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

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

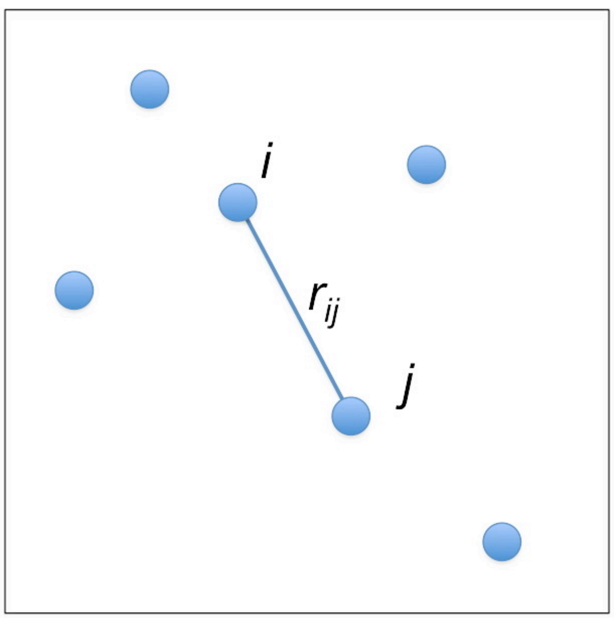
Pair Distribution

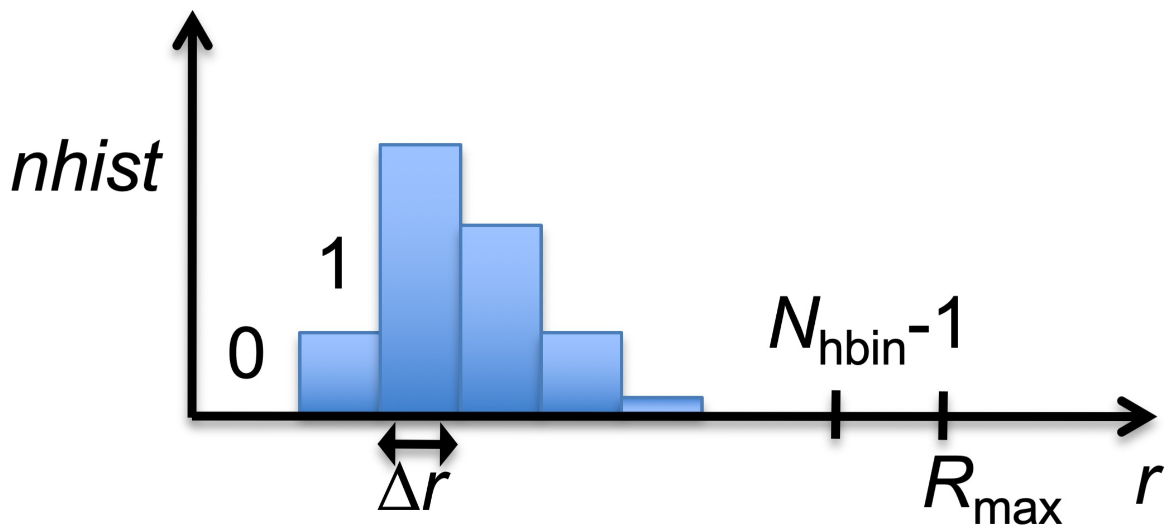
- **Pair-distance histogram,** `nhist[Nhbin]`

```
for all histogram bins i
  nhist[i] = 0
for all atomic pairs (i,j)
  ++nhist[⌊|r_ij|/Δr⌋]
```

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,

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

`rhmax`

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

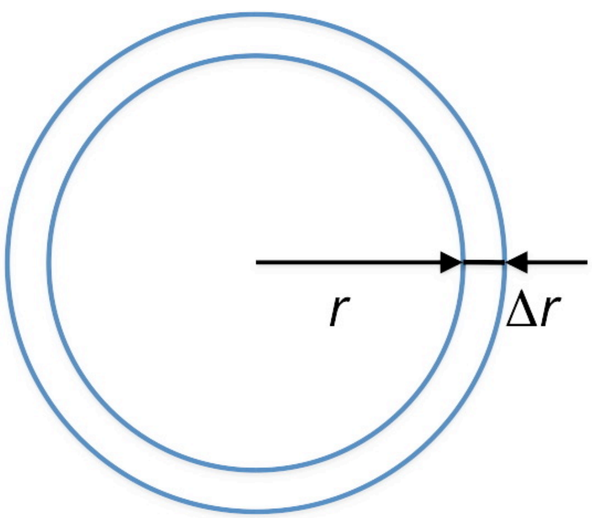
`drh`

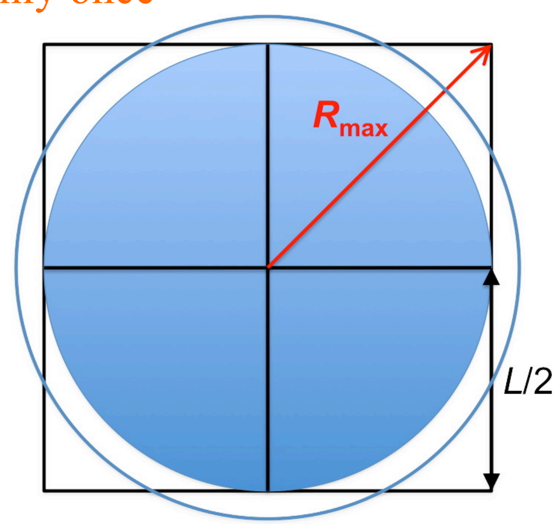
$$\because\ g(r_i) = \boxed{\frac{2\times nhist(i)}{N}} \times \frac{1}{\boxed{4\pi r_i^2 \Delta r} \times \boxed{\rho}}$$

# 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;
     }
     rij = sqrt(rij); // Pair distance
     ih = rij/drh;
     nhis[ih] += 1.0; // Entry to the histogram
   }  // End for j
 }  // Endo for i
```

Minimum-image convention (*cf.* MD lecture)
https://aiichironakano.github.io/cs596/01MD.pdf

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

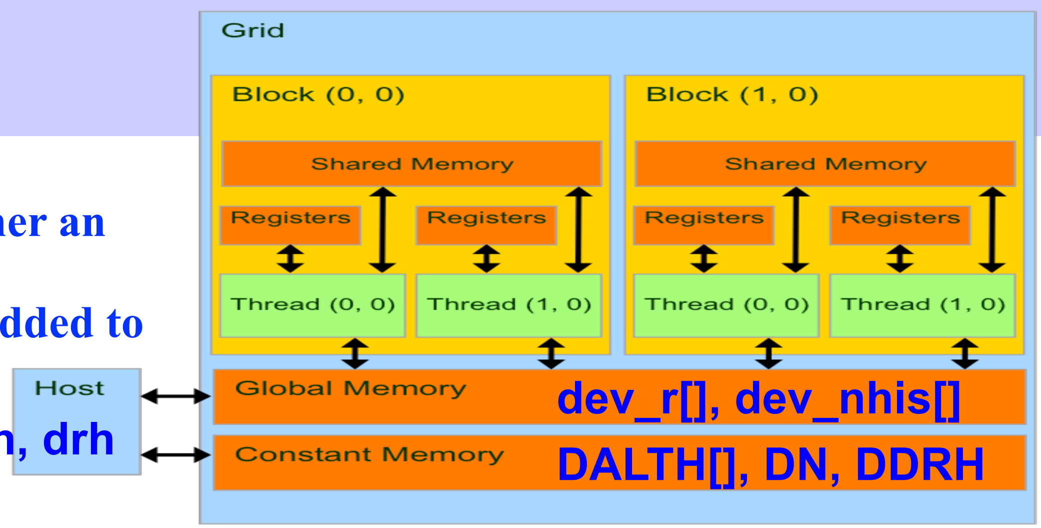
Variables in Device Memory

```
__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);
```

In read-only constant memory

memory offset

- `cudaMemcpyToSymbol:`
  Destination (in device) is either an address or variable name
  Memory offset (in bytes) is added to destination

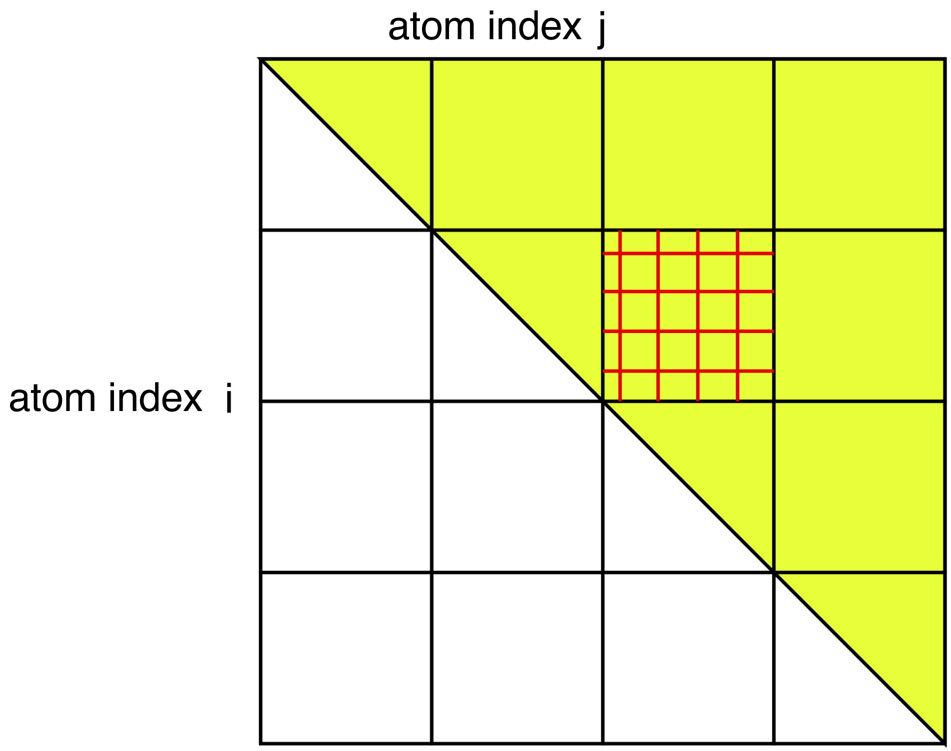


Who Does What: Nested Decompositions

- **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

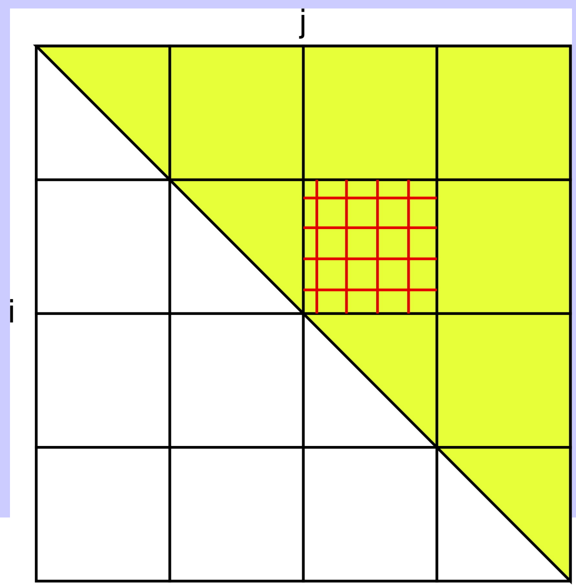
```
__device__ float d_SignR(float v,float x) {if (x > 0) return v; else return -v;}
```

This is only called from the device program

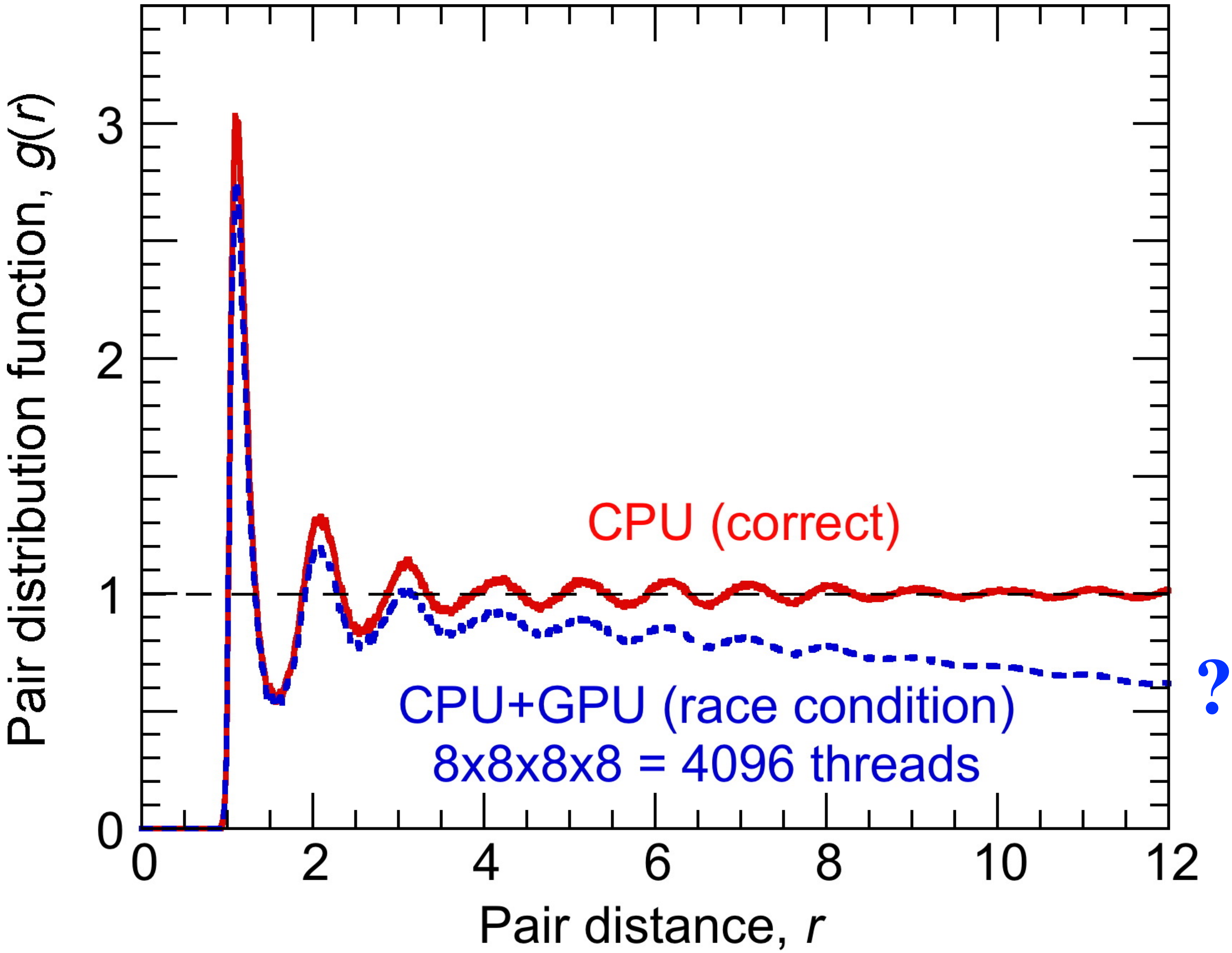
```
__global__ void gpu_histogram_kernel(float *r,float *nhis) {

  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

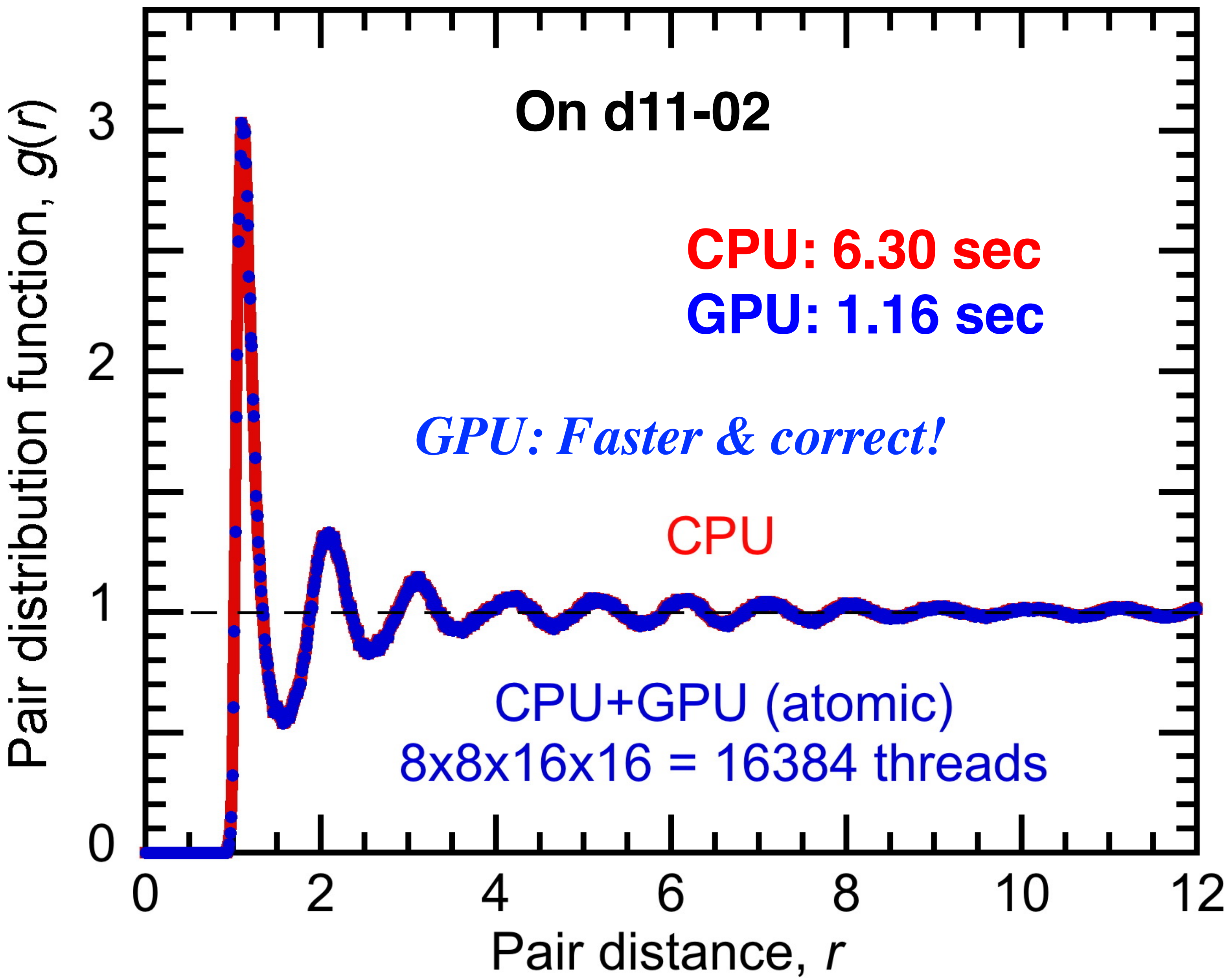
```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --gres=gpu:1
#SBATCH --time=00:00:59
#SBATCH --output=pdf.out
#SBATCH -A anakano_429
echo '##### CPU: gcc -o pdf0 pdf0.c -lm #####'
./pdf0
echo '##### GPU: nvcc -o pdf pdf.cu   #####'
./pdf
```

Output

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

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*

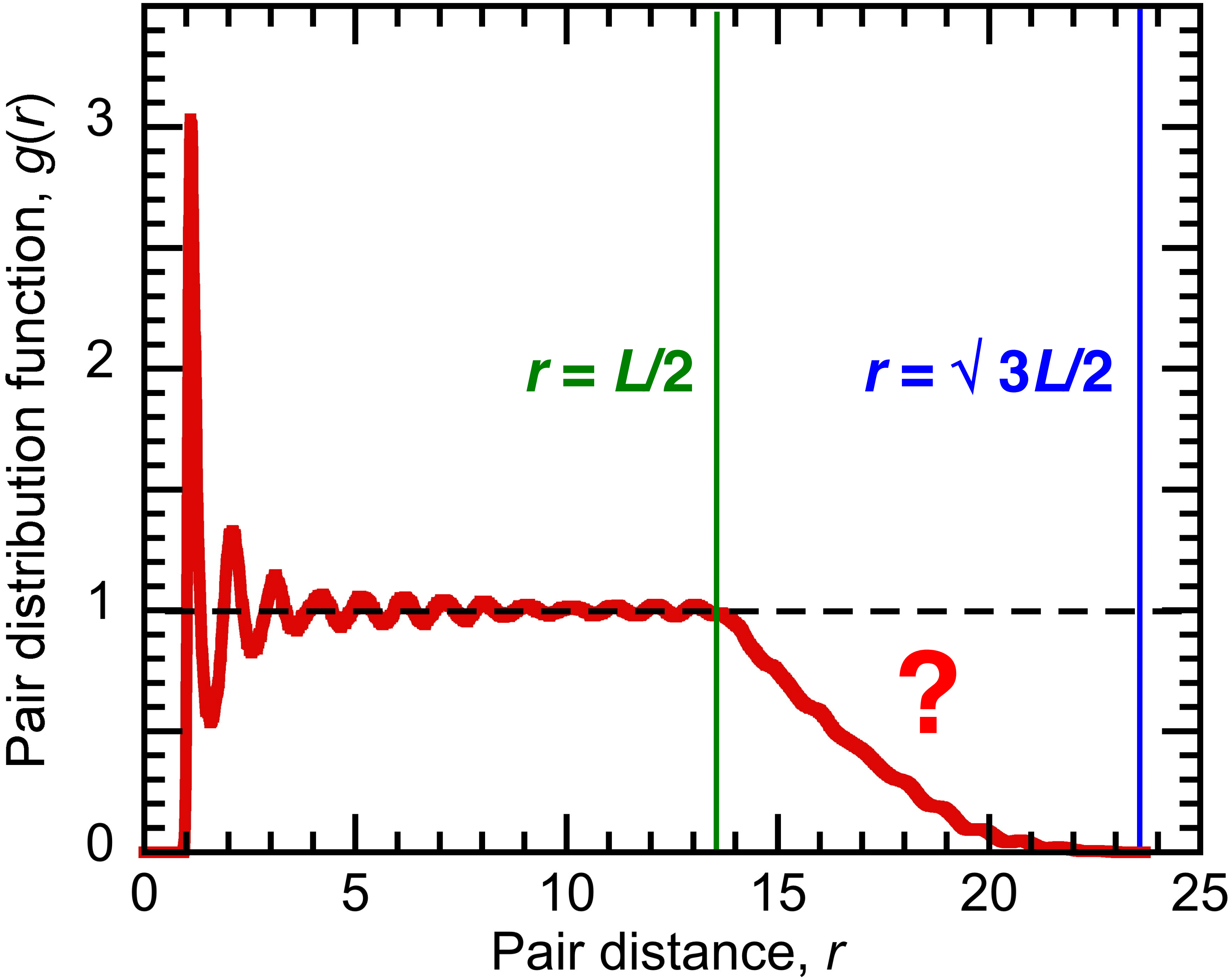
Multithreading (SPMD):

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

copy: host ← device

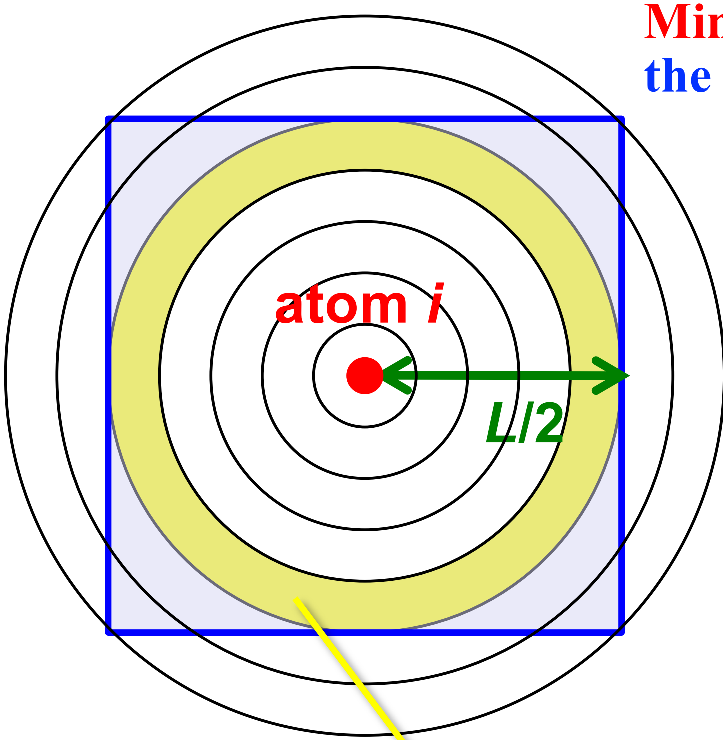
output: *nhis*[]

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

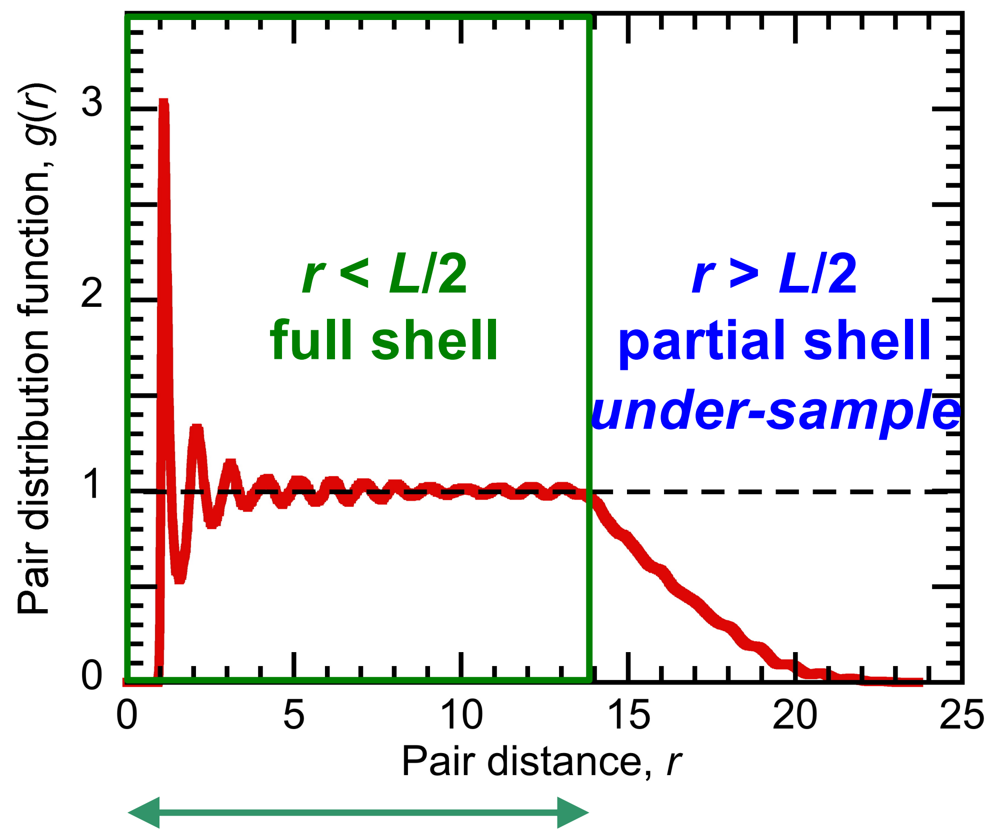


$$g(r) = \boxed{\frac{2 \times nhist(i)}{N}} \times \frac{1}{\boxed{4\pi r^2 \Delta r} \times \boxed{(N/V)}}$$

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

Volume of the shell

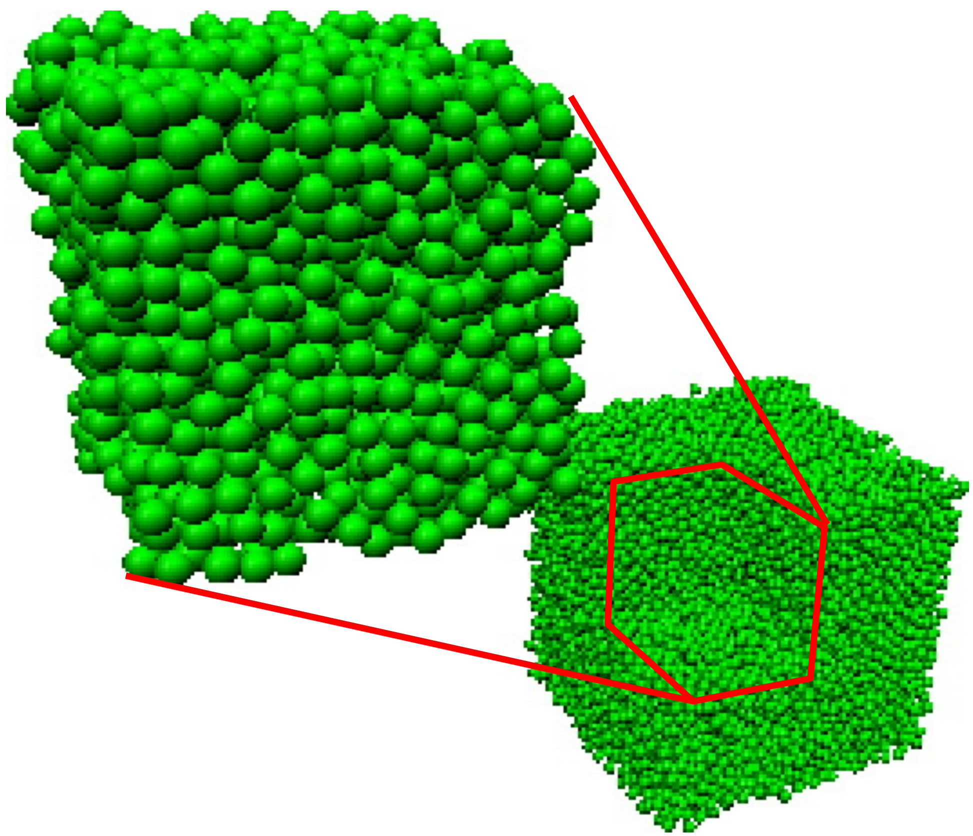
Average density



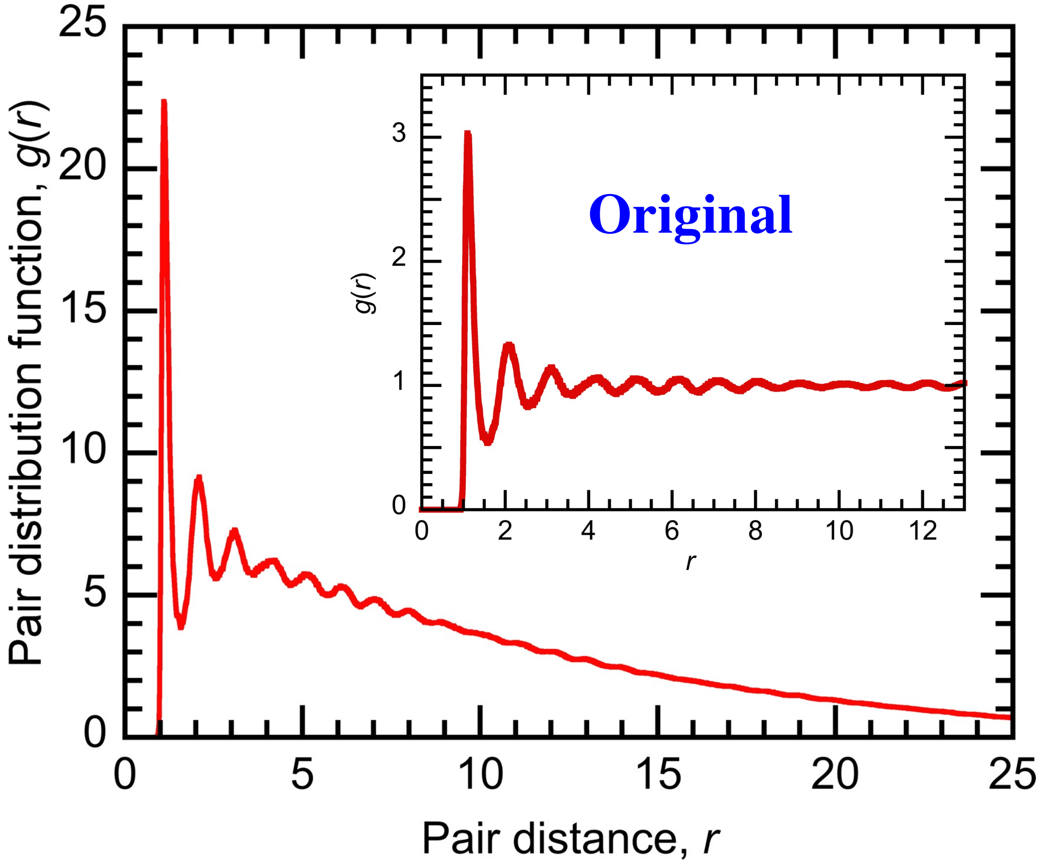
Physically meaningful result

Large-scale Correlation in $g(r)$

One octant of the system cut-out & displaced



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

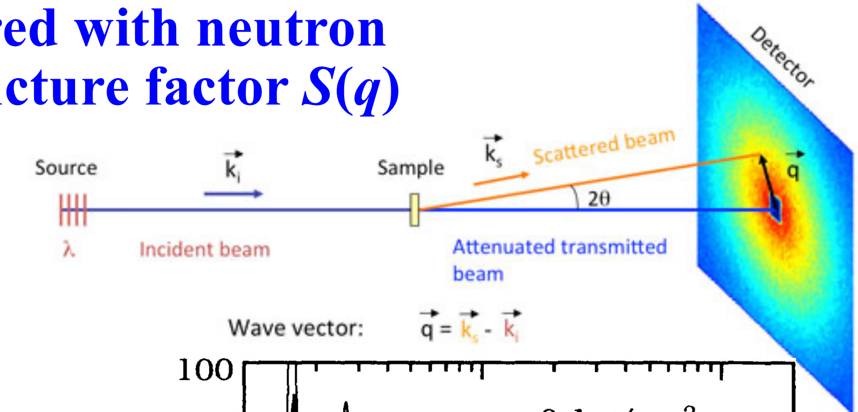


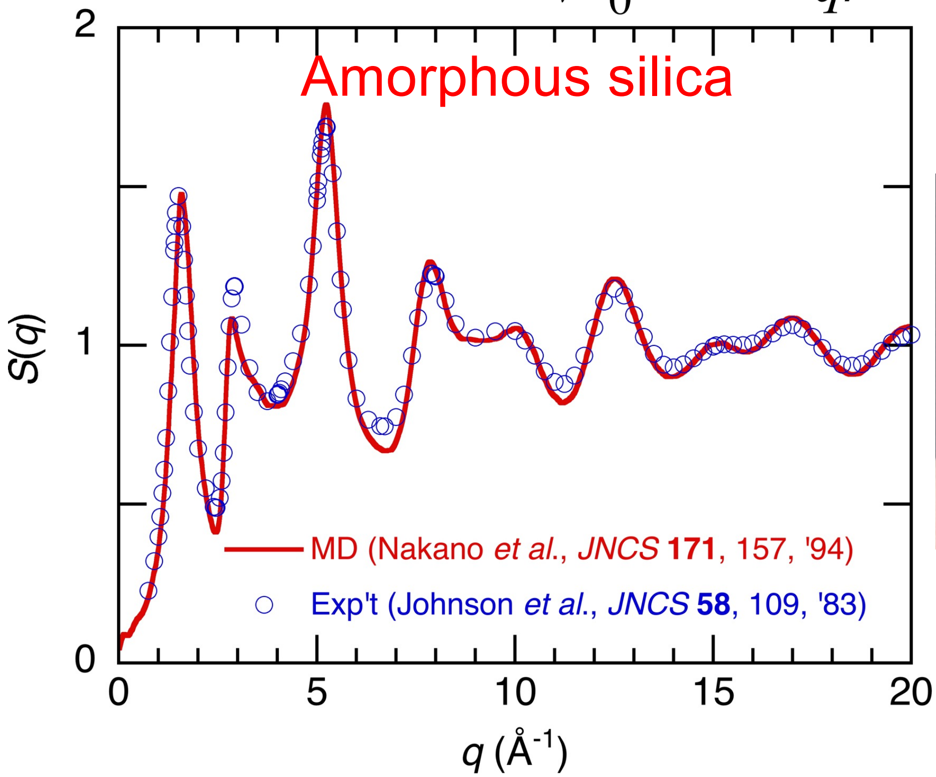
- **Short-range correlation (*i.e.* peak positions) unchanged, just magnified by the lower average density, N/V_{expanded}**
- **Superimposed with larger length-scale geometric factors**

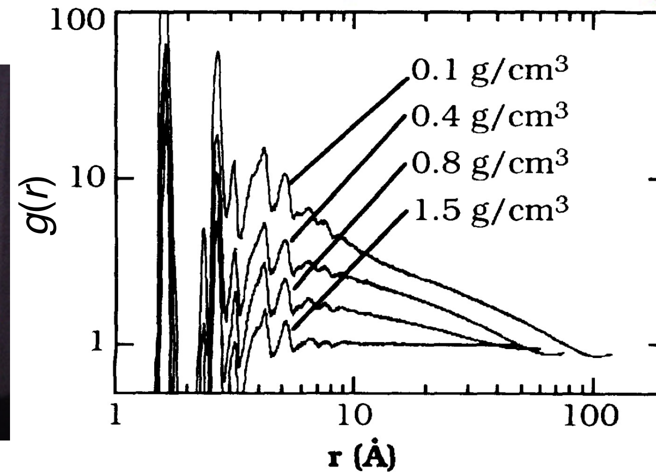
Experimental Connection

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

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



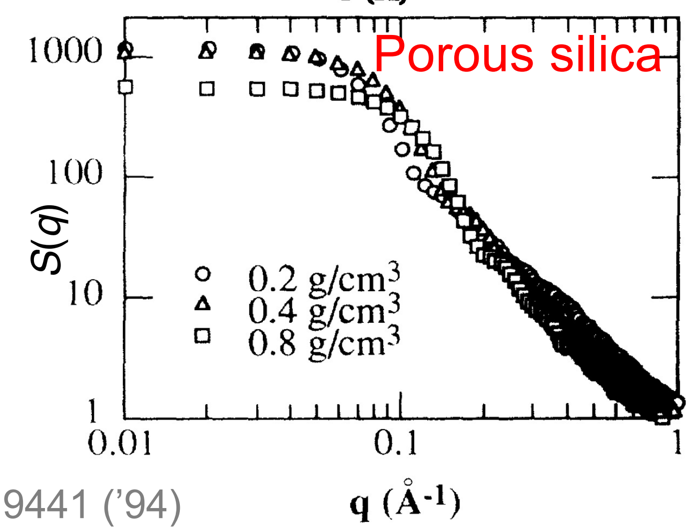




- **Long-range correlations are measured by small-angle neutron or X-ray scattering structure factors (SANS or SAXS)**

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

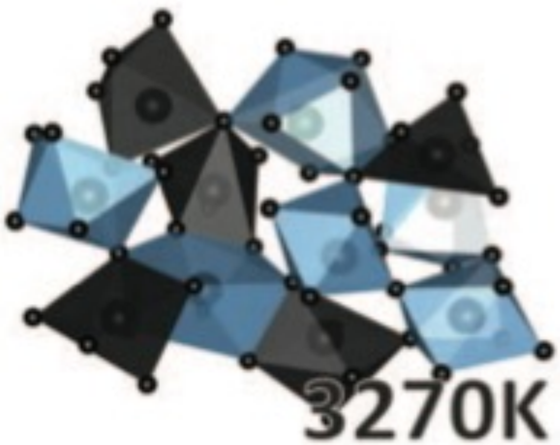
d_f: Fractal dimension

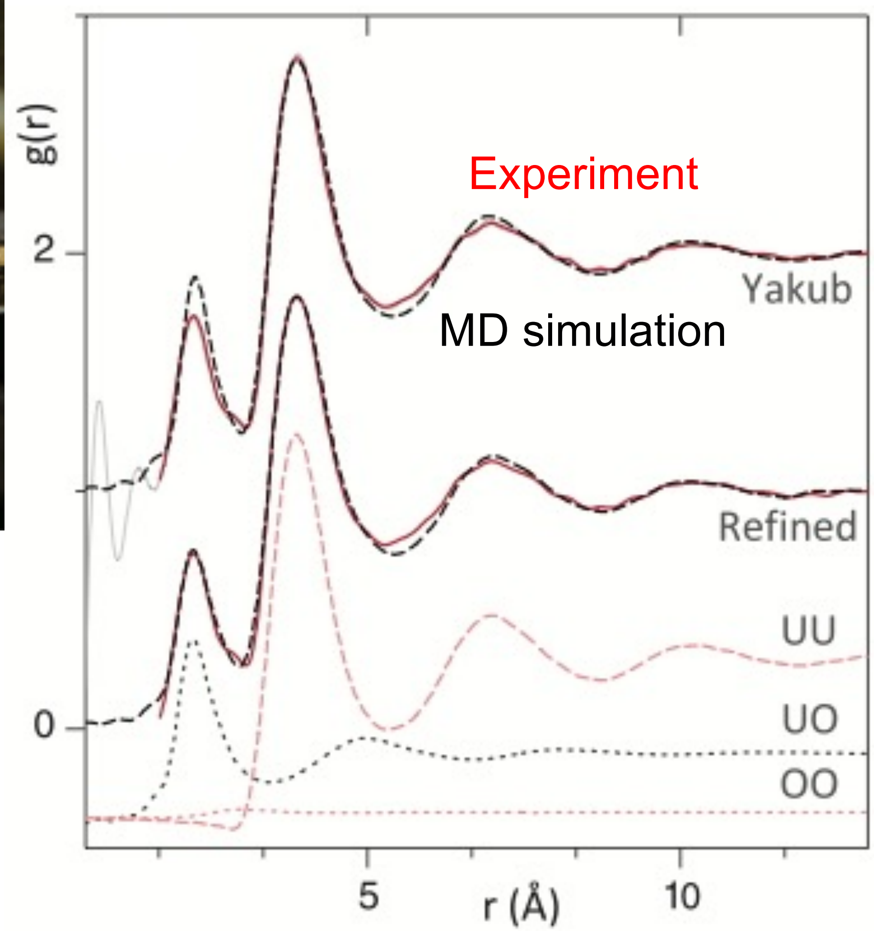


Nakano *et al.*, *PRL* **71**, 85 ('93); *PRB* **49**, 9441 ('94)

$g(r)$ 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

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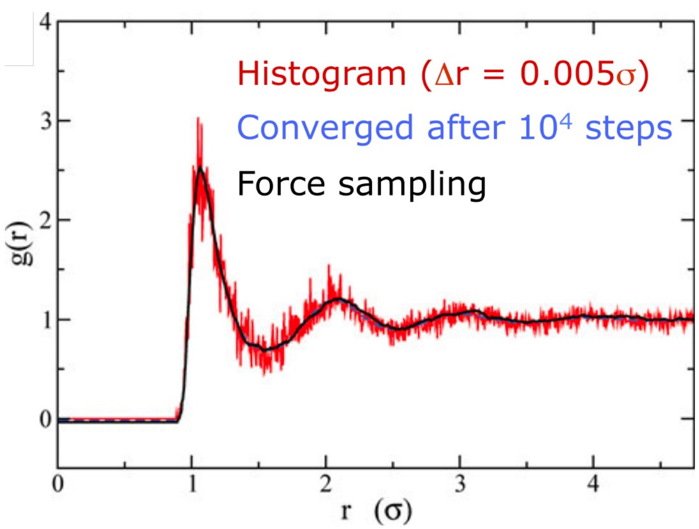
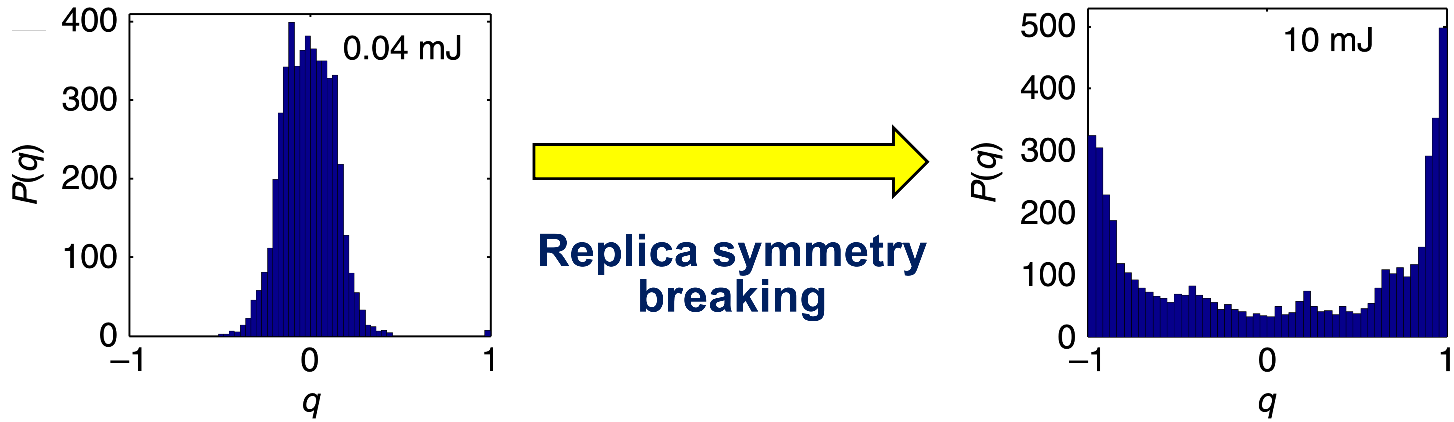


https://aiichironakano.github.io/cs596/Rotenberg-UseTheForce-JCP20.pdf

Extension: Replica Pair Correlation

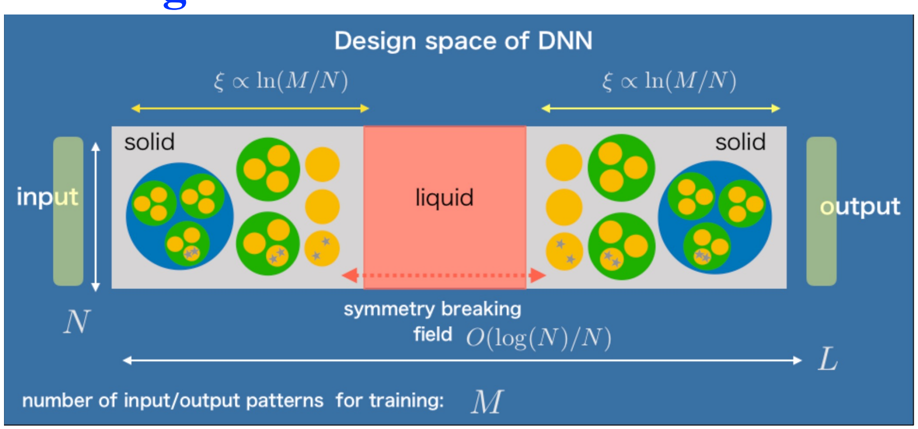
- **Pair correlation beyond Euclidean distance?**
- **Replica-pair correlation (cosine similarity) to detect replica symmetry breaking (Giorgio Parisi, Nobel physics prize, 2021)**

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
Princeton University, USA

Klaus Hasselmann
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