Pair Distribution Computation on GPU

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Quantitative & Computational Biology
University of Southern California

Email: anakano@usc.edu

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

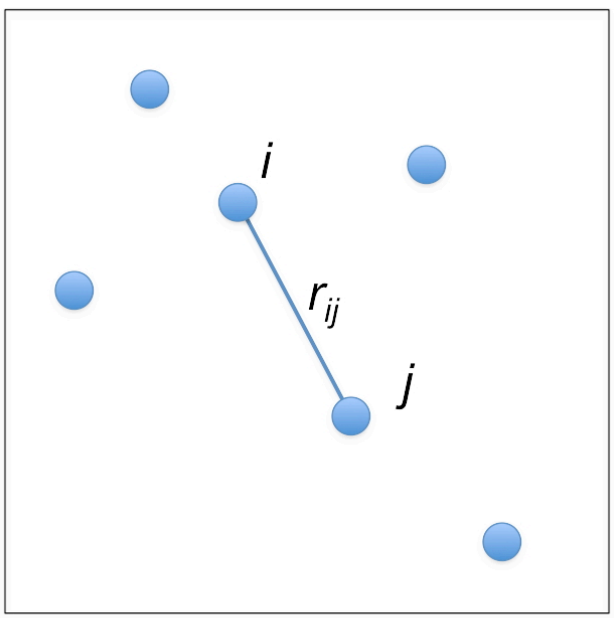
- **Pair-distance histogram,** `nhist[Nhbin]`

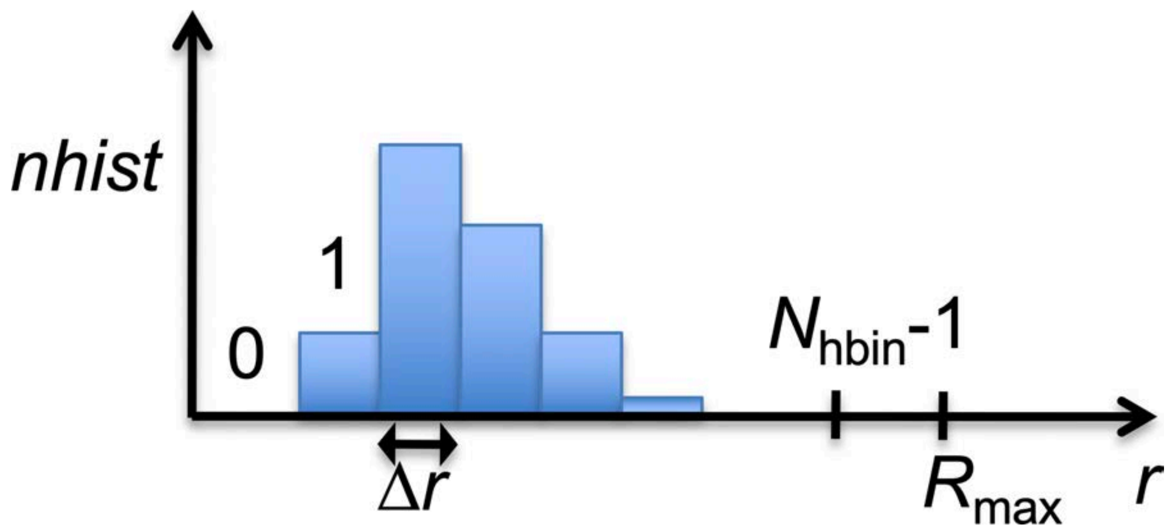
```
for all histogram bins i
  nhist[i] = 0
for all atomic pairs (i,j)
  ++nhist[⌊|r_ij|/Δr⌋]
```

$$\texttt{++nhist[}\lfloor |\vec{r}_{ij}|/\Delta r \rfloor\texttt{]}$$

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 $r = 0$

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

# 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

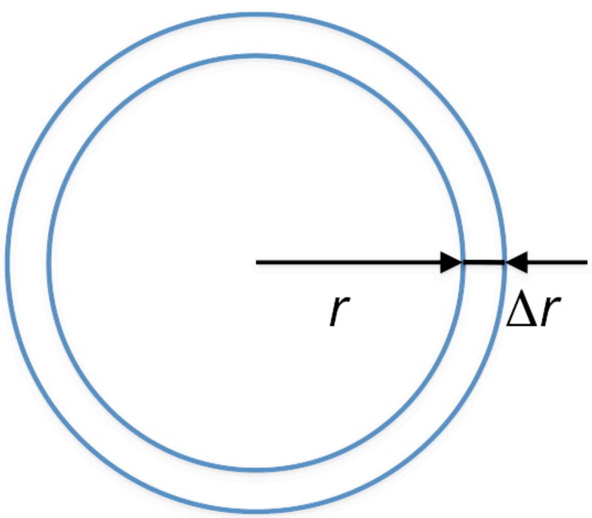
With minimum-image convention,

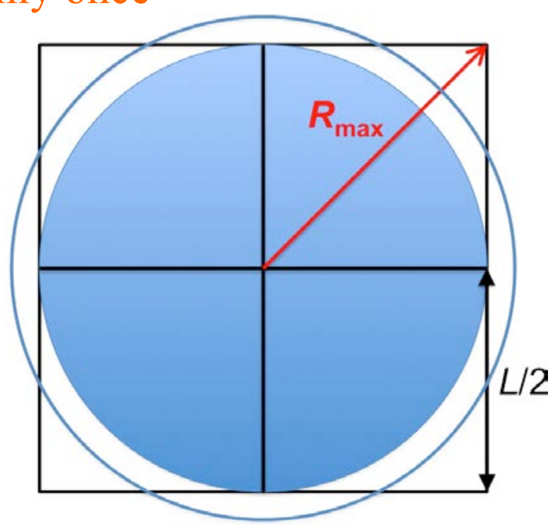
$$R_{\max} = \sqrt{\sum_{\alpha=x,y,z} \left(\frac{\mathrm{al}[\alpha]}{2}\right)^2}$$

`rhmax`

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

`drh`





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

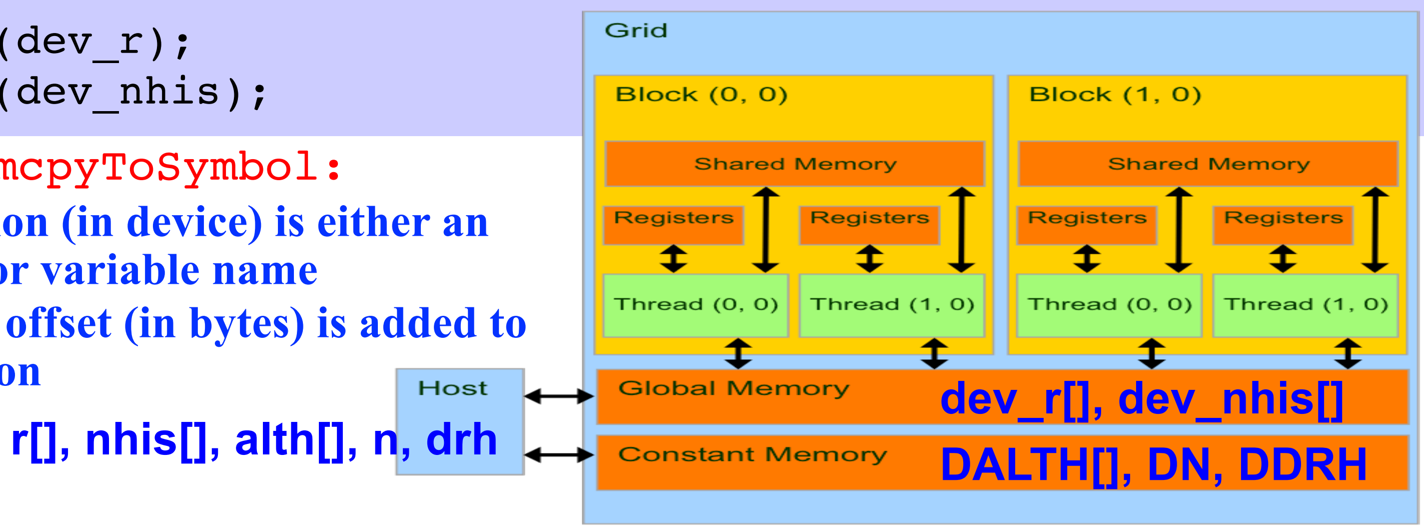
Variables in Device Memory

```
__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

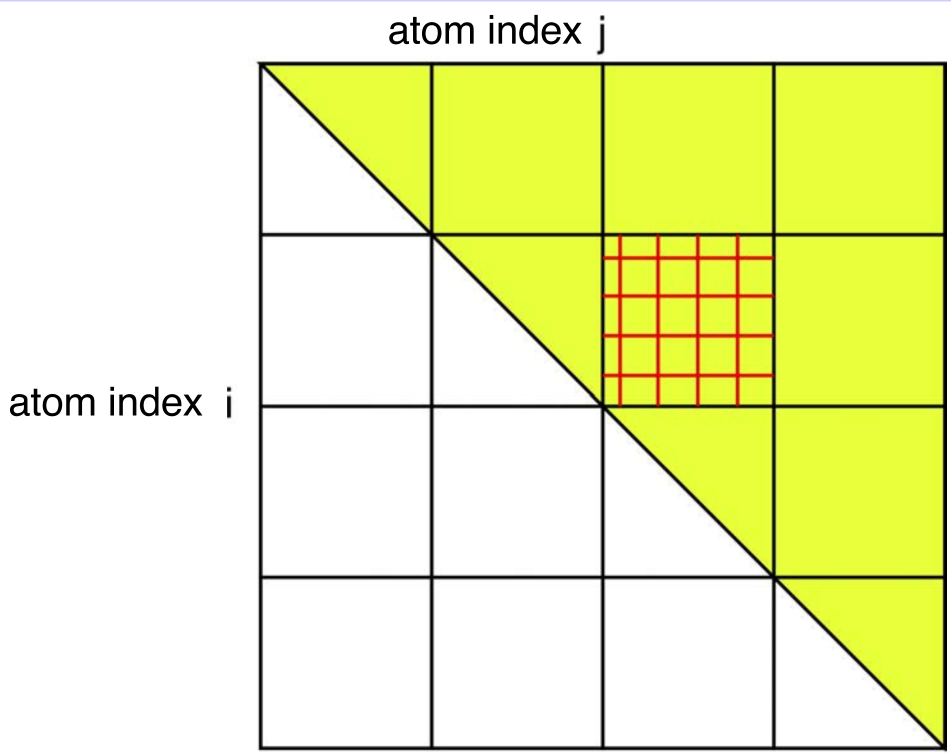


Who Does What: Nested Decompositions

- **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

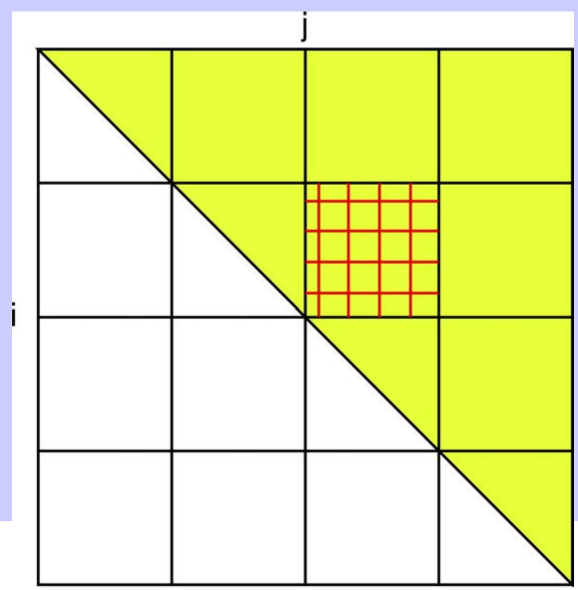
```
__device__ float d_SignR(float v,float x) {if (x > 0) return v; else return -v;}
```

This is only called from the device program

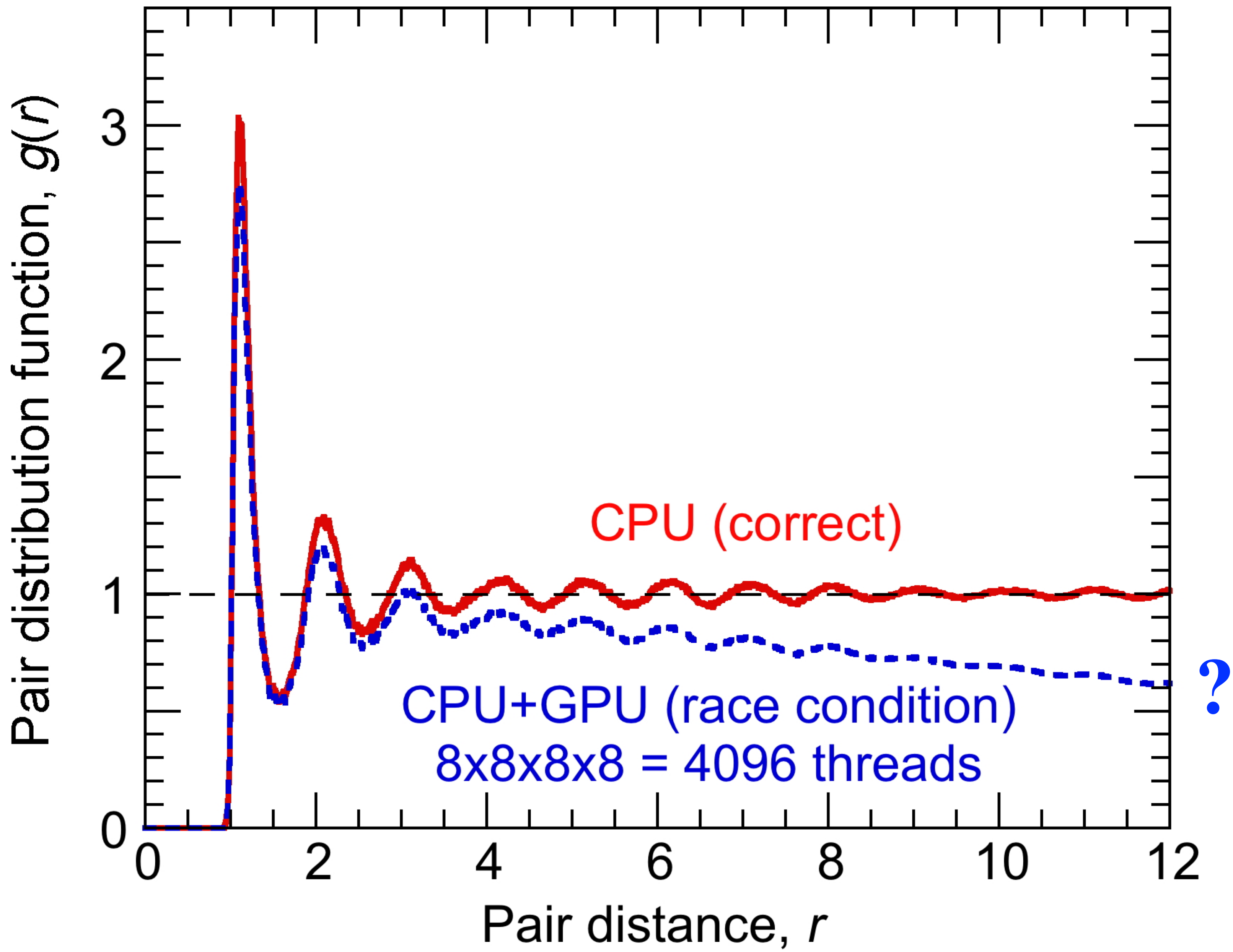
```
__global__ void gpu_histogram_kernel(float *r,float *nhis) {

  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 (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

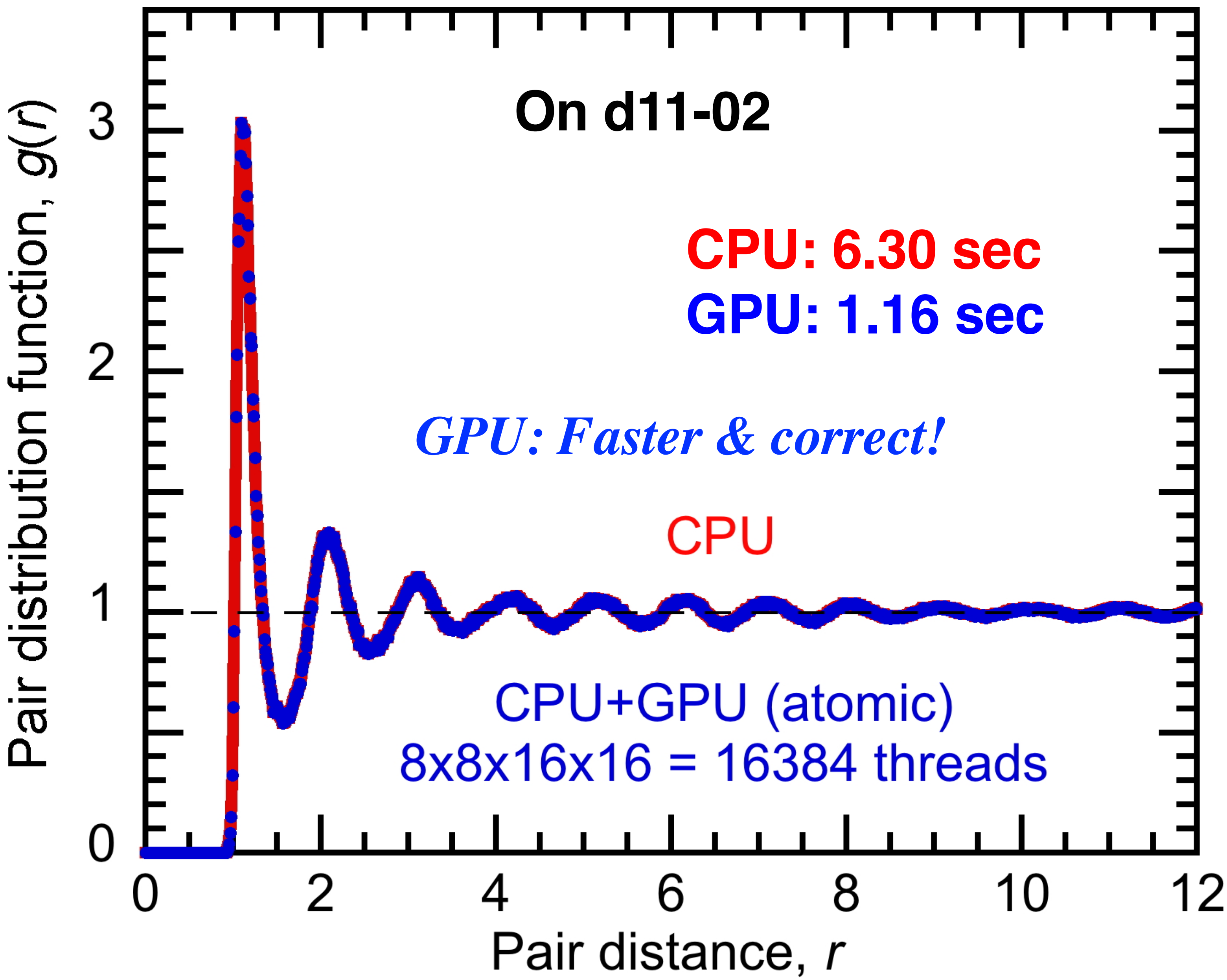
Script

```
#!/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*

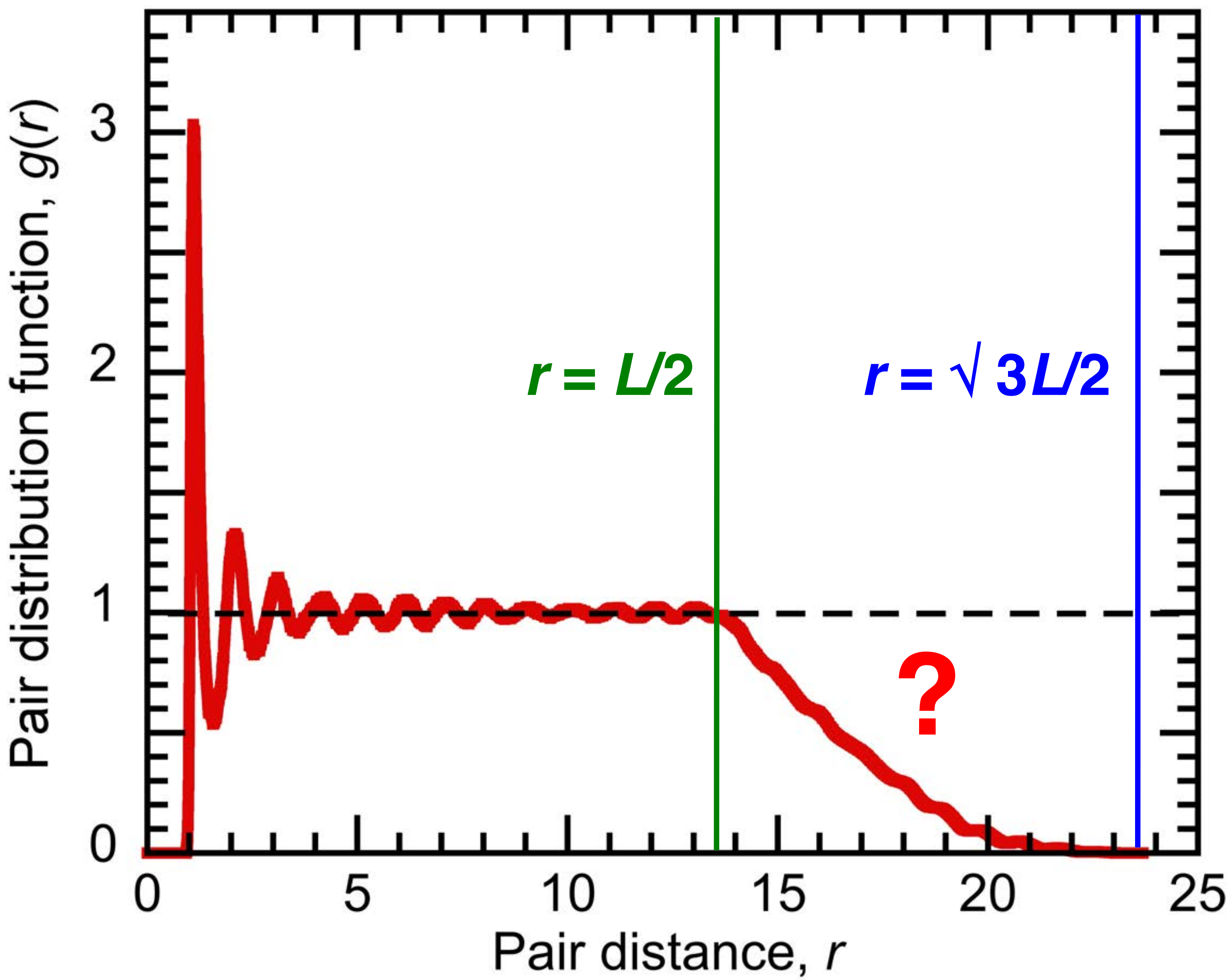
Multithreading (SPMD):

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

copy: host ← device

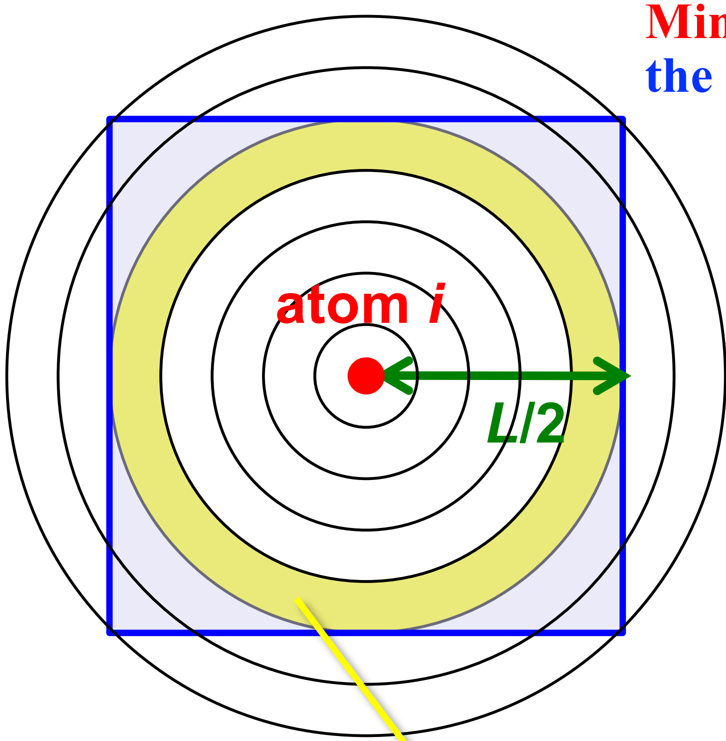
output: *nhis*[]

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

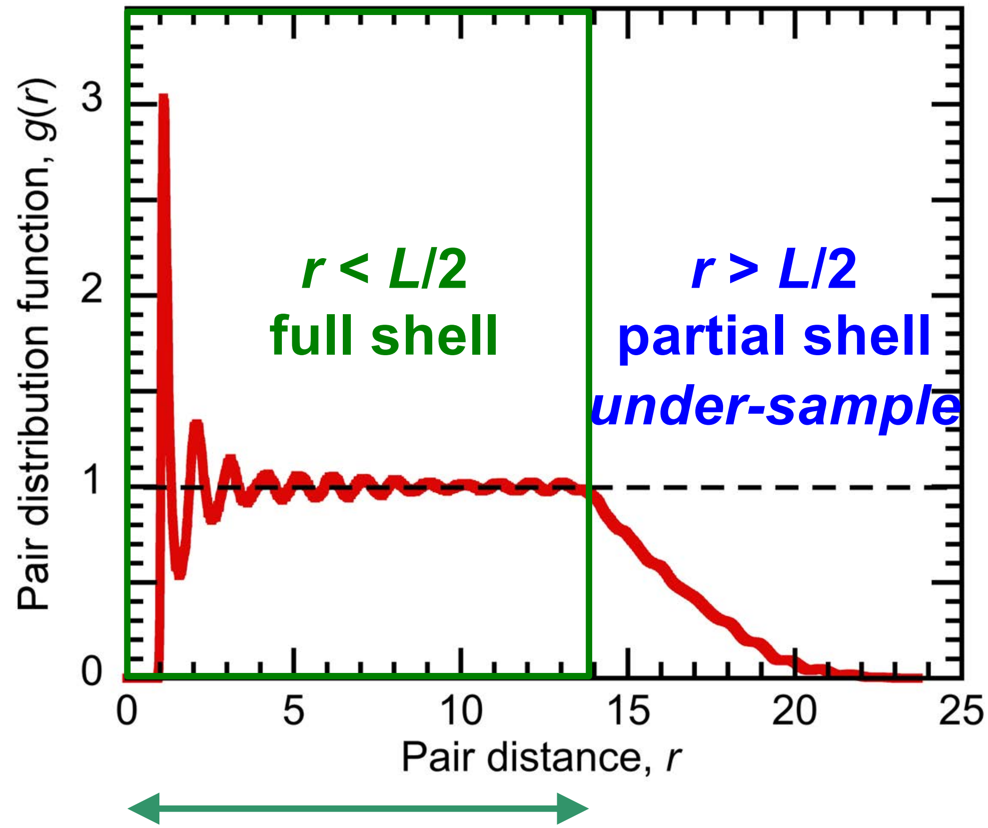


$$g(r) = \boxed{\frac{2\times nhist(i)}{N}} \times \frac{1}{\boxed{4\pi r^2 \Delta r} \times \boxed{(N/V)}}$$

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

Volume of the shell

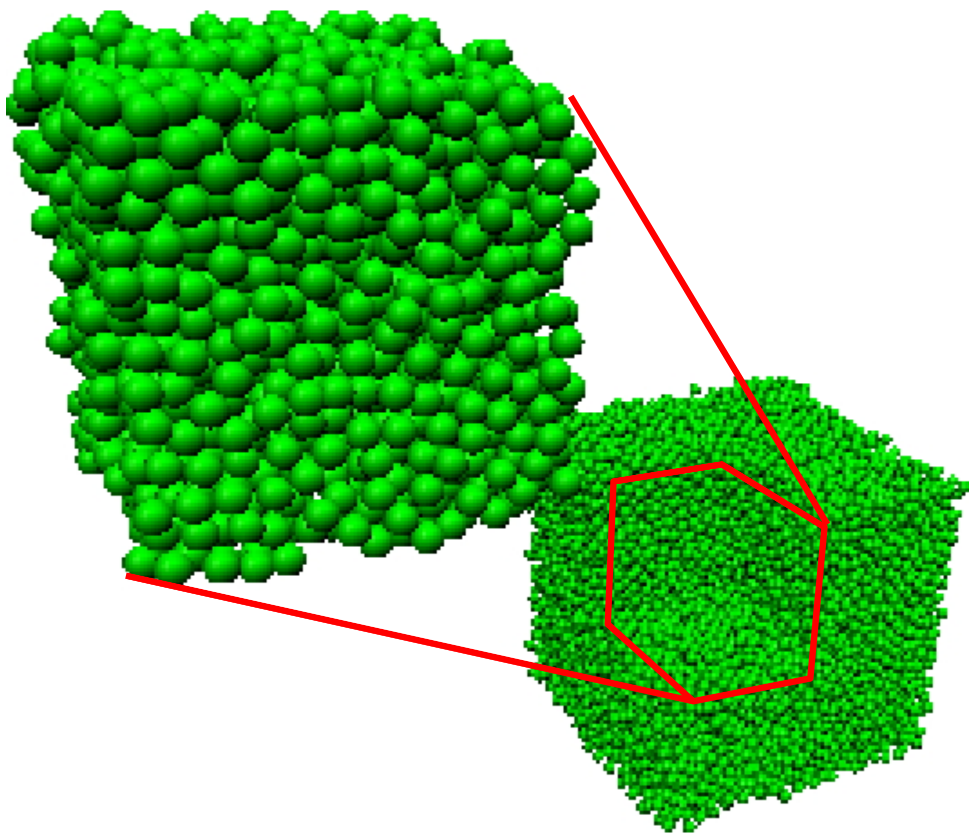
Average density



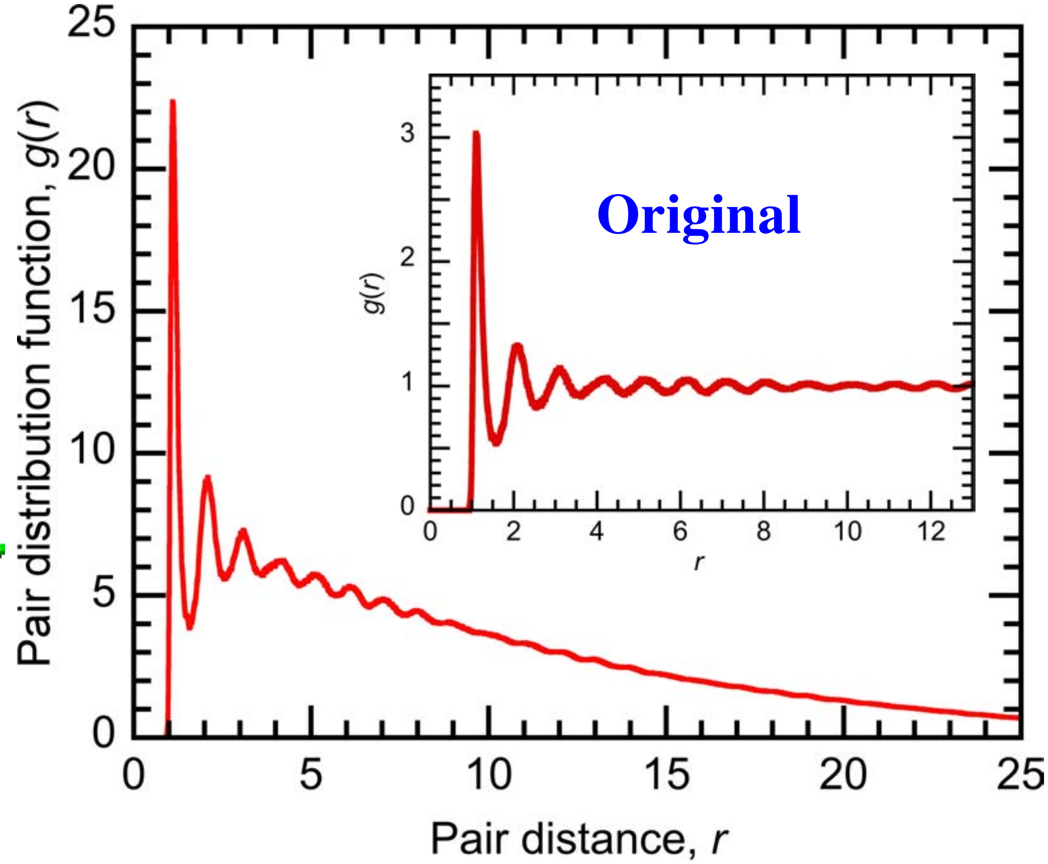
Physically meaningful result

Large-scale Correlation in $g(r)$

One octant of the system cut-out & displaced



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

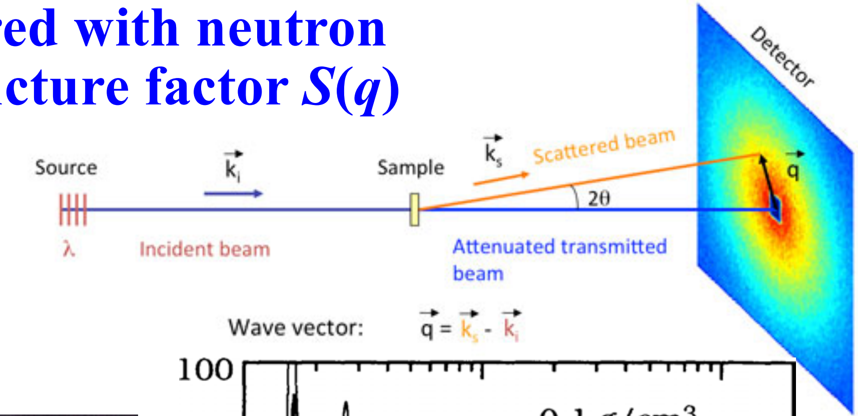


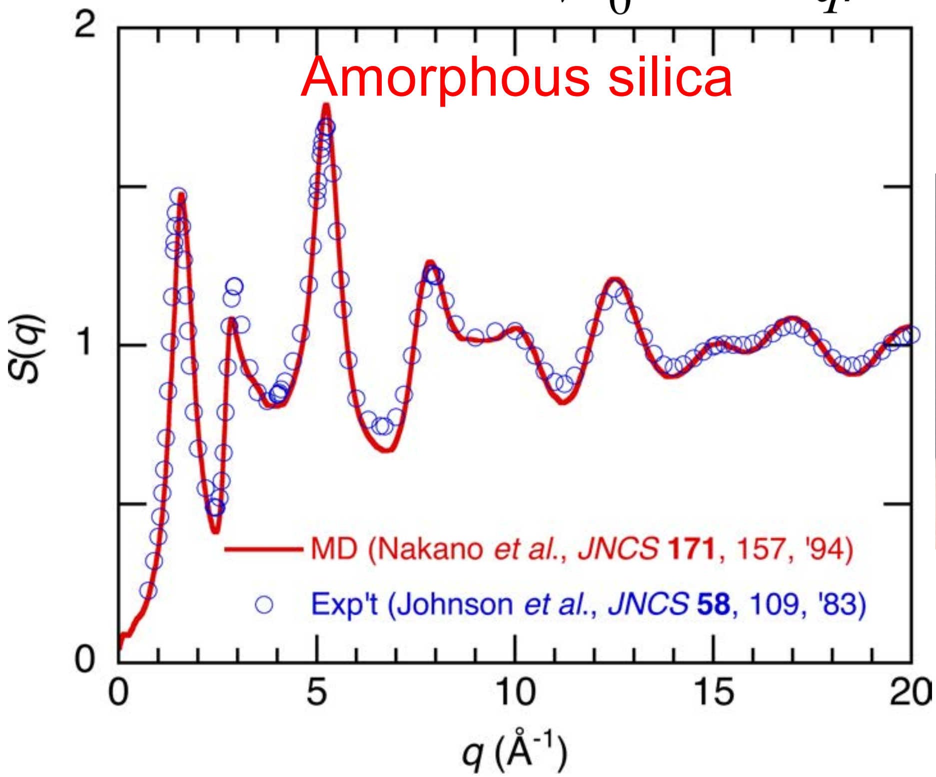
- **Short-range correlation (*i.e.* peak positions) unchanged, just magnified by the lower average density, $N/V_{expanded}$**
- **Superimposed with larger length-scale geometric factors**

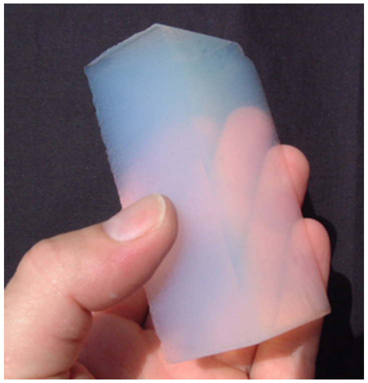
Experimental Connection

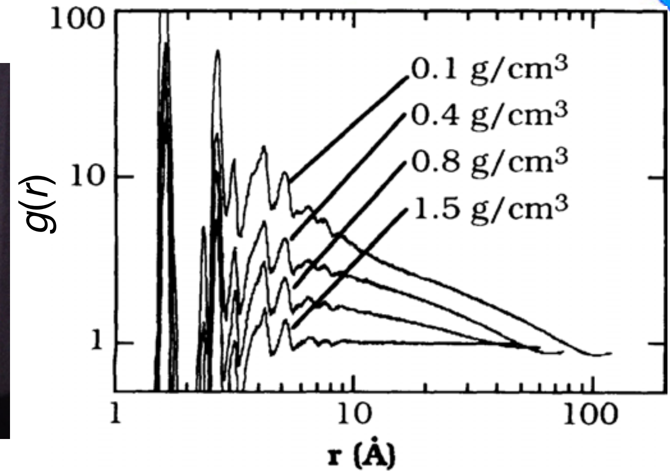
- **Short-range correlations are directly compared with neutron or X-ray scattering measurements of the structure factor $S(q)$**

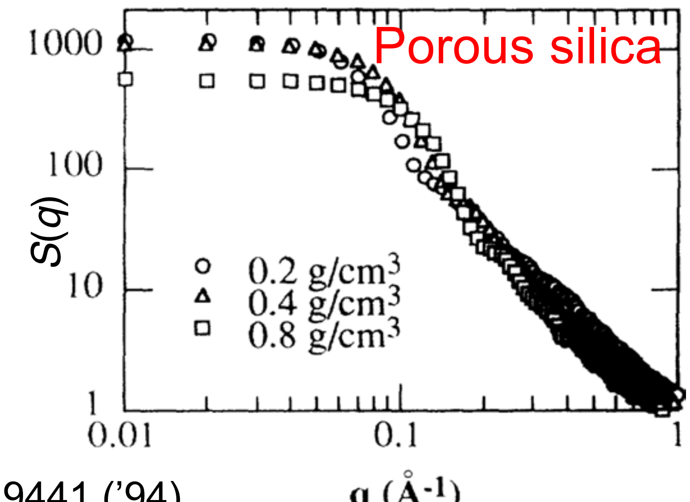
$$S(q) = 1 + 4\pi \frac{N}{V} \int_0^\infty dr r^2 \frac{\sin(qr)}{qr} [g(r) - 1]$$











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

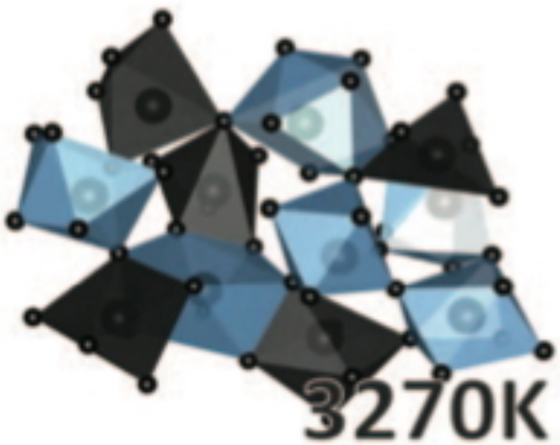
$S(q) \propto q^{-d_f}$

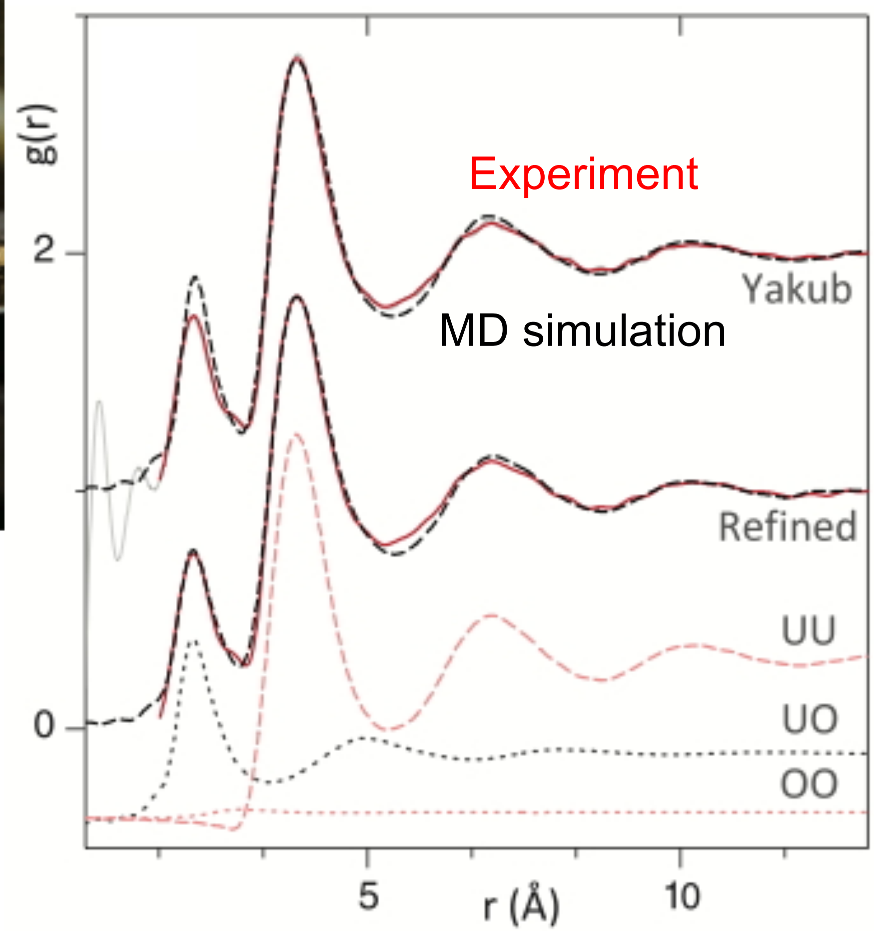
d_f: Fractal dimension

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

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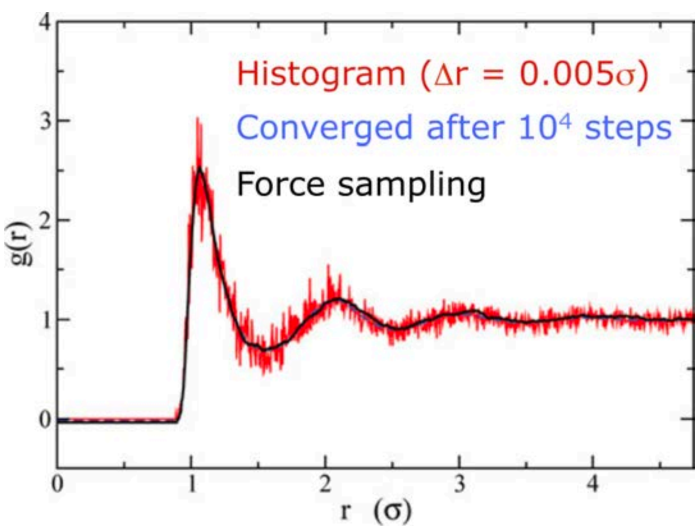
AFFILIATIONS

Sorbonne Université, CNRS, Physico-Chimie des électrolytes et Nanosystèmes Interfaciaux, F-75005 Paris, France

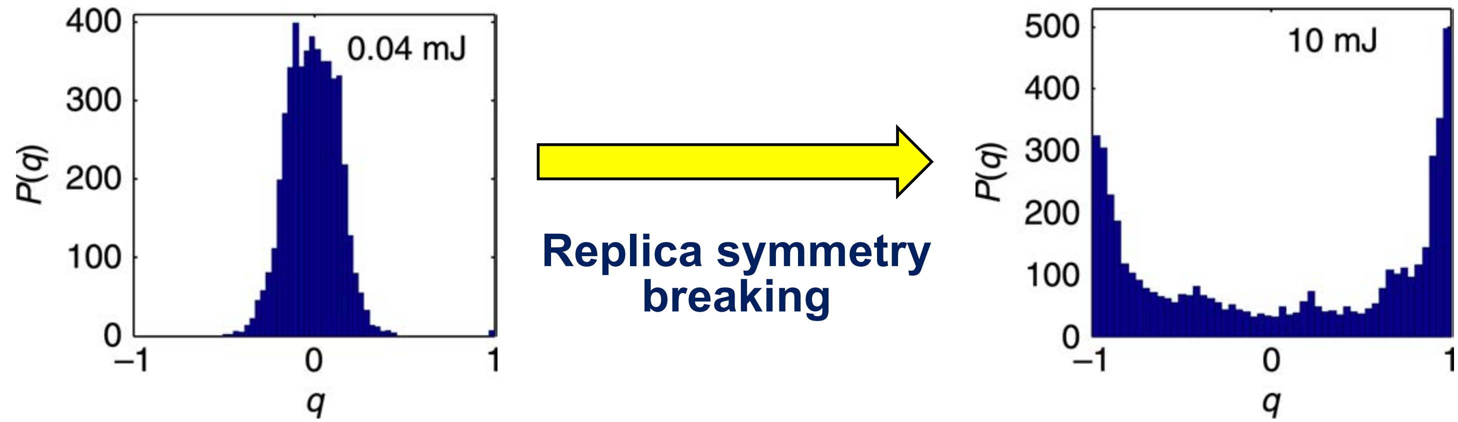


https://aiichironakano.github.io/cs596/Rotenberg-UseTheForce-JCP20.pdf

Extension: Replica Pair Correlation

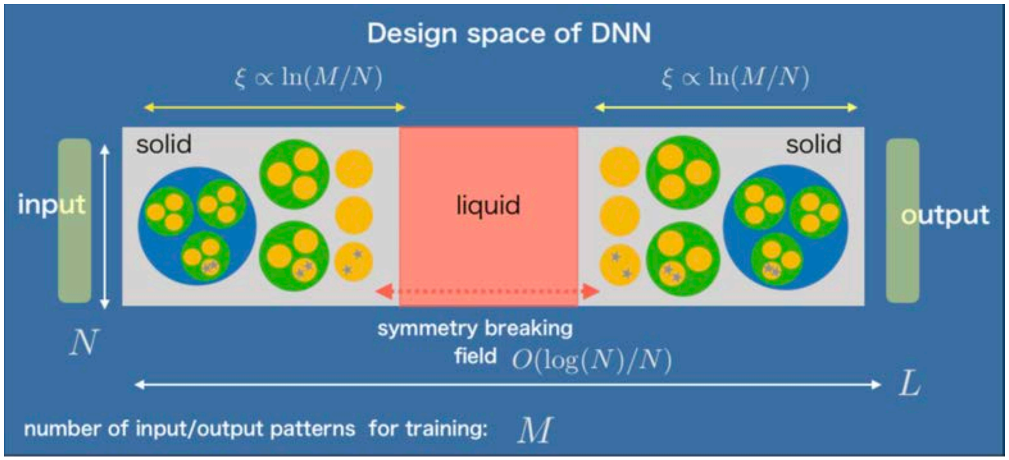
- **Pair correlation beyond Euclidean distance?**
- **Replica-pair correlation (cosine similarity) to detect replica symmetry breaking (Giorgio Parisi, Nobel physics prize, 2021)**

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)