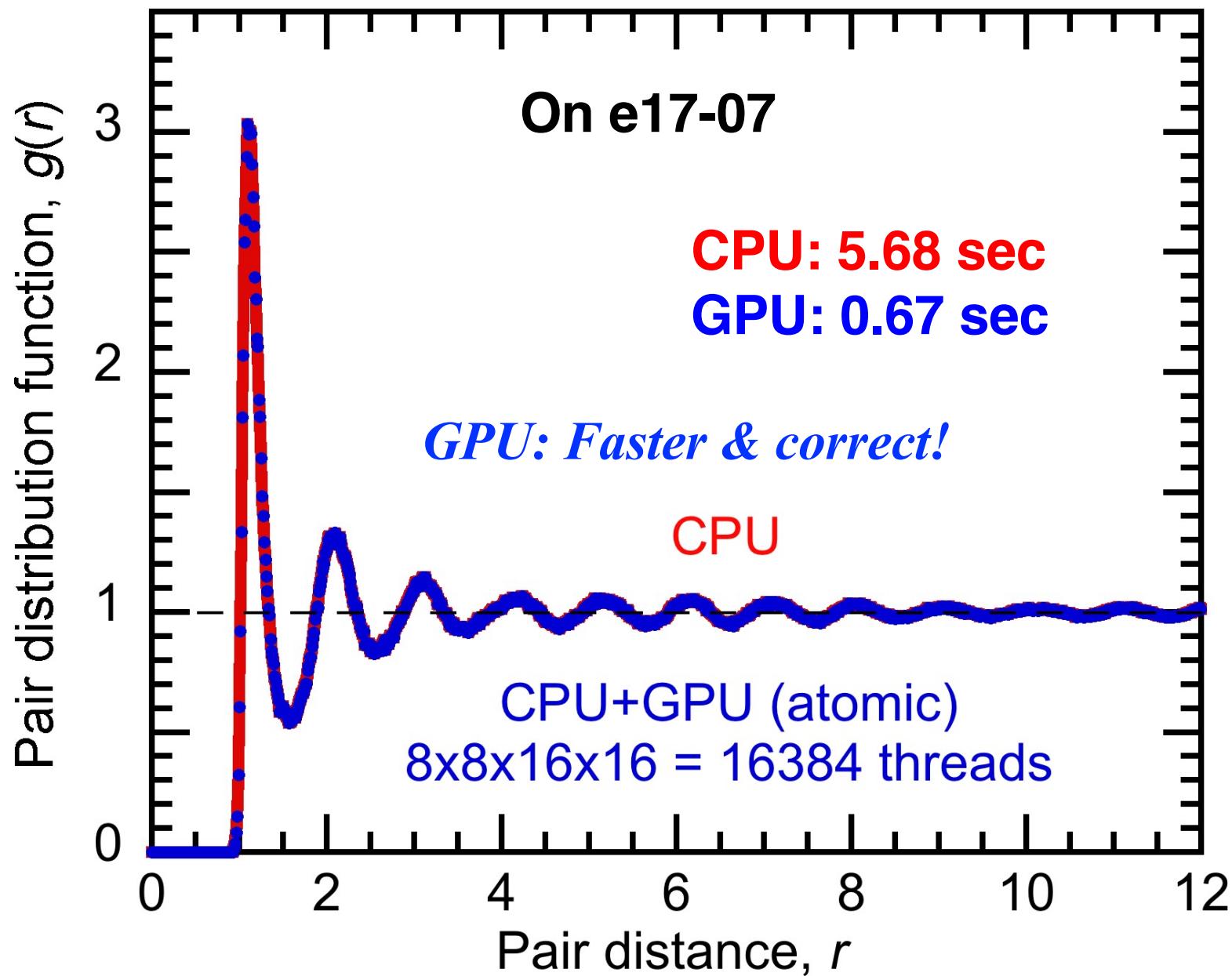
```
##### CPU: gcc -o pdf0 pdf0.c -lm #####
Execution time (s) = 5.680000e+00
##### GPU: nvcc -o pdf pdf.cu      #####
Execution time (s) = 6.700000e-01
```



Faster!

The histogram file, pdf.d, calculated by pdf0 will be overwritten by that by pdf

Numerical Results



Summary: CUDA Pair-Distribution Computing

copy: host → device

input: $r[]$

constants: $alth[], n, drh$

Multithreading
(SPMD):

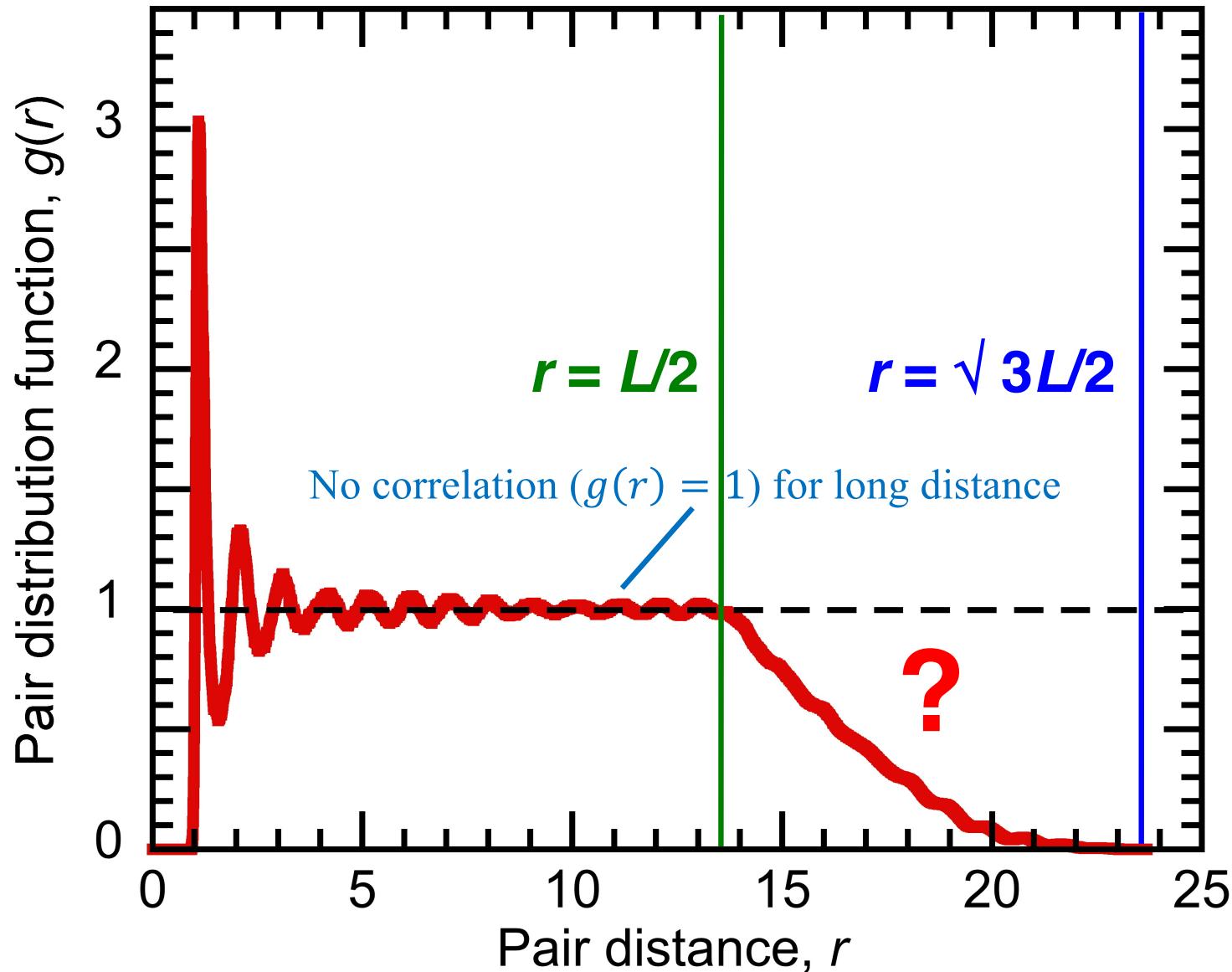
big (i, j) loop —
hybrid block
(SM) spatial
decomposition
& thread (SP)
interleaving

copy: host

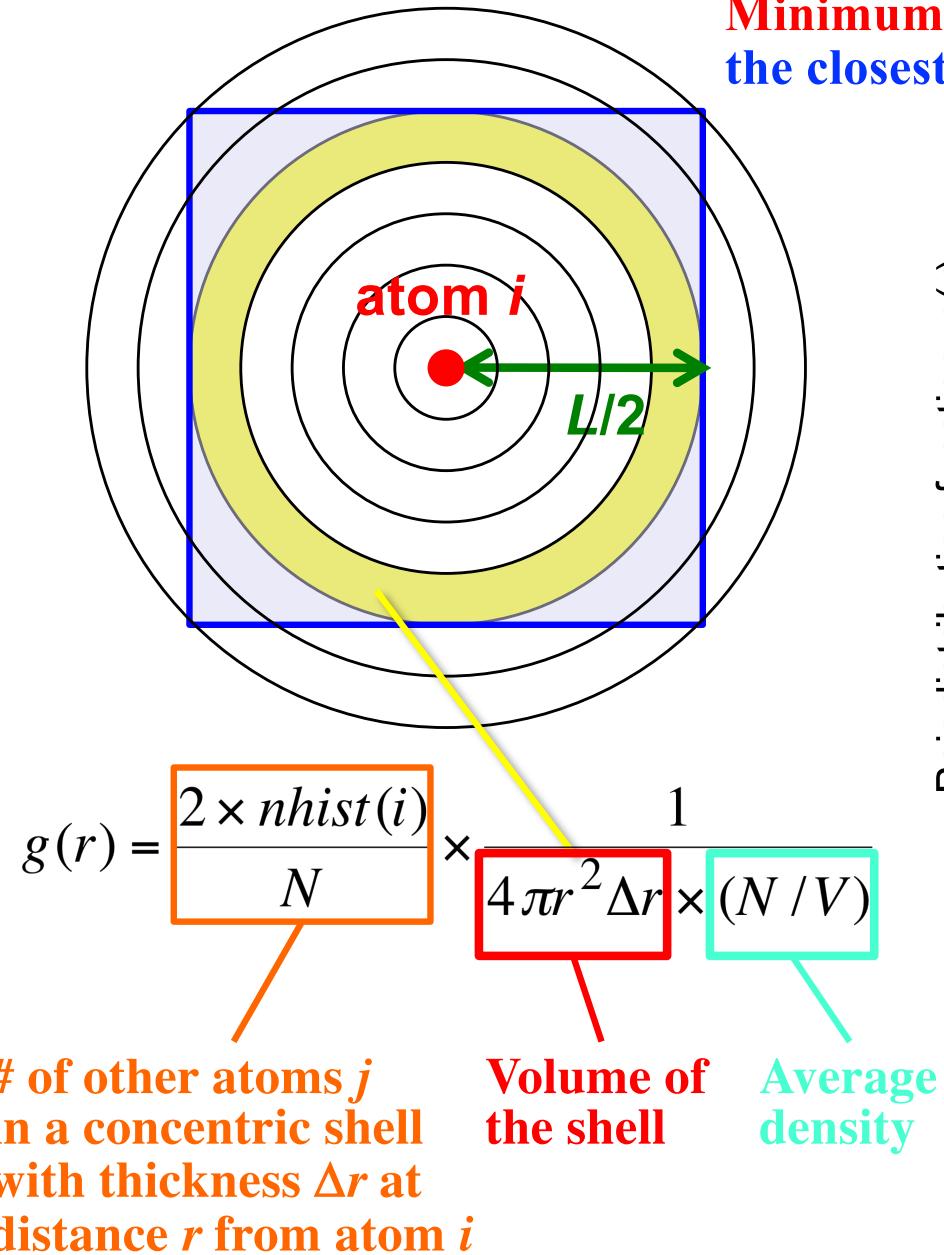
device

output: $nhis[]$

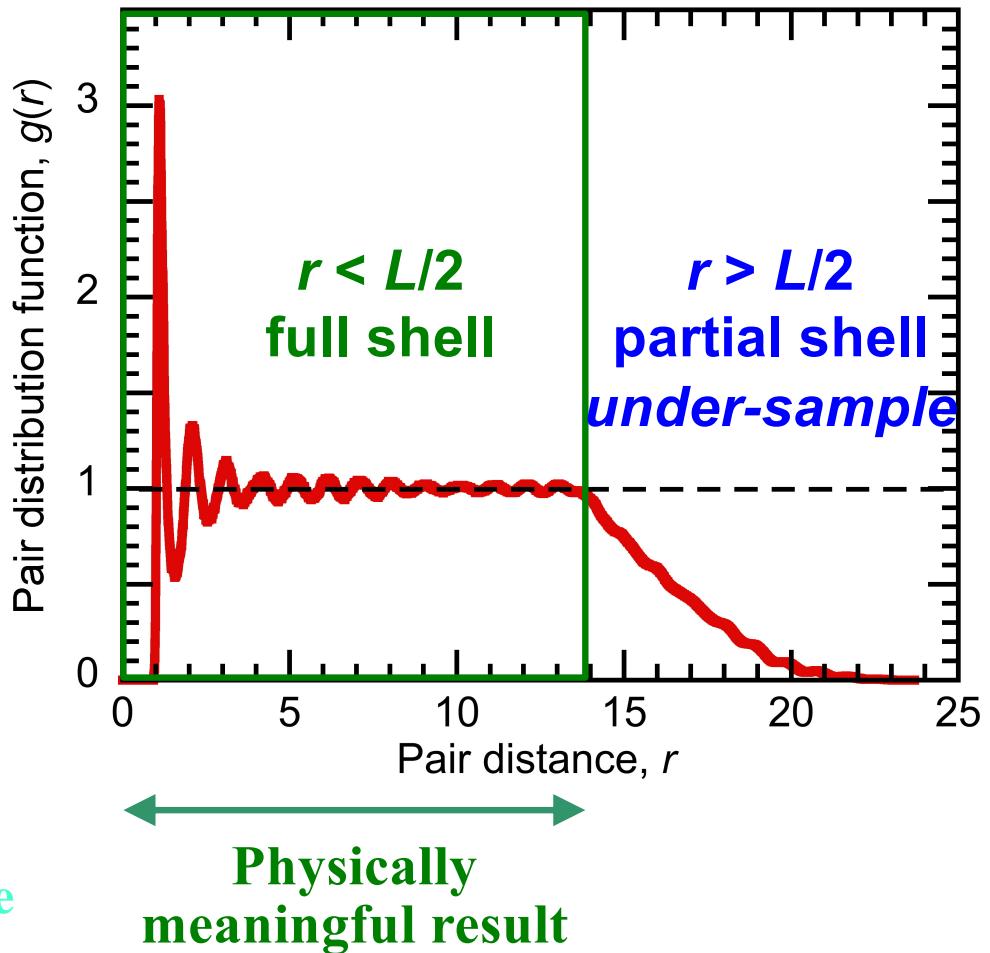
Finite-Size Effect on $g(r)$



Geometric Factor in $g(r)$

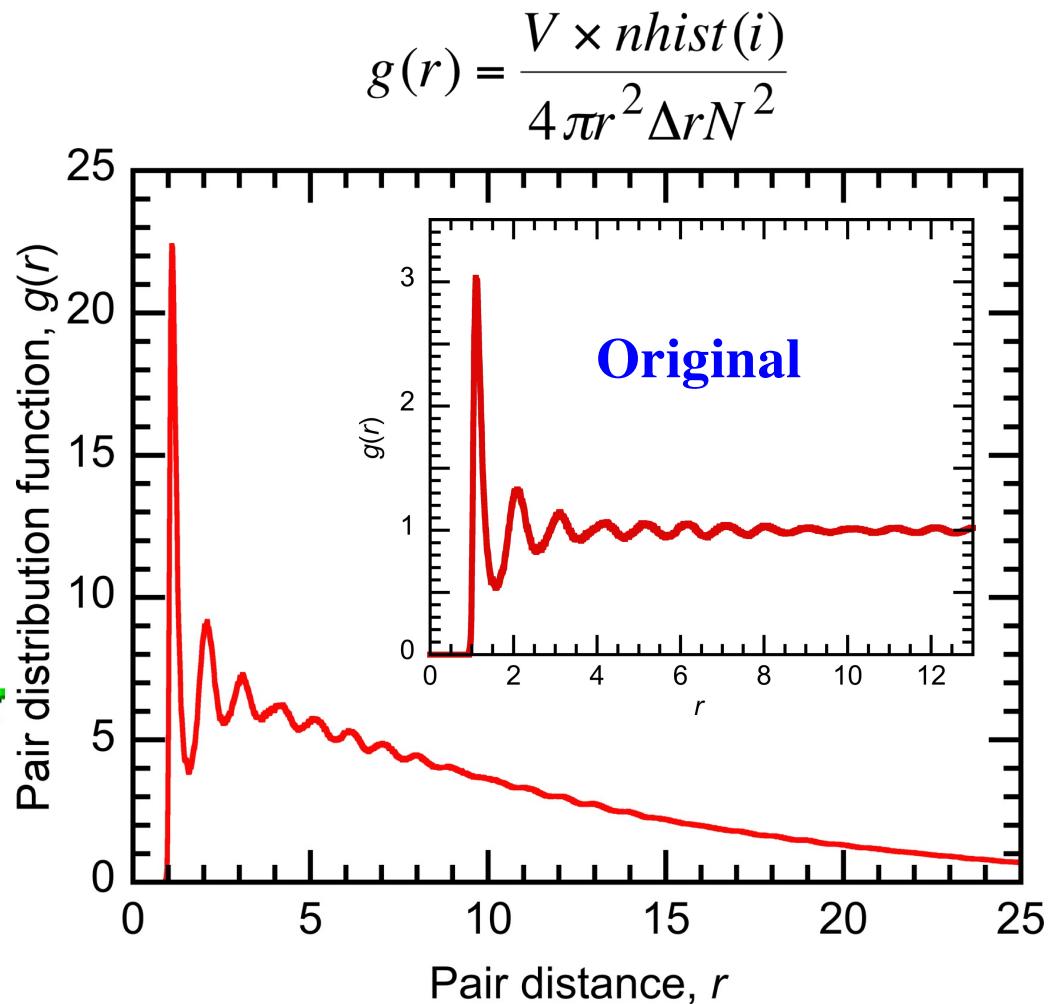
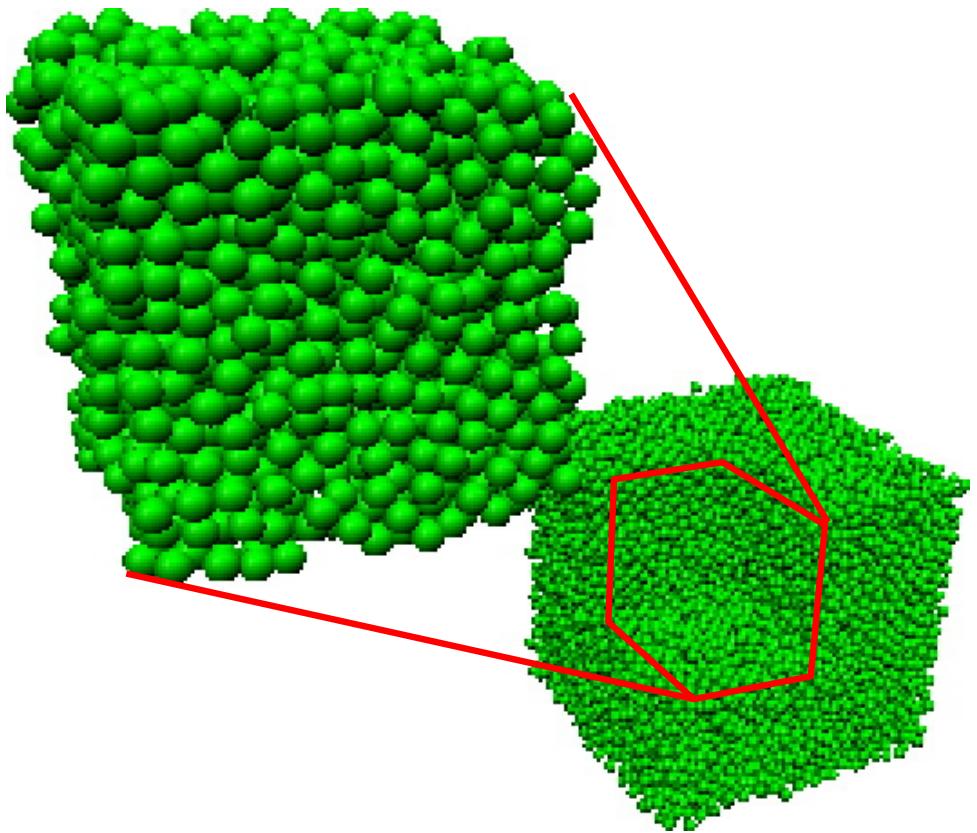


Minimum-image convention: For atom i , pick the closest periodic image of neighbor atom j



Large-scale Correlation in $g(r)$

One octant of the system
cut-out & displaced

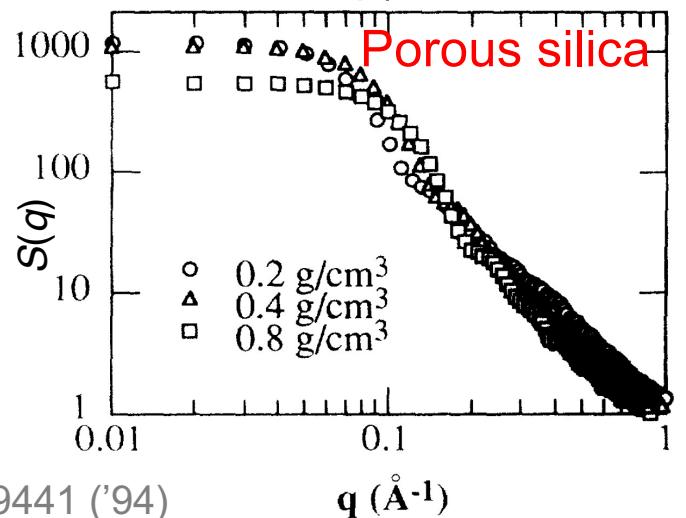
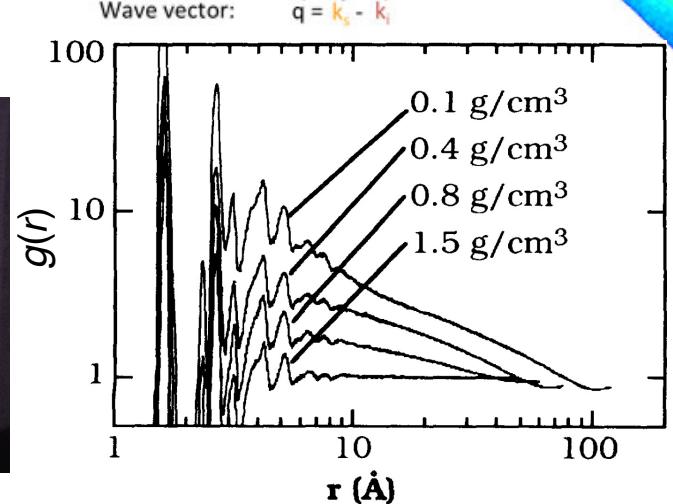
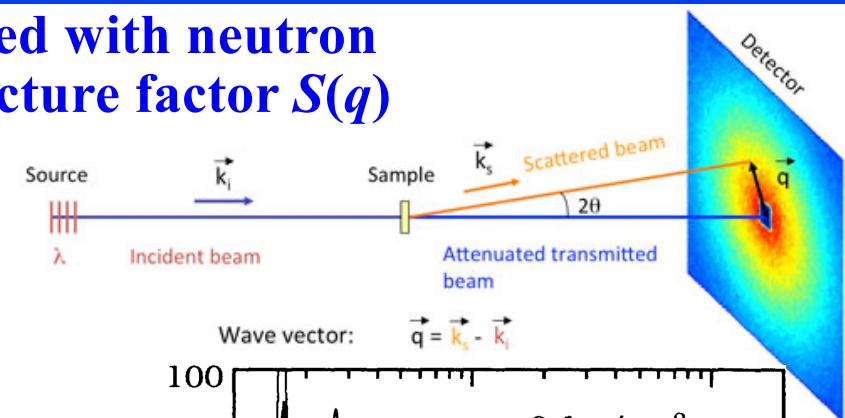
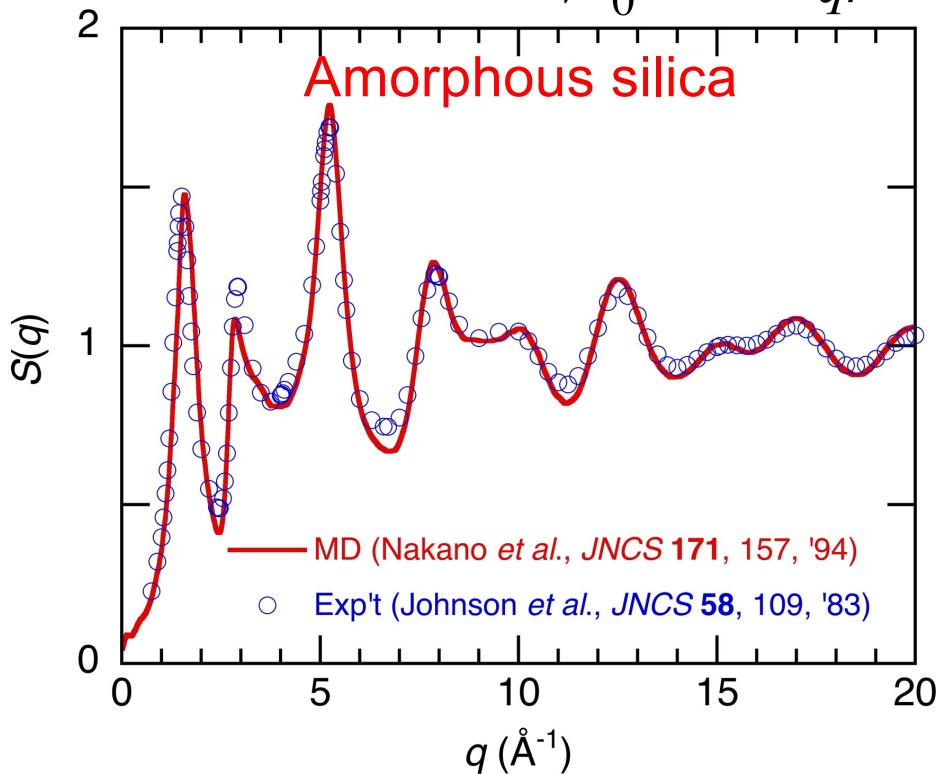


- Short-range correlation (*i.e.* peak positions) unchanged, just magnified by the lower average density, N/V_{expanded}
- Superimposed with larger length-scale geometric factors

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)

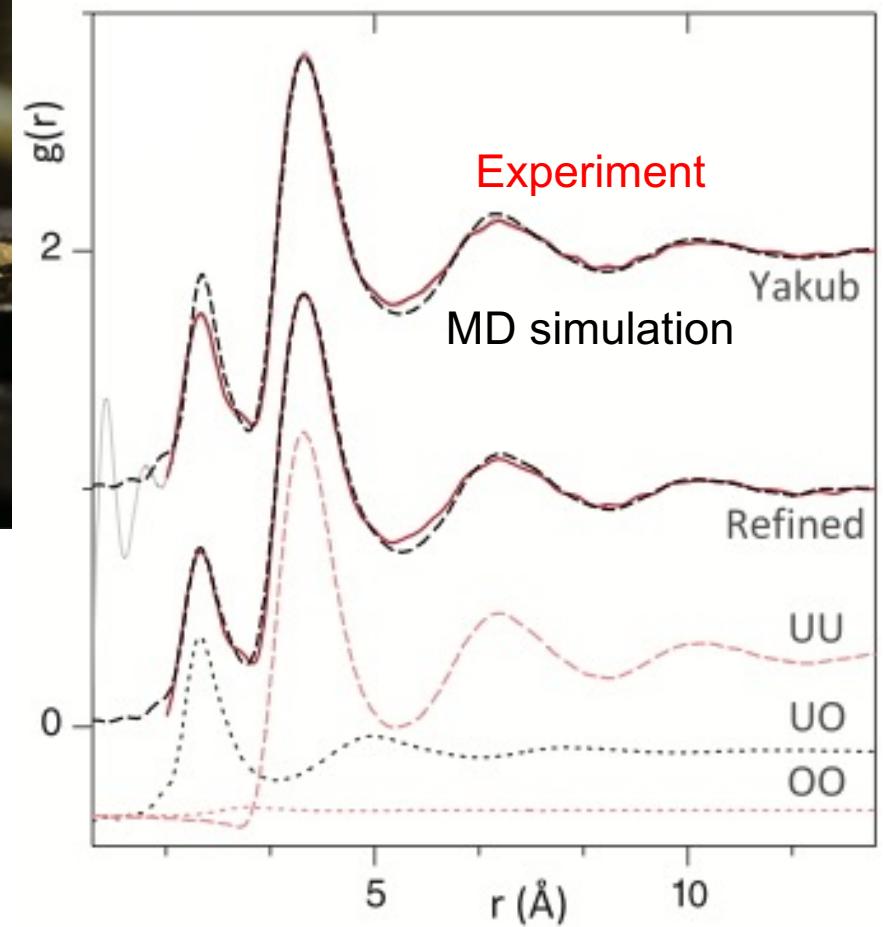
$$S(q) \propto q^{-d_f}$$

d_f : Fractal dimension

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

$g(r)$ of Molten UO_2

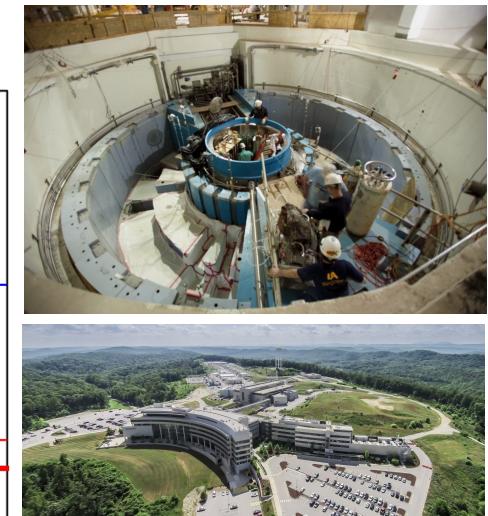
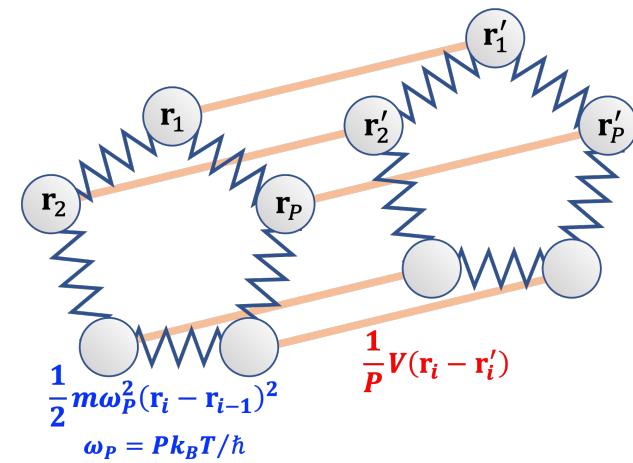
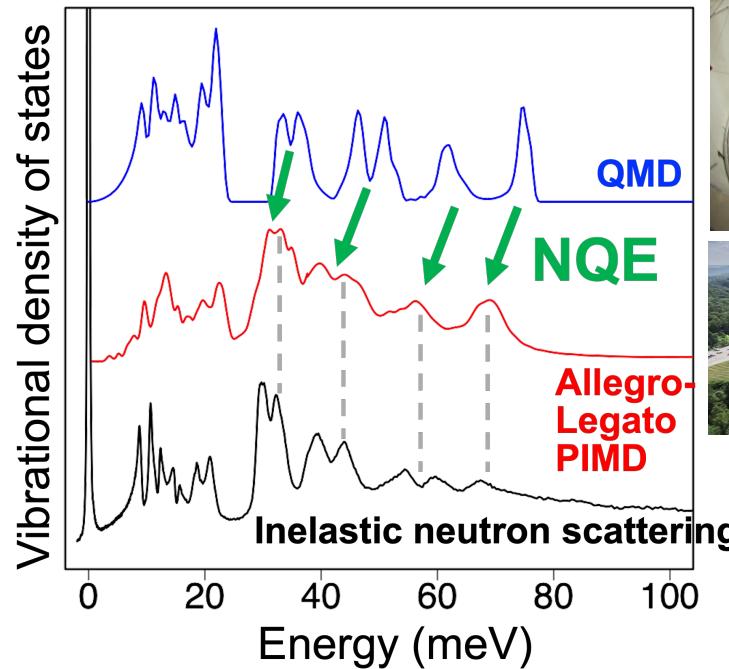
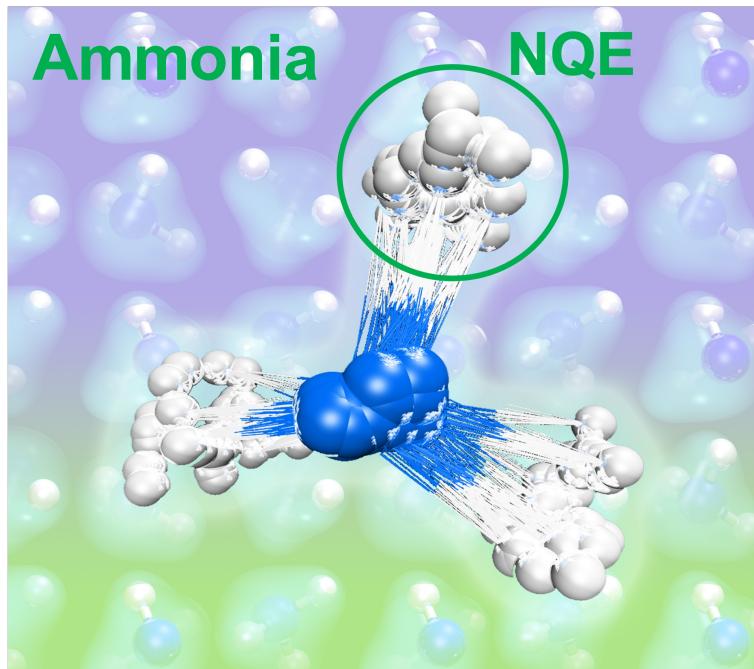
- X-ray scattering measurement using synchrotron radiation from 7 GeV electrons at the Advanced Photon Source of the Argonne National Lab.



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

Neutron Scattering Meets Quantum Neural Network

- Allegro-Legato-PIMD: Incorporate nuclear quantum effect (NQE) through path-integral molecular dynamics (PIMD)
- Neural-network quantum molecular dynamics (NNQMD) trained by quantum molecular dynamics (QMD) achieves long-time Hamiltonian dynamics to resolve fine vibrational structures
- NQE down-shifts inter-molecular vibrational modes in ammonia to explain high-resolution inelastic neutron scattering experiments



More Pair-Distribution Computation

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

Cite as: J. Chem. Phys. 153, 150902 (2020); doi: [10.1063/5.0029113](https://doi.org/10.1063/5.0029113)

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

Published Online: 16 October 2020



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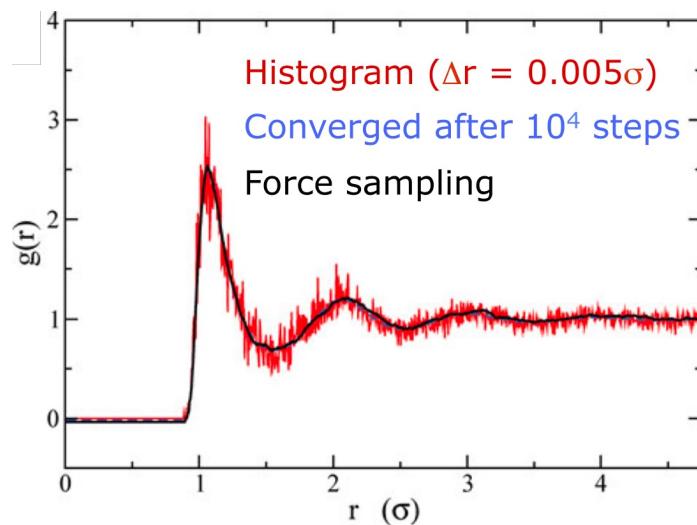


CrossMark

Benjamin Rotenberg^{a)} 

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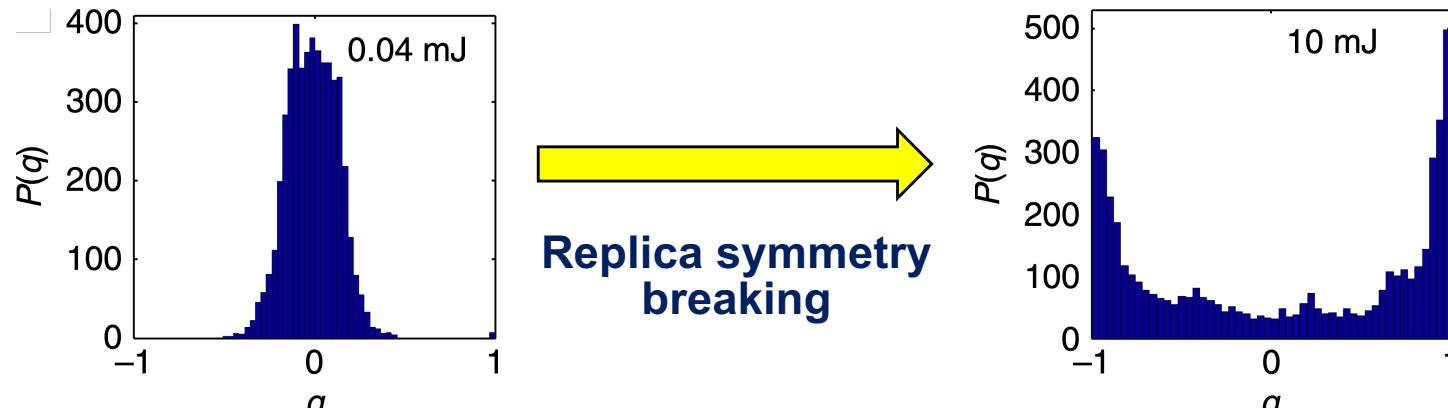


<https://aiichironakano.github.io/cs596/Rotenberg-UseTheForce-JCP20.pdf>

Extension: Replica Pair Correlation

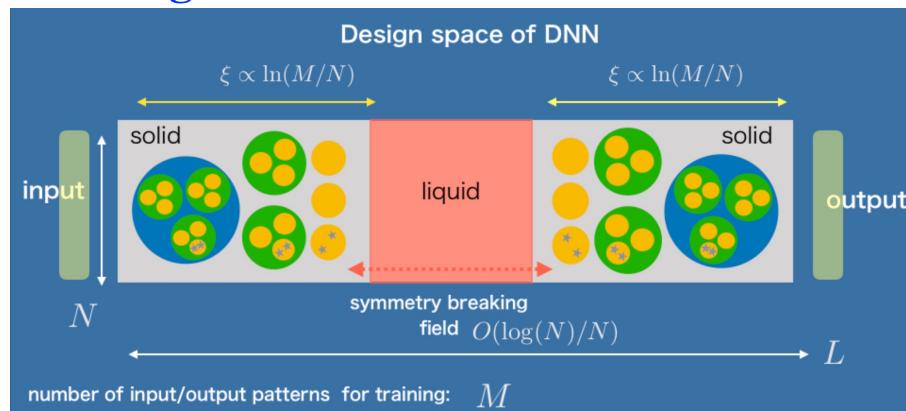
- Pair correlation beyond Euclidean distance?
- Replica-pair correlation (cosine similarity) to detect replica symmetry breaking (Giorgio Parisi, Nobel physics prize, 2021)

Histogram of correlation between replica pairs (random laser pattern)



https://www.nobelprize.org/uploads/2021/10/sciback_fy_en_21.pdf

- Used to analyze “freezing transitions” of deep neural networks with increasing training data size



H. Yoshino, *SciPost Phys. Core* 2, 005 ('20)

The Nobel Prize in Physics 2021

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Physics 2021

"for groundbreaking contributions to our understanding of complex physical systems"

with one half jointly to

Syukuro Manabe **Klaus Hasselmann**

Princeton University, USA Max Planck Institute for Meteorology,
Hamburg, Germany

"for the physical modelling of Earth's climate,
quantifying variability and reliably predicting
global warming"

and the other half to

Giorgio Parisi

Sapienza University of Rome, Italy

"for the discovery of the interplay of
disorder and fluctuations in physical
systems from atomic to planetary scales"

Replica symmetry breaking