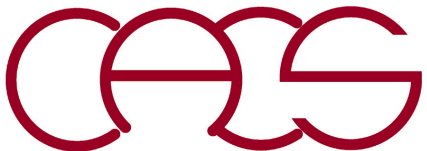# Parallel Pair Distribution Computation

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Pair Distribution Function

- **Pair-distance histogram, nhist**

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

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

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

With minimum-image convention,

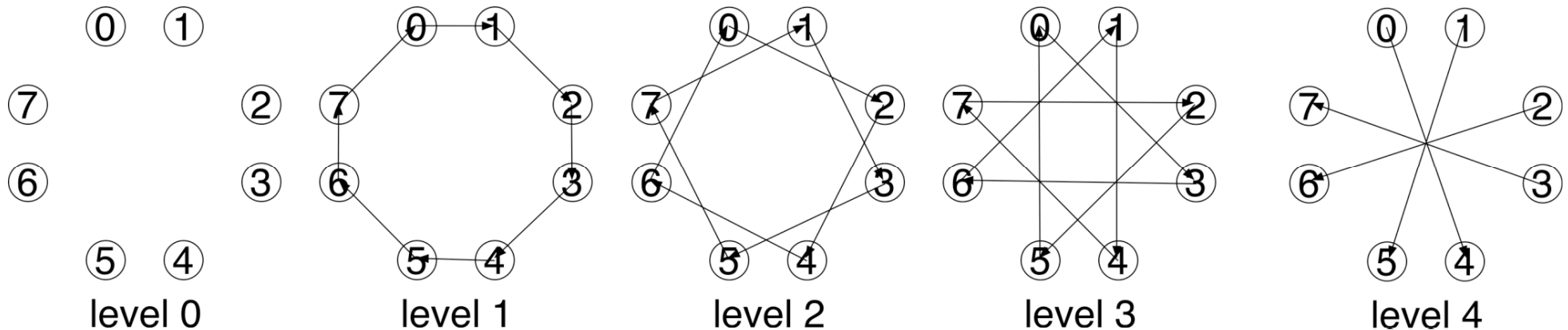$$R_{max} = \sqrt{\sum_{\alpha=x,y,z} \left(\frac{al[\alpha] \times vproc[\alpha]}{2} \right)^2}$$

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

Parallel All-Pair Algorithm

Inter-processor computations with spatial decomposition

```
for level = 0 to nproc/2
  if (level < nproc/2 or myid >= nproc/2) then
    process ∀pairs between processors
    myid & (myid-level)%nproc
```


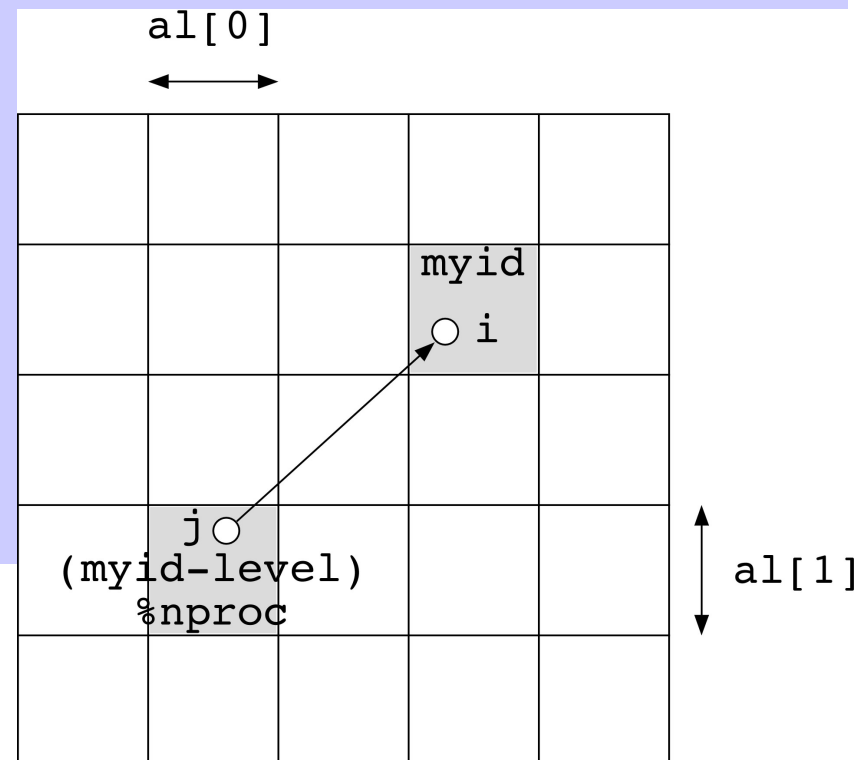level 0   level 1   level 2   level 3   level 4

$$\sum_{level=0}^{nproc/2-1} nproc + \frac{nproc}{2} = \frac{nproc(nproc+1)}{2}$$

Coordinate Shifts & Wrap-Around

```
compose a message: r[i][0:2] to dbuf[3*i:3*i+2] (i=0,n-1)
(asynchronously) receive idguest, nguest & dbufr[0:3*nguest-1]
send myid, n & dbuf[0:3*n-1] to (myid+level)%nproc
locally add (i: host, j: guest) pairs to nhist
  for (rij = 0.0, a=0; a<3; a++) {
    /* Guest positions need to be shifted */
    dr = r[i][a]+dl[a]-dbufr[3*j+a];
    /* Periodic boundary condition: min. image convention */
    dr = dr-SignR(alth[a],dr-alth[a])-SignR(alth[a],dr+alth[a]);
    rij += dr*dr;
  }
rij = sqrt(rij);
nhis[(int)rij/drh] += 1.0;


1. dl[a]?
2. alth[a] = al[a]*vproc[a]/2
```

al[0]

myid

○ i

j ○
(myid-level)
%nproc

al[1]

Numerical Result

Pair distribution function vs. Pair distance (Lennard-Jones unit)