Parallel Pair Distribution Computation

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Biological Sciences
University of Southern California

Email: anakano@usc.edu
Pair Distribution Function

- Pair-distance histogram, \( \text{nhist} \)

\[
\text{nhist}[i] = 0 \\
\text{for all atomic pairs } (i,j) \\
++\text{nhist}[
\left\lfloor \frac{|\vec{r}_{ij}|}{\Delta r} \right\rfloor]
\]

- Pair-distribution function, \( g(r) \)

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

With minimum-image convention,

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

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

\[
\sum_{level=0}^{nproc/2-1} nproc + \frac{nproc}{2} = \frac{nproc(nproc + 1)}{2}
\]
Compose a message: \( r[i][0:2] \) to \( \text{dbuf}[3*i:3*i+2] \) (\( i=0,n-1 \)) (asynchronously) receive idguest, nguest & \( \text{dbuffr}[0:3*\text{nguest}-1] \)

Send myid, n & \( \text{dbuf}[0:3*n-1] \) to \((\text{myid}+\text{level})\%\text{nproc}\)

Locally add \((i: \text{host}, j: \text{guest})\) pairs to nhist

For \((rij = 0.0, a=0; a<3; a++)\) {
  /* Guest positions need to be shifted */
  \( dr = r[i][a]+dl[a]-\text{dbuffr}[3*j+a]; \)
  /* Periodic boundary condition: min. image convention */
  \( dr = dr-\text{SignR}(alth[a],dr-alth[a])-\text{SignR}(alth[a],dr+alth[a]); \)
  \( rij += dr*dr; \)
}

\( rij = \sqrt{rij}; \)

\( \text{nhis}[(\text{int})rij/\text{drh}] += 1.0; \)

1. \( dl[a]? \)
2. \( alth[a] = al[a]*vproc[a]/2 \)