

Parallel Molecular Dynamics

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Objective: Operationally understand spatial decomposition (who does what) & message passing using a real-world application (pmd.c)



<https://aiichironakano.github.io/cs596/src/pmd>
<https://github.com/KenichiNomura/binary-LJ-pmd>



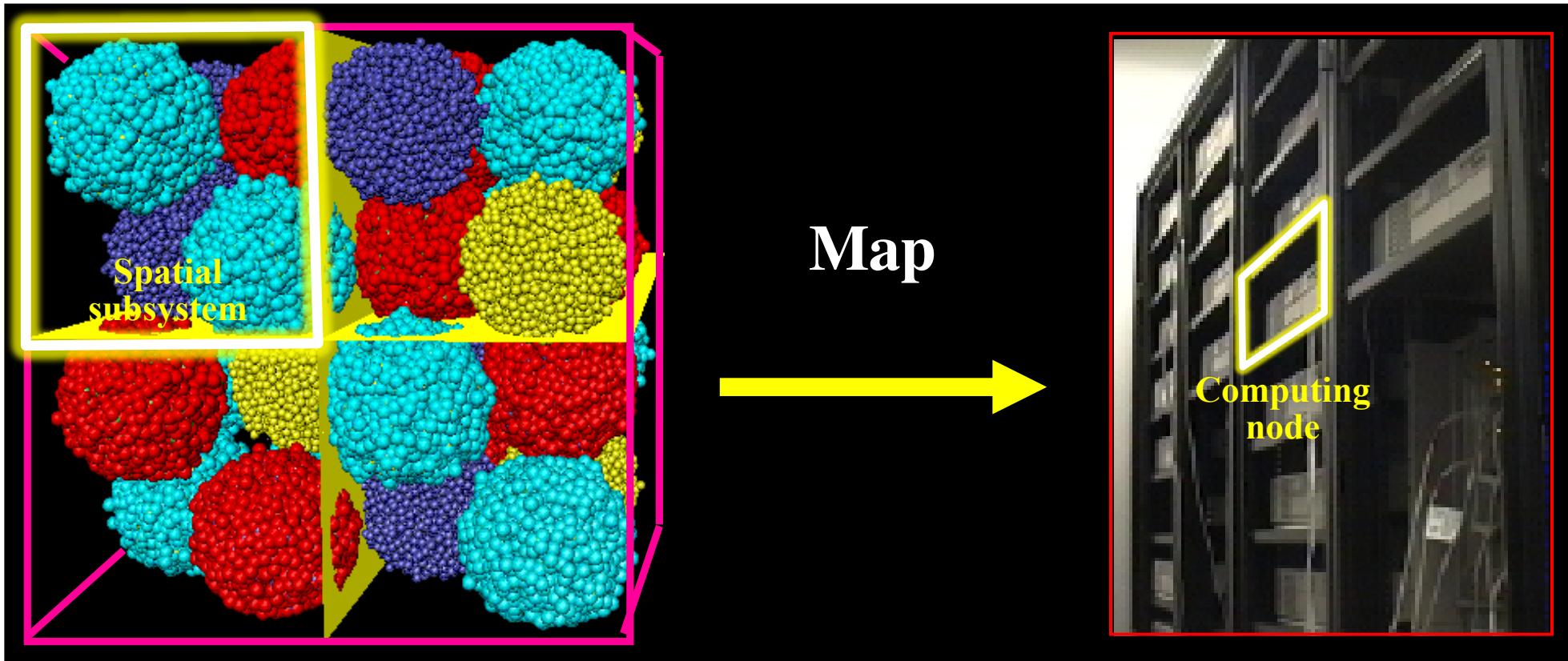
Parallel Molecular Dynamics

Spatial decomposition (short-ranged):

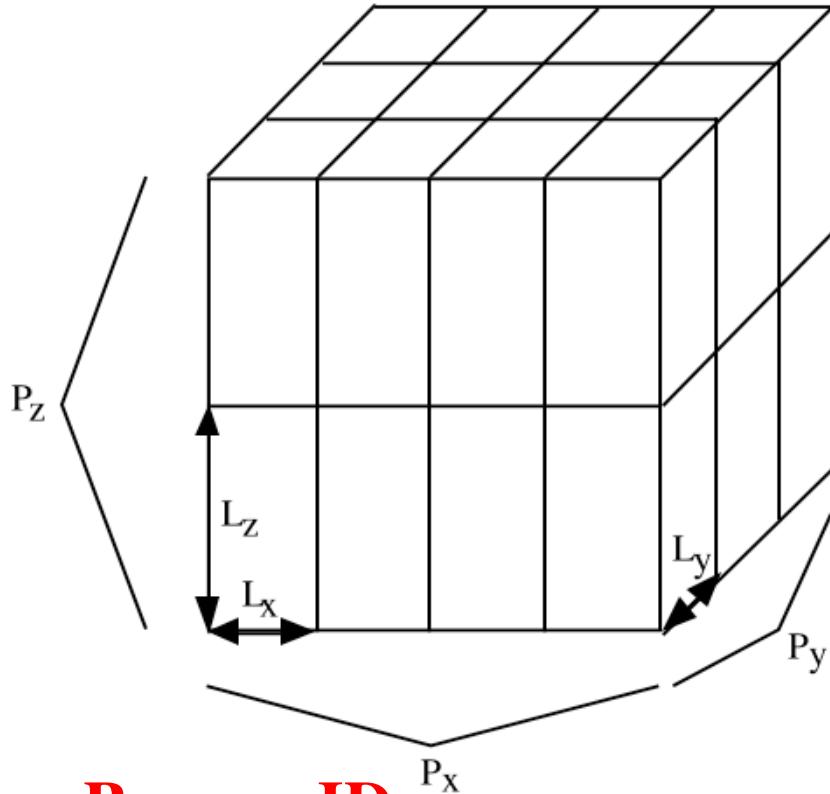
Will learn other decomposition schemes later:
<http://cacs.usc.edu/education/cs596/NT.pdf>

1. Divide the physical space into subspaces of equal volume
2. Assign each subspace to a computing node (more generally, to a process) in a parallel computer
3. Each node computes forces on the atoms in its subspace & updates their positions & velocities

Who does what



Spatial Decomposition



- Process ID P
- Vector*

$$p_x = p / (P_y P_z)$$

$$p_y = (p / P_z) \bmod P_y$$

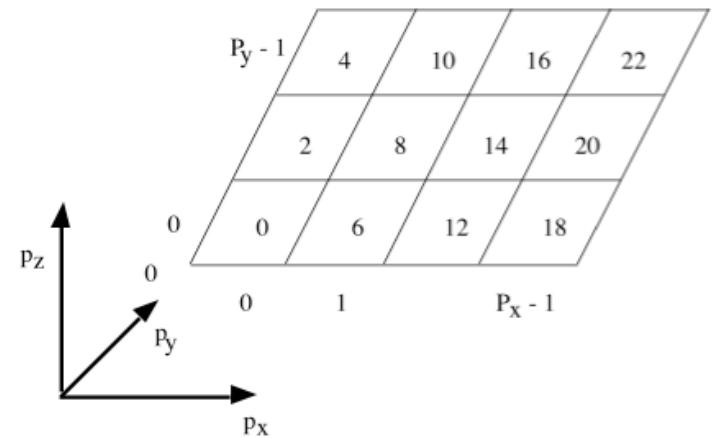
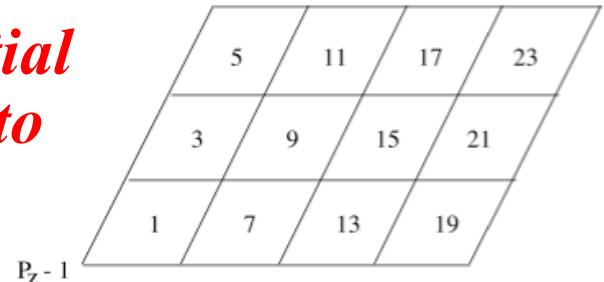
$$p_z = p \bmod P_z$$

Scalar

$$p = p_x \times P_y P_z + p_y \times P_z + p_z \quad \text{Rank}$$

Which 3D
subspace?

Map a spatial subsystem to a process!



$$\text{nproc} = \text{vproc}[0] \times \text{vproc}[1] \times \text{vproc}[2]$$

In **pmd.h** P_x P_y P_z

```
int vproc[3] = {1,1,2}, nproc = 2;
```

In **pmd.c**

```
rank
MPI_Comm_rank(MPI_COMM_WORLD, &sid);
vid[0] = sid/(vproc[1]*vproc[2]);
vid[1] = (sid/vproc[2])%vproc[1];
vid[2] = sid%vproc[2];
```

Neighbor Process ID

$$p'_{\alpha}(\kappa) = [p_{\alpha} + \delta_{\alpha}(\kappa) + P_{\alpha}] \bmod P_{\alpha} \quad (\kappa = 0, \dots, 5; \alpha = x, y, z) \quad \text{neighbor's vector}$$

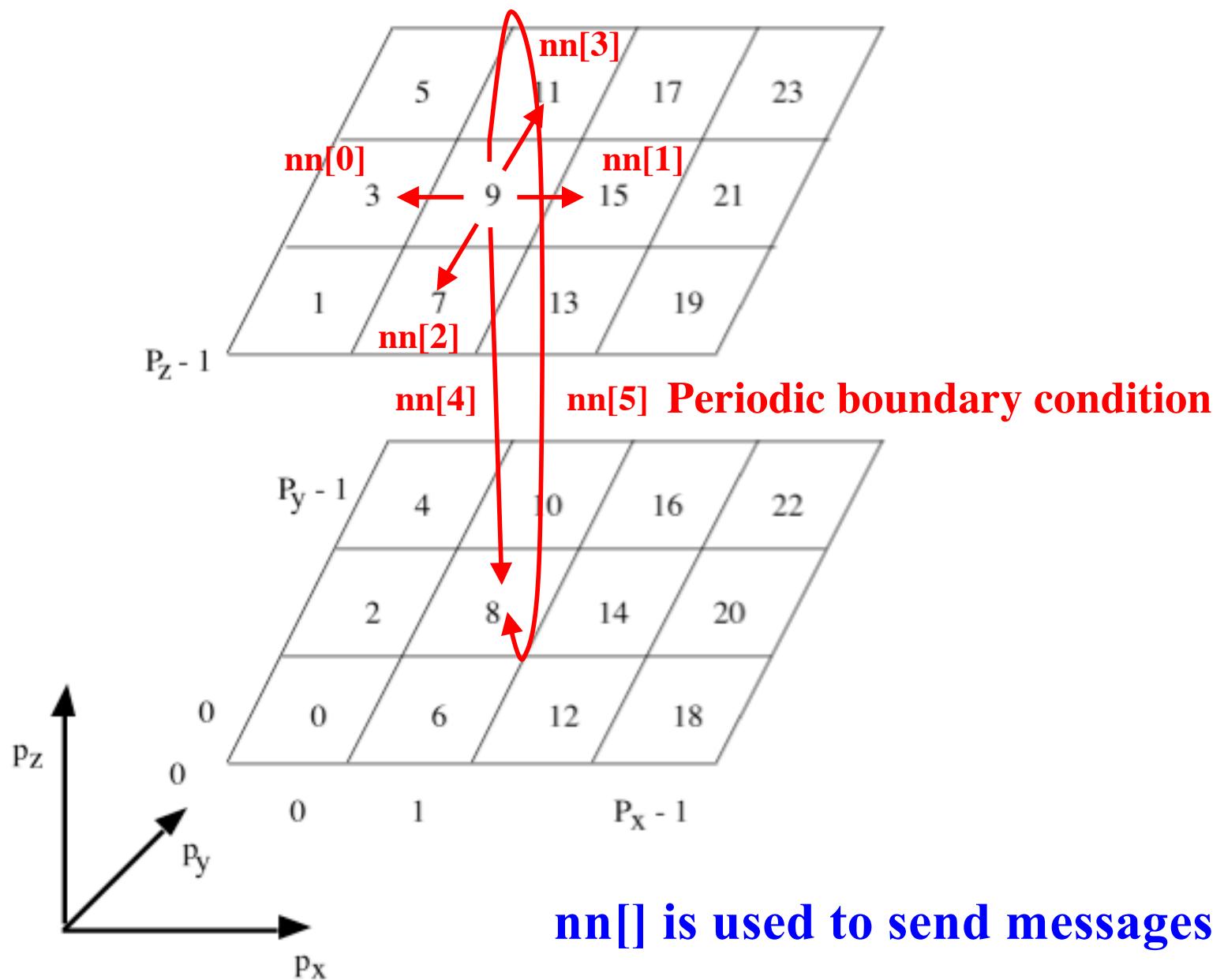
$$p'(\kappa) = p'_x(\kappa) \times P_y P_z + p'_y(\kappa) \times P_z + p'_z(\kappa) \quad \text{process ID}$$

Neighbor ID, κ	$\vec{\delta} = (\delta_x, \delta_y, \delta_z)$	$\vec{\Delta} = (\Delta_x, \Delta_y, \Delta_z)$
0 (east)	(-1, 0, 0)	($-L_x$, 0, 0)
1 (west)	(1, 0, 0)	(L_x , 0, 0)
2 (north)	(0, -1, 0)	(0, $-L_y$, 0)
3 (south)	(0, 1, 0)	(0, L_y , 0)
4 (up)	(0, 0, -1)	(0, 0, $-L_z$)
5 (down)	(0, 0, 1)	(0, 0, L_z)

- L_x , L_y & L_z are the box lengths *per process* in the x , y & z directions
 - Atom coordinates are in the range $[0, L_\alpha]$ ($\alpha = x, y, z$) in each process

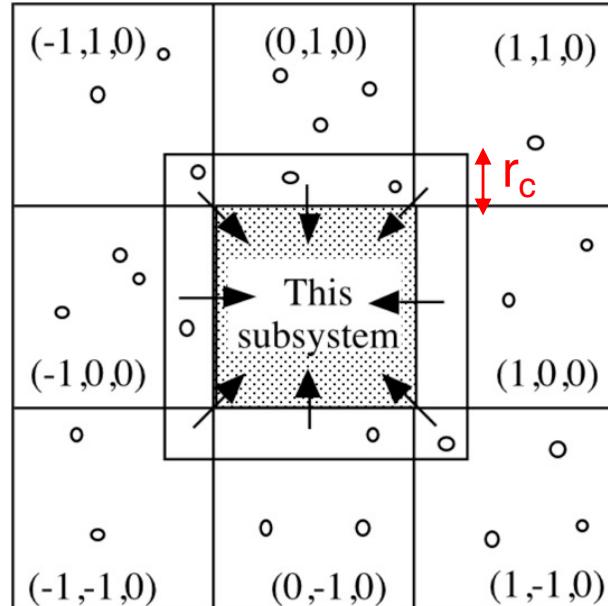
In pmd.c

Neighbor Process ID Example

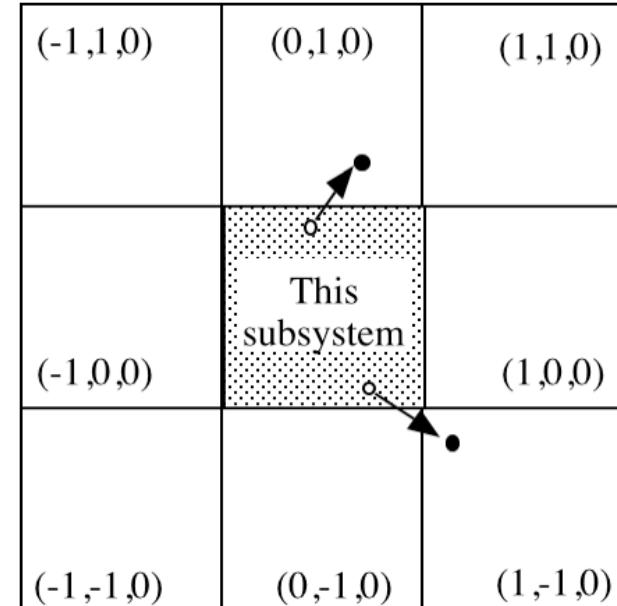


Parallel MD Concepts

Atom caching

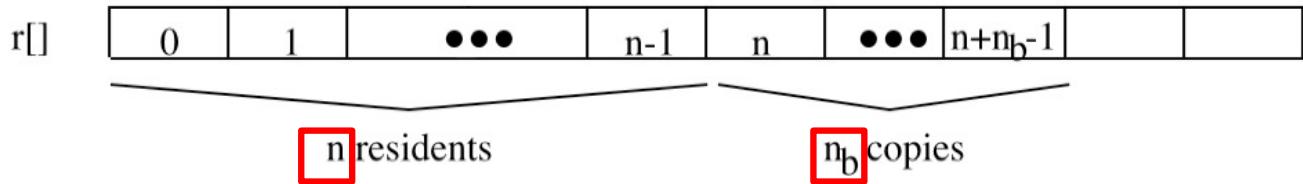


Atom migration



1. First half kick to obtain $v_i(t+Dt/2)$
2. Update atomic coordinates to obtain $r_i(t+Dt)$
3. `atom_move()`: Migrate the moved-out atoms to the neighbor processes
4. `atom_copy()`: Copy the surface atoms within distance r_c from the neighbors
5. `compute_accel()`: Compute new accelerations, $a_i(t+Dt)$, including the contributions from the cached atoms
6. Second half kick to obtain $v_i(t+Dt)$

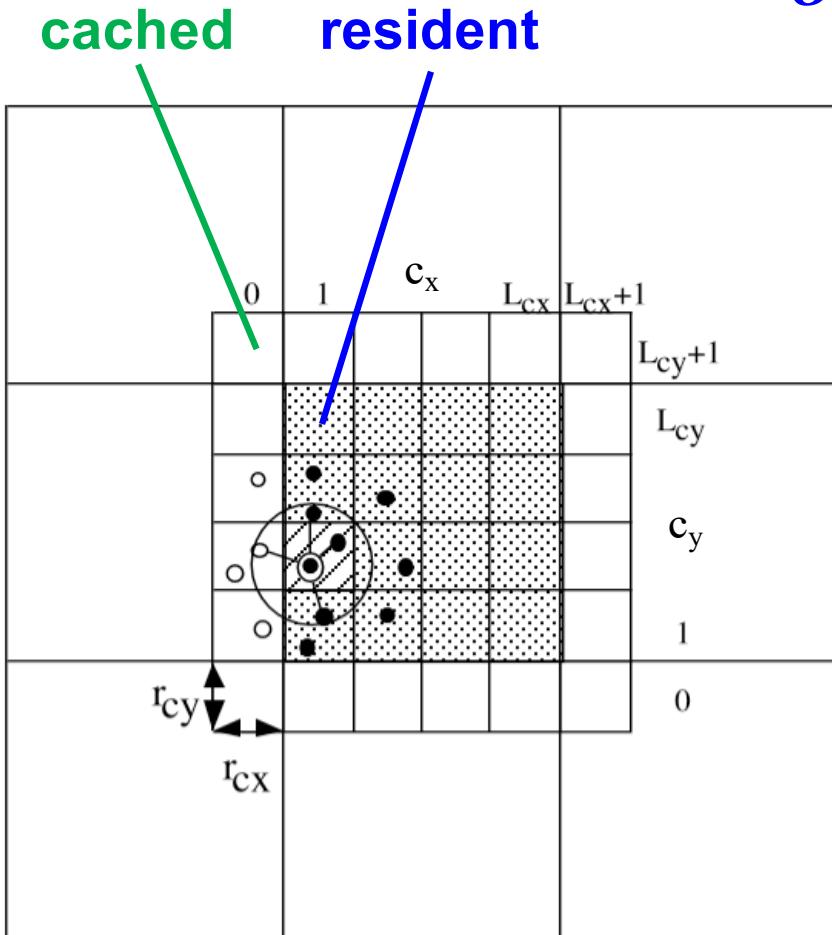
Data structure



Linked-List Cell Method

Search for pairs only within the nearest neighbor cells:

$$O(N^2) \rightarrow O(N)$$



- **Cell size**

$$L_{ca} = \lfloor L_\alpha / r_{ca} \rfloor$$
$$r_{ca} = L_\alpha / L_{ca} \quad (\alpha = x, y, z)$$

- **Cell index**

$$c = c_x(L_{cy}+2)(L_{cz}+2) + c_y(L_{cz}+2) + c_z$$

$$c_x = c / [(L_{cy}+2)(L_{cz}+2)]$$

$$c_y = [c / (L_{cz}+2)] \bmod (L_{cy}+2)$$

$$c_z = c \bmod (L_{cz}+2)$$

- **Atom → cell mapping**

$$c_\alpha = \lfloor (r_\alpha + r_{ca}) / r_{ca} \rfloor \quad (\alpha = x, y, z)$$

Only change from serial lmd.c in green:
Augmented cells to include cached atoms

List Construction Algorithm

```
/* Reset the headers, head */
for (c=0; c<lcxyz2; c++) head[c] = EMPTY;
/* Scan atoms to construct headers, head, & linked lists, lscl */
for (i=0; i<n+nb; i++) { Consider nb cached atoms
    /* Vector cell index to which this atom belongs */
    for (a=0; a<3; a++) mc[a] = (r[i][a]+rc[a])/rc[a]; Position offset by one cell
    /* Translate the vector cell index, mc, to a scalar cell index */
    c = mc[0]*lcyz2+mc[1]*lc2[2]+mc[2];
    /* Link to the previous occupant (or EMPTY if you're the 1st) */
    lscl[i] = head[c];
    /* The last one goes to the header */
    head[c] = i;
}
```

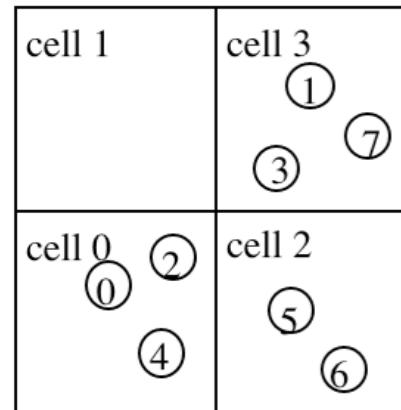
In the above:

$$\text{lcyz2} = \text{lc2}[1]*\text{lc2}[2]$$

where

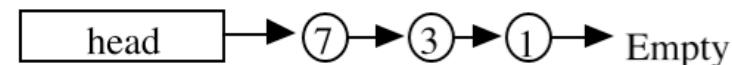
$$\text{lc2}[a] = \text{lc}[a]+2 \quad (a = 0, 1, 2)$$

$$\text{lcxyz2} = \text{lcyz2}*\text{lc2}[0]$$



head	0	1	2	3	4	5	6	7
lscl	E	E	0	1	2	E	5	3

Change from serial lmd.c in green



Interaction Computation

```

/* Scan inner cells (resident) */
for (mc[0]=1; mc[0]<=lc[0]; (mc[0])++)
for (mc[1]=1; mc[1]<=lc[1]; (mc[1])++)
for (mc[2]=1; mc[2]<=lc[2]; (mc[2])++) {
    /* Calculate a scalar cell index */
    c = mc[0]*lcyz2+mc[1]*lc2[2]+mc[2];
    /* Scan the neighbor cells (including itself) of cell c (resident + cached) */
    for (mc1[0]=mc[0]-1; mc1[0]<=mc[0]+1; (mc1[0])++)
    for (mc1[1]=mc[1]-1; mc1[1]<=mc[1]+1; (mc1[1])++)
    for (mc1[2]=mc[2]-1; mc1[2]<=mc[2]+1; (mc1[2])++) {
        /* Calculate the scalar cell index of the neighbor cell */
        c1 = mc1[0]*lcyz2+mc1[1]*lc2[2]+mc1[2];
        /* Scan atom i in cell c */
        i = head[c];
        while (i != EMPTY) {
            /* Scan atom j in cell c1 */
            j = head[c1];
            while (j != EMPTY) {
                ...
                if (i<j && rij<rc2) Process pair (i, j)
                ...
                j = lscl[j];
            }
            i = lscl[i];
        }
    }
}

```

Change from serial lmd.c in green

Who does what: Each rank computes forces on the **resident** atoms in its subspace & updates their positions & velocities

Resident atoms may interact with cached atoms (cf. slide 7)

cell 1	cell 3
0, 2, 4	1, 3, 7

cell 0	cell 2
0, 2, 4	5, 6

head	0	1	2	3
	4	E	6	7

lscl	0	1	2	3	4	5	6	7
	E	E	0	1	2	E	5	3

head → 7 → 3 → 1 → Empty

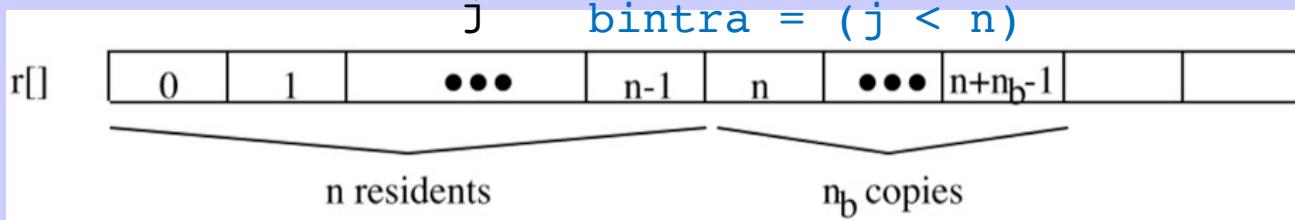
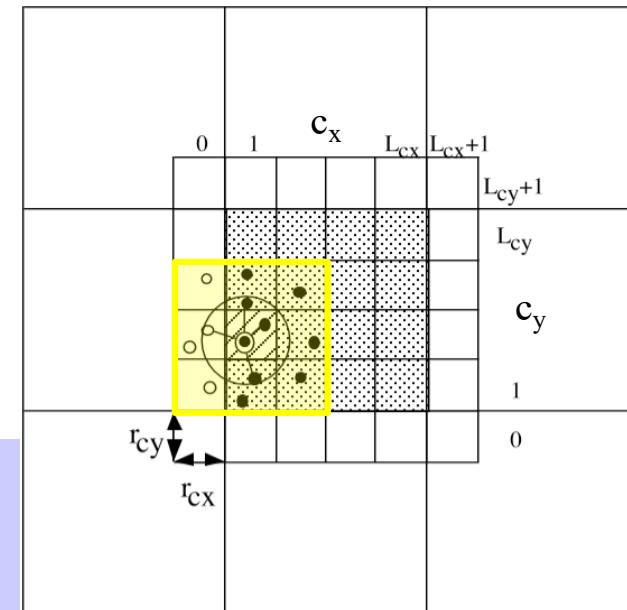
Parallel Interaction Computation

SPMD: Who does what?

Each process computes:

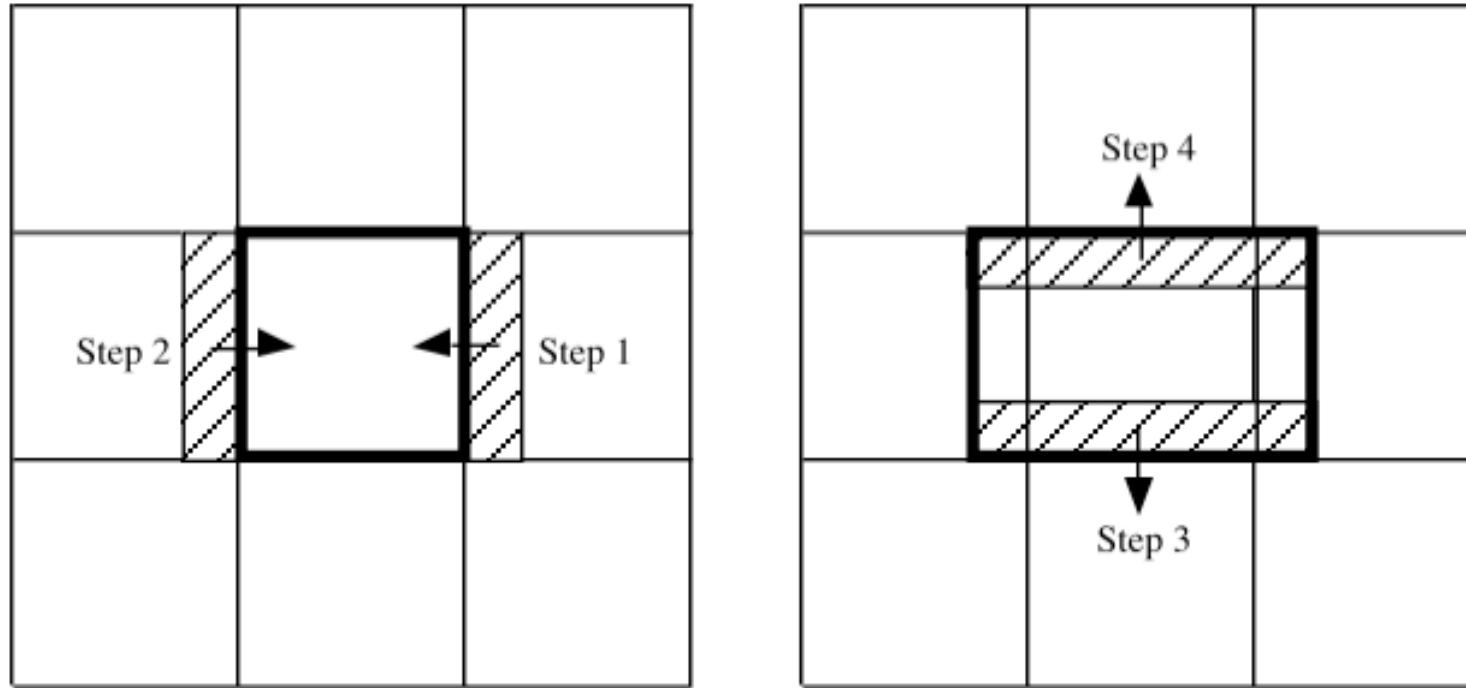
1. The forces on its resident atoms
2. The potential energy between resident pairs & 1/2 of that between resident-cached pairs

```
for resident cells, c {  
    for neighbor (resident or cached) cells, c1 {  
        scan atom i in cell c using c's linked list {  
            scan atom j in cell c1 using c1's linked list {  
                ...  
                if (i<j && rij<rc2) {  
                    compute pair force aij & potential u(rij)  
                    bintra = j < n; // j is resident?  
                    ai += aij; if (bintra) aj -= aij;  
                    if (bintra) lpe += u(rij); else lpe += u(rij)/2;  
                }  
            }  
        }  
    }  
}  
MPI_Allreduce(&lpe, &potEnergy,...,MPI_SUM,...);
```



Atom Caching: atom_copy()

Caching from 26 neighbors in 6 steps (by forwarding)



Reset the number of received cache atoms, nbnew = 0

for x, y, and z directions

Make boundary-atom lists, lsb, for lower and higher directions **including both resident, n, and cache, nbnew, atoms** (within r_c from boundary)

for lower and higher directions

Send/receive boundary-atom coordinates to/from the neighbor

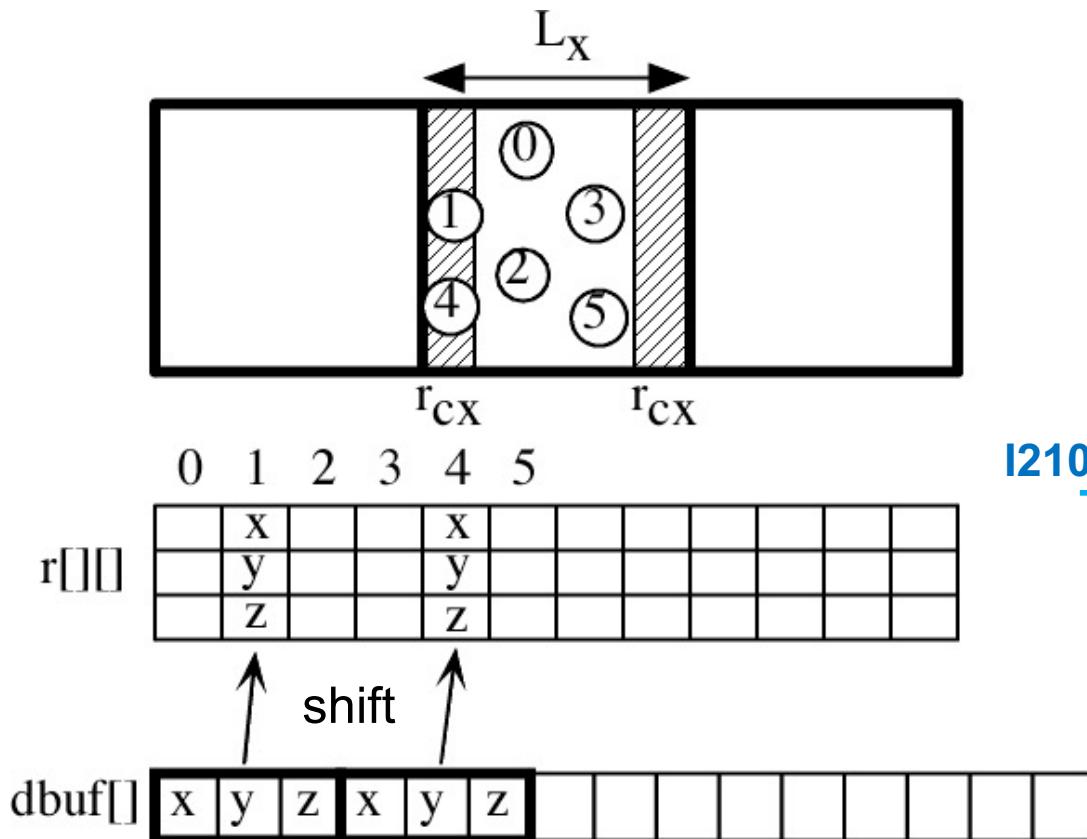
Increment nbnew;

endfor

endfor

nb = nbnew

Implementing Atom Caching



Copying condition

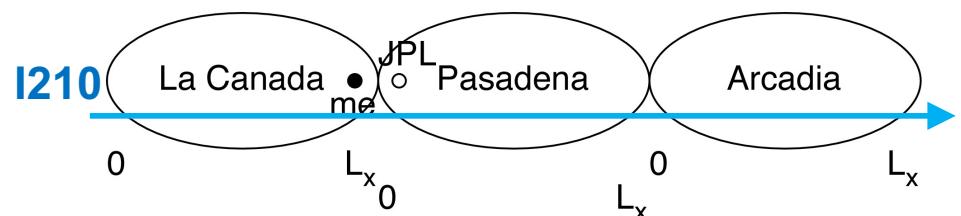
```
bbd(ri[],ku) {  
    kd = ku / 2 (= 0|1|2) x|y|z  
    kdd = ku % 2 (= 0|1) lower|higher  
    if (kdd == 0)  
        return ri[kd] < RCUT  
    else  
        return al[kd] - RCUT < ri[kd]  
}
```

3 phases of message passing

1. Message buffering: $dbuf \leftarrow r\text{-sv (shift)}$, gather
2. Message passing: $dbuf_{fr} \leftarrow dbuf$
Send dbuf
Receive dbufr
3. Message storing: $r \leftarrow dbufr$, append after the residents

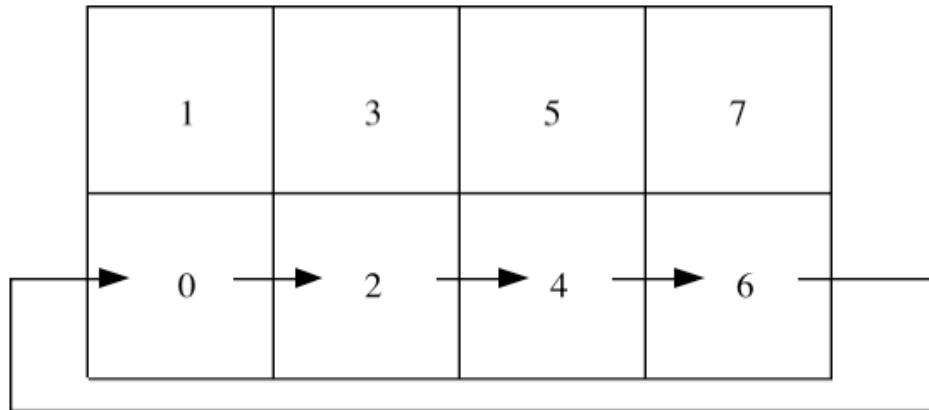
See `atom_copy()` in [pmd.c](#)

Self-centric coordinate systems

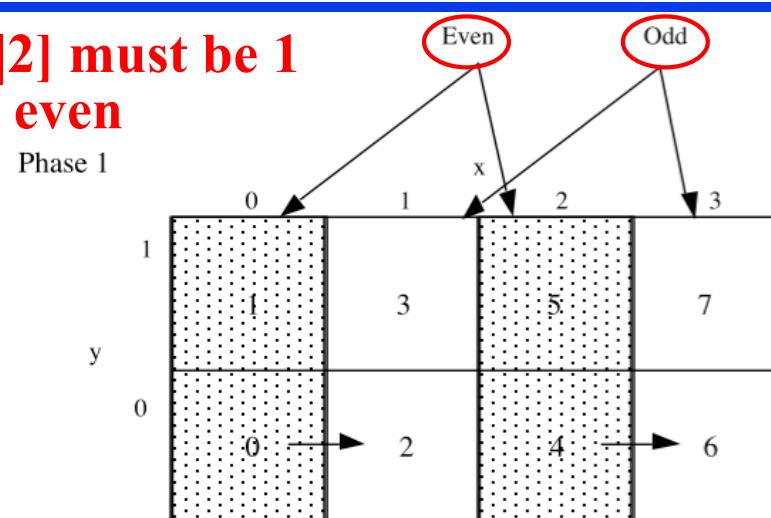


Deadlock Avoidance

Cyclic dependence



vproc[0|1|2] must be 1 or even



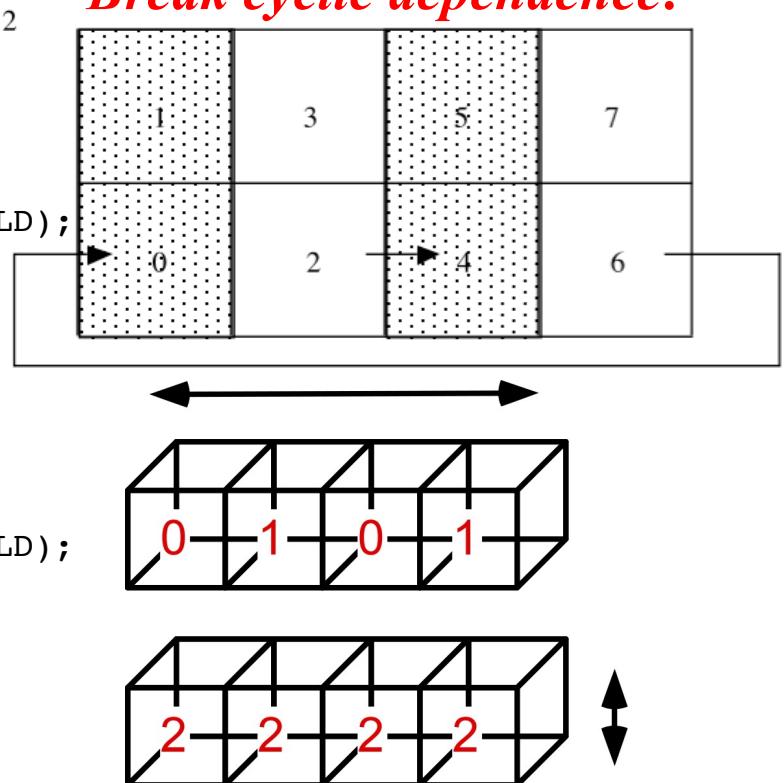
3-phase (deadlock-free) message passing

```

1. Message buffering: dbuf ← r, gather
2. Message passing: dbufr ← dbuf
/* Even node: send & recv, if not empty */
if (myparity[kd] == 0) {
    MPI_Send(dbuf, 3*nsd, MPI_DOUBLE, inode, 120, MPI_COMM_WORLD);
    MPI_Recv(dbufr, 3*nrc, MPI_DOUBLE, MPI_ANY_SOURCE, 120,
             MPI_COMM_WORLD, &status);
}
/* Odd node: recv & send, if not empty */
else if (myparity[kd] == 1) {
    MPI_Recv(dbufr, 3*nrc, MPI_DOUBLE, MPI_ANY_SOURCE, 120,
             MPI_COMM_WORLD, &status);
    MPI_Send(dbuf, 3*nsd, MPI_DOUBLE, inode, 120, MPI_COMM_WORLD);
}
/* Single layer: Exchange information with myself */
else
    for (i=0; i<3*nrc; i++) dbufr[i] = dbuf[i];
3. Message storing: r ← dbufr, append

```

Break cyclic dependence!



ANL IBM SP1 User's Guide ('94)

11. Q: My parallel program runs on other parallel machines but seems to deadlock on the SP-1 when using EUI, EUI-H, or Chameleon.

A: The following parallel program can deadlock on *any* system when the size of the message being sent is large enough:

```
send( to=partner, data, len, tag )
recv( from=partner, data, maxlen, tag )
```

where these are blocking send's and receives (`mp_bsенд` in EUI/EUI-H and `PIbsend` in Chameleon). For many systems, deadlock does not occur until the message is very long (often 128 KBytes or more). For EUI, the size is (roughly) 128 bytes (*not* KBytes) and for EUI-H, the size if (again roughly) 4 KBytes. The limit for Chameleon is the same as the underlying transport layer (i.e., the EUI or EUI-H limits).

To fix this you have several choices:

- pmd.c**
- Reorder your send and receive calls so that they are pair up. For example, if there are always an even number of processors, you could use

```
if (myid is even) {
    send( to=partner, data, len, tag )
    recv( from=partner, data, maxlen, tag )
}
else {
    recv( from=partner, data, maxlen, tag )
    send( to=partner, data, len, tag )
}
```

- assignment**
- Use non-blocking sends and receives instead



MPI_Irecv();
MPI_Send();
MPI_Wait();

Digress: Polyacetylene & Peierls Distortion

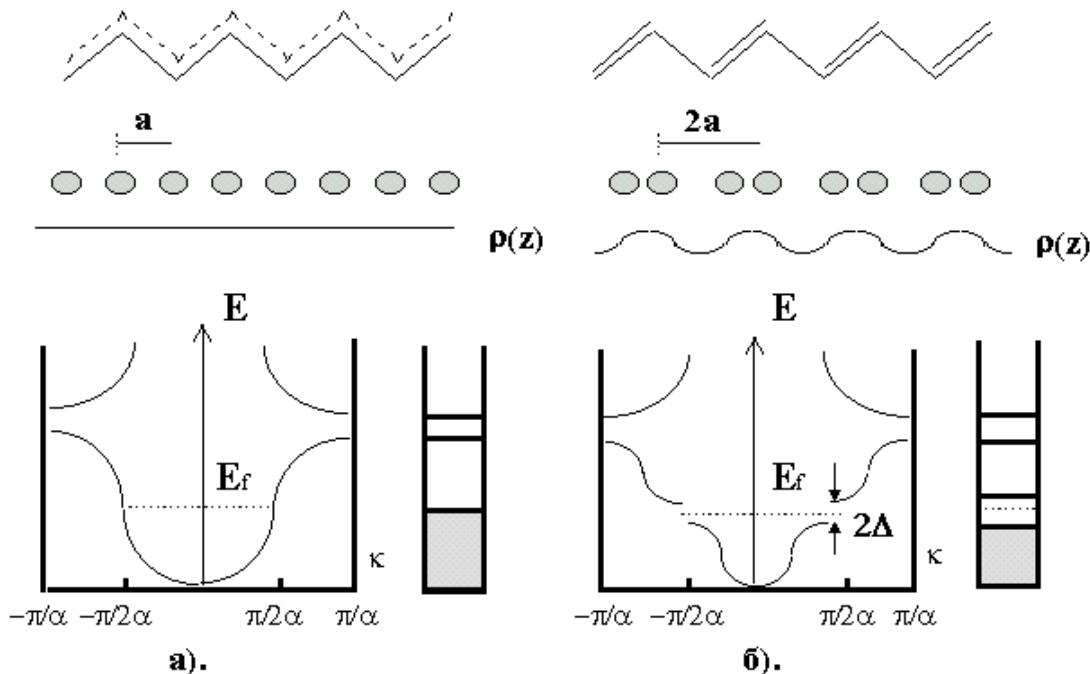


Fig. 1. Electron dispersion and a band pattern of one-dimensional molecular system:
a). metallic and b). insulator state, ($\rho(z)$)—a electronic density, a —a lattice period).



Alan J. Heeger
Prize share: 1/3

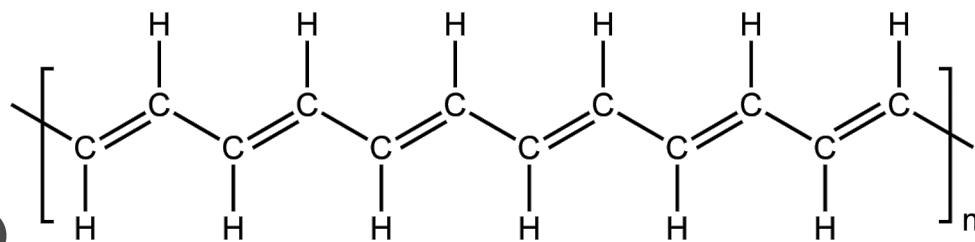
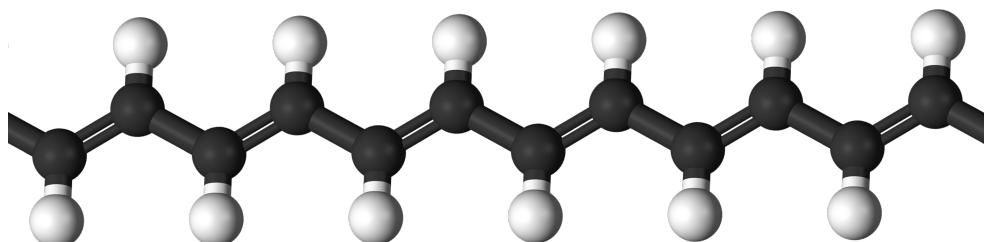


Alan G. MacDiarmid
Prize share: 1/3



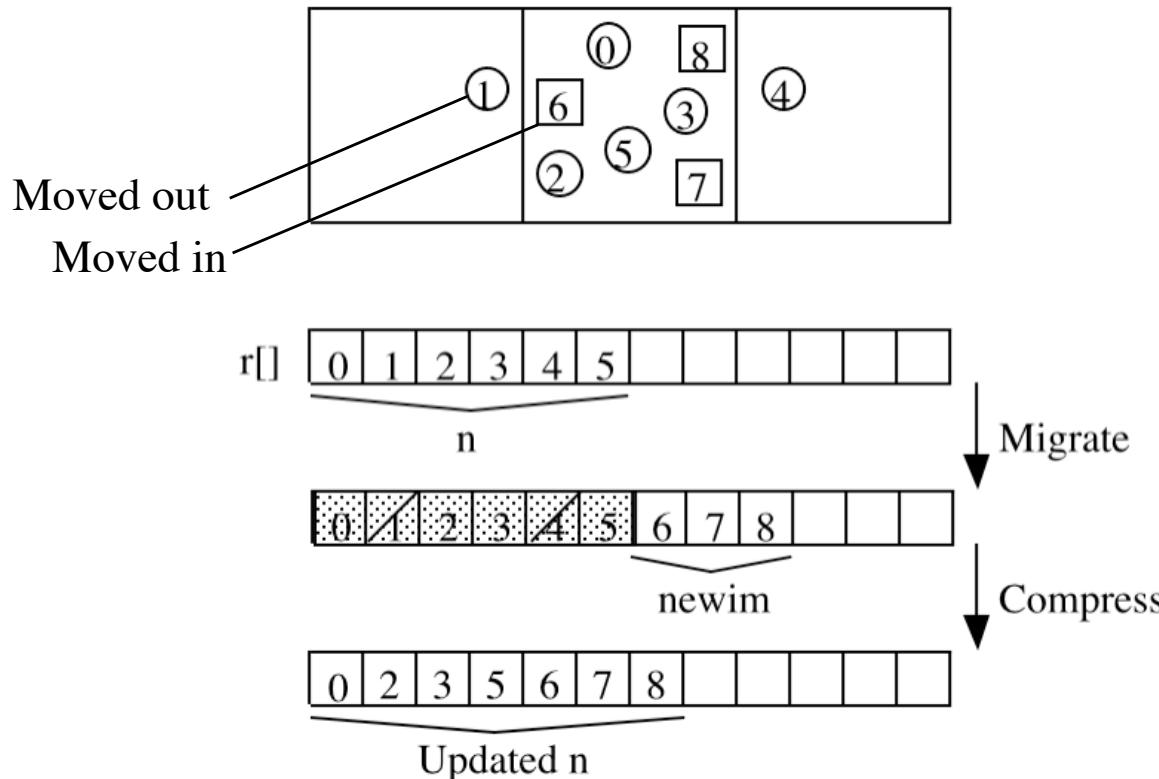
Hideki Shirakawa
Prize share: 1/3

The Nobel Prize in Chemistry 2000 was awarded jointly to Alan J. Heeger, Alan G. MacDiarmid and Hideki Shirakawa "for the discovery and development of conductive polymers".



Nature's spontaneous even-odd symmetry breaking

Atom Migration: atom_move()



Reset the number of received new immigrants, $newim = 0$

for x, y, and z directions

Make moving-atom lists, $mvque$, for lower and higher directions **including both resident, n , and immigrant, $newim$, atoms but excluding those already moved out for lower and higher directions**

Send/receive moving-atom coordinates to/from the neighbor

(When moving, $r[0] \leftarrow MOVED_OUT = -10^{10}$)

Increment $newim$

endfor

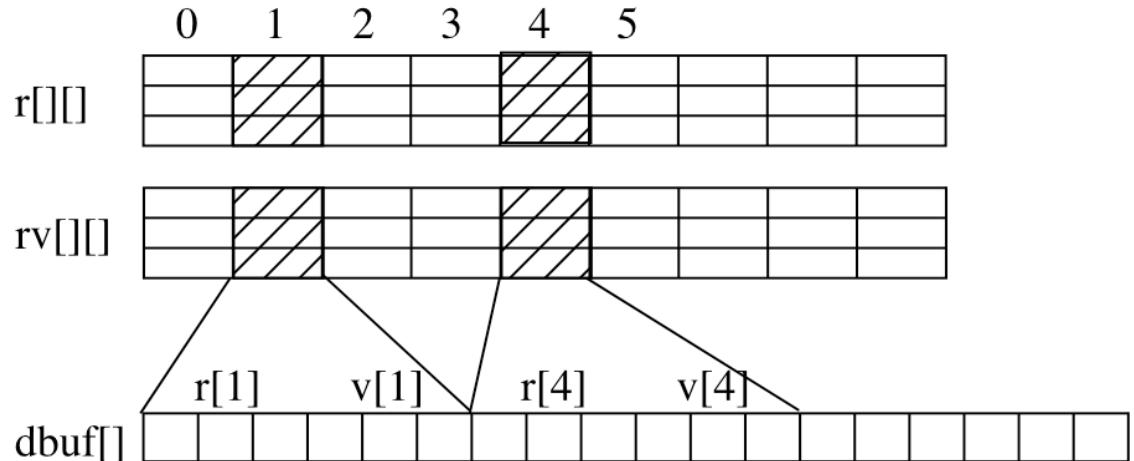
endfor

Compress the r array to eliminate the moved-out atoms

Implementing Atom Migration

Moving condition

```
bmv(ri[],ku) {  
    kd = ku / 2 (= 0|1|2)  
    kdd = ku % 2 (= 0|1)  
    if (kdd == 0)  
        return ri[kd] < 0.0  
    else  
        return al[kd] < ri[kd]  
}
```



3 phases of message passing

1. Message buffering: $\text{dbuf} \leftarrow \text{r-sv}$ (shift) & rv , gather
Mark **MOVED_OUT** in r
2. Message passing: $\text{dbufr} \leftarrow \text{dbuf}$
Send dbuf
Receive dbufr
3. Message storing: $\text{r} \& \text{rv} \leftarrow \text{dbufr}$, append after the residents

See `atom_move()` in [pmd.c](#)

Bottom Line: Parallel MD

Parallel computing:
Specifies who does what — decomposition

Parallel molecular dynamics (spatial decomposition):
Who does what = each processor computes forces on
only resident atoms in the subspace assigned to it &
updates their positions & velocities

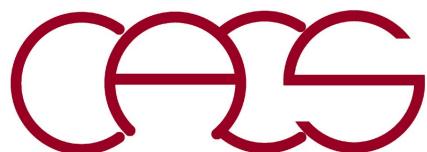
Scalability Metrics for Parallel Molecular Dynamics

Aiichiro Nakano

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Department of Physics & Astronomy
Department of Quantitative & Computational Biology
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Objective: Consolidate your understanding of scalability analysis
(e.g., fixed-problem vs. isogranular scaling) using a real-world
example of pmd.c



Recap: Parallel Efficiency

Parallel computing = solving a big problem (W) in a short time (T) using many processors (P)

- Execution time: $T(W,P)$
 W : Workload
 P : Number of processors

- Speed: $S(W,P) = \frac{W}{T(W,P)}$

- Speedup: $S_P = \frac{S(W_P,P)}{S(W_1,1)} = \frac{W_P T(W_1,1)}{W_1 T(W_P,P)}$

- Efficiency: $E_P = \frac{S_P}{P} = \frac{W_P T(W_1,1)}{P W_1 T(W_P,P)}$

How to scale W_P with P ?

Fixed Problem-Size (Strong) Scaling

Solve the same problem faster using more processors

$W_P = W$ —constant (strong scaling)

$$S_P = \frac{T(W,1)}{T(W,P)} \leq P$$

- **Speedup:** $S_P = \frac{W_P T(W_1,1)}{W_1 T(W_P,P)} = \frac{T(W,1)}{T(W,P)}$ $S_P = \frac{S(W_P,P)}{S(W_1,1)} = \frac{W_P T(W_1,1)}{W_1 T(W_P,P)}$
- **Efficiency:** $E_P = \frac{T(W,1)}{P T(W,P)}$ $E_P = \frac{S_P}{P} = \frac{W_P T(W_1,1)}{P W_1 T(W_P,P)}$
- **Amdahl's law:** f (= sequential fraction of the workload) limits the asymptotic speedup

$$\begin{aligned} T(W,P) &= f T(W,1) + \frac{(1-f) T(W,1)}{P} \\ \therefore S_P &= \frac{T(W,1)}{T(W,P)} = \frac{1}{f + (1-f)/P} \\ \therefore S_P &\rightarrow \frac{1}{f} \quad (P \rightarrow \infty) \end{aligned}$$

Isogranular (Weak) Scaling

Solve a larger problem within the same time duration using more processors

$$E_P = \frac{T(w,1)}{T(Pw,P)} \leq 1$$

$W_P = Pw$ (weak scaling)

w = constant workload per processor (granularity)

- **Speedup:** $S_P = \frac{S(P \bullet w, P)}{S(w, 1)} = \frac{P \bullet w / T(P \bullet w, P)}{w / T(w, 1)} = \frac{P \bullet T(w, 1)}{T(P \bullet w, P)}$

- **Efficiency:** $E_P = \frac{S_P}{P} = \frac{T(w, 1)}{T(P \bullet w, P)}$

$$S_P = \frac{S(W_P, P)}{S(W_1, 1)} = \frac{W_P T(W_1, 1)}{W_1 T(W_P, P)}$$

$$E_P = \frac{S_P}{P} = \frac{W_P T(W_1, 1)}{P W_1 T(W_P, P)}$$

Analysis of Parallel MD

- Parallel execution time:
Workload \propto Number of atoms, N (linked-list cell algorithm)

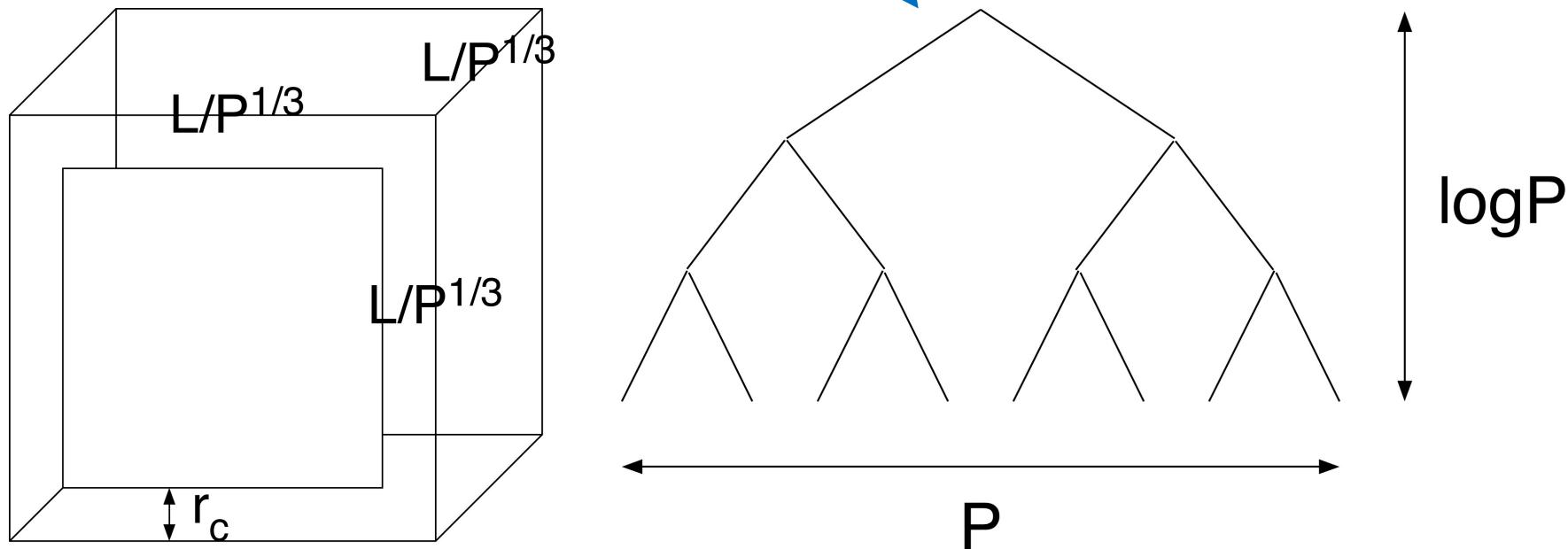
$$T(N, P) = T_{\text{comp}}(N, P) + T_{\text{comm}}(N, P) + T_{\text{global}}(P)$$

$$= a \frac{N}{P} + b \left(\frac{N}{P} \right)^{2/3} + c \log P$$

MPI_Allreduce()

facets $\hat{6}$ cached volume $\overbrace{\frac{L^2}{P^{2/3}} r_c}$ atom density $\hat{\rho}$
 $= 6r_c \frac{N^{2/3}/\rho^{2/3}}{P^{2/3}} \rho$
 $= 6r_c \rho^{1/3} \left(\frac{N}{P} \right)^{2/3}$

$$\left(\because \frac{N}{L^3} = \rho \Rightarrow L^2 = \frac{N^{2/3}}{\rho^{2/3}} \right)$$



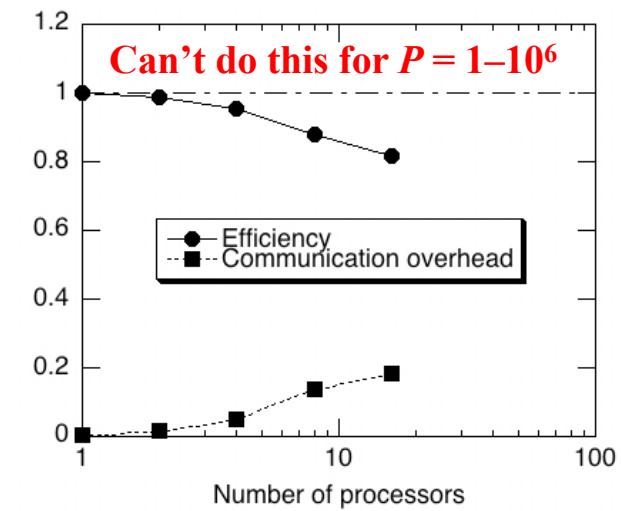
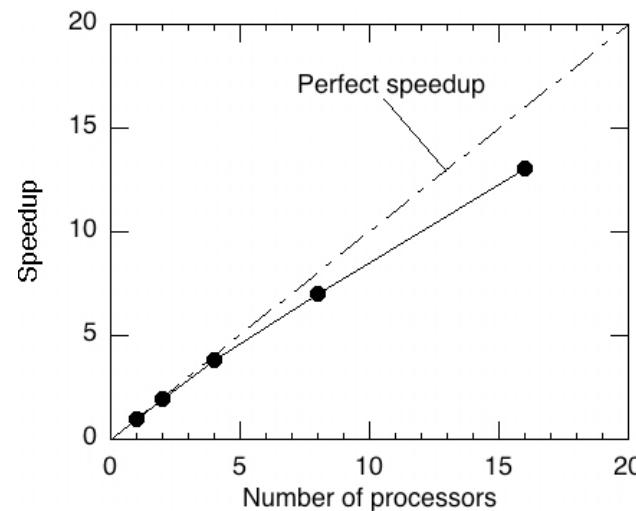
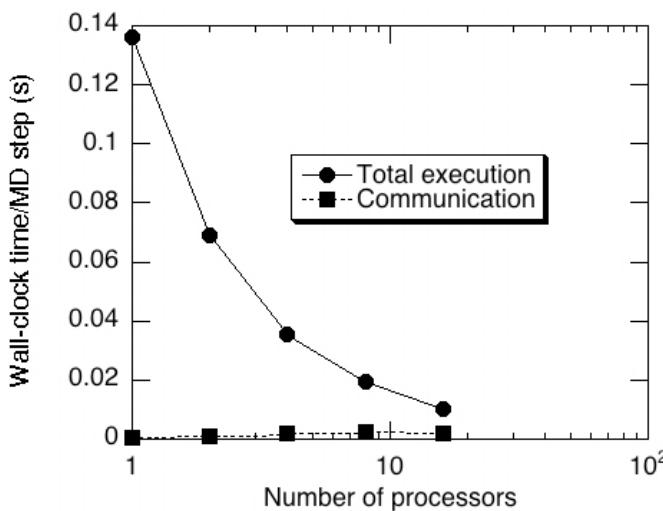
Fixed Problem-Size Scaling

- Speedup:

$$\begin{aligned} S_P &= \frac{T(N,1)}{T(N,P)} = \frac{aN}{aN/P + b(N/P)^{2/3} + c \log P} \\ &= \frac{P}{1 + \frac{b}{a} \left(\frac{P}{N} \right)^{1/3} + \frac{c}{a} \frac{P \log P}{N}} \end{aligned}$$

- Efficiency:

$$E_P = \frac{S_P}{P} = \frac{1}{1 + \frac{b}{a} \left(\frac{P}{N} \right)^{1/3} + \frac{c}{a} \frac{P \log P}{N}}$$

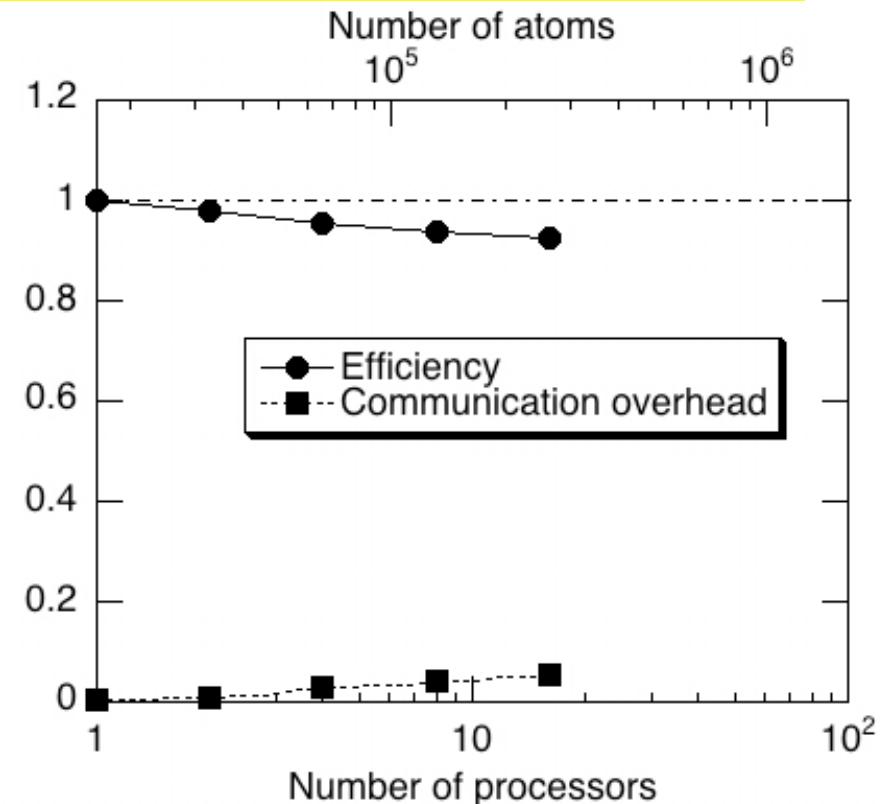
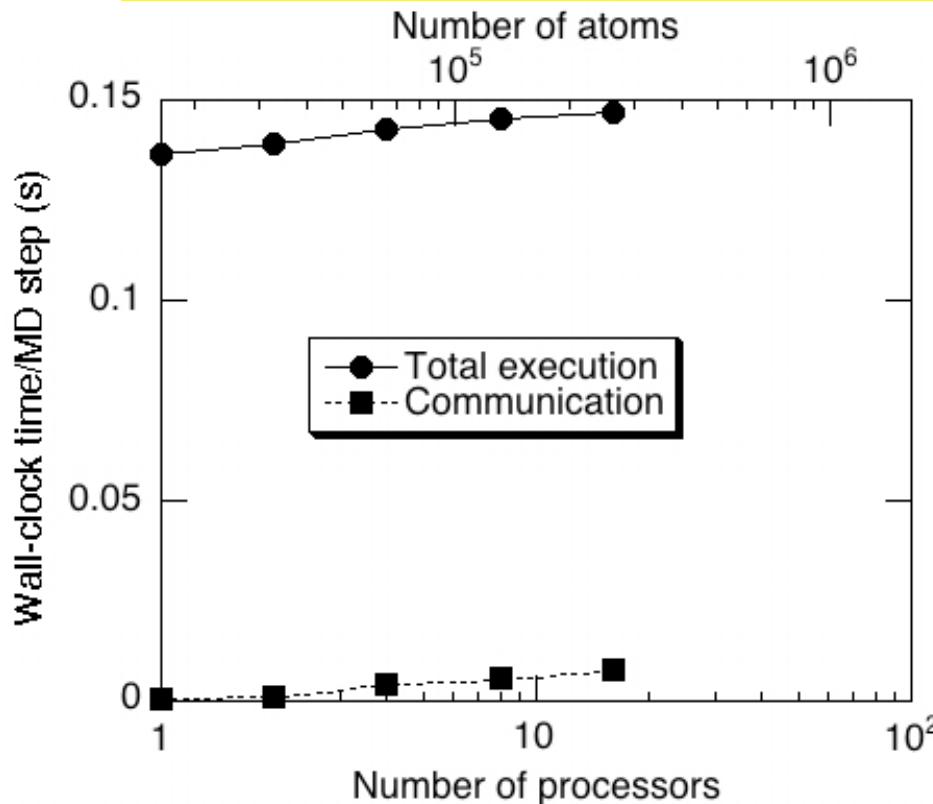


pmd.c: $N = 16,384$, on HPC (predecessor of CARC)

Isogranular Scaling of Parallel MD

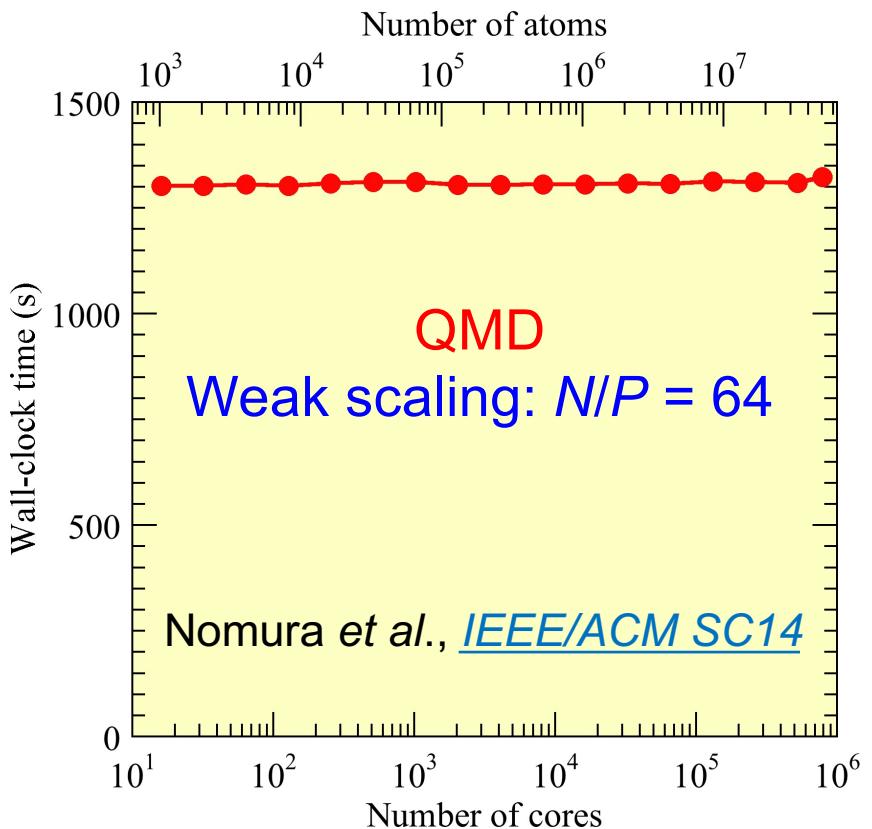
- $n = N/P = \text{constant}$: doable for arbitrarily large P
- Efficiency:

$$E_P = \frac{T(n,1)}{T(nP,P)} = \frac{an}{an + bn^{2/3} + c \log P} = \frac{1}{1 + \frac{b}{a} n^{-1/3} + \frac{c}{an} \log P}$$



pmd.c: $N/P = 16,384$, on HPC (predecessor of CARC)

High-End Parallel MD



- **4.9 trillion-atom space-time multiresolution MD (MRMD) of SiO₂**
- **8.5 billion-atom fast reactive force-field (F-ReaxFF) RMD of RDX**
- **39.8 trillion grid points (50.3 million-atom) DC-DFT QMD of SiC parallel efficiency 0.984 on 786,432 Blue Gene/Q cores**

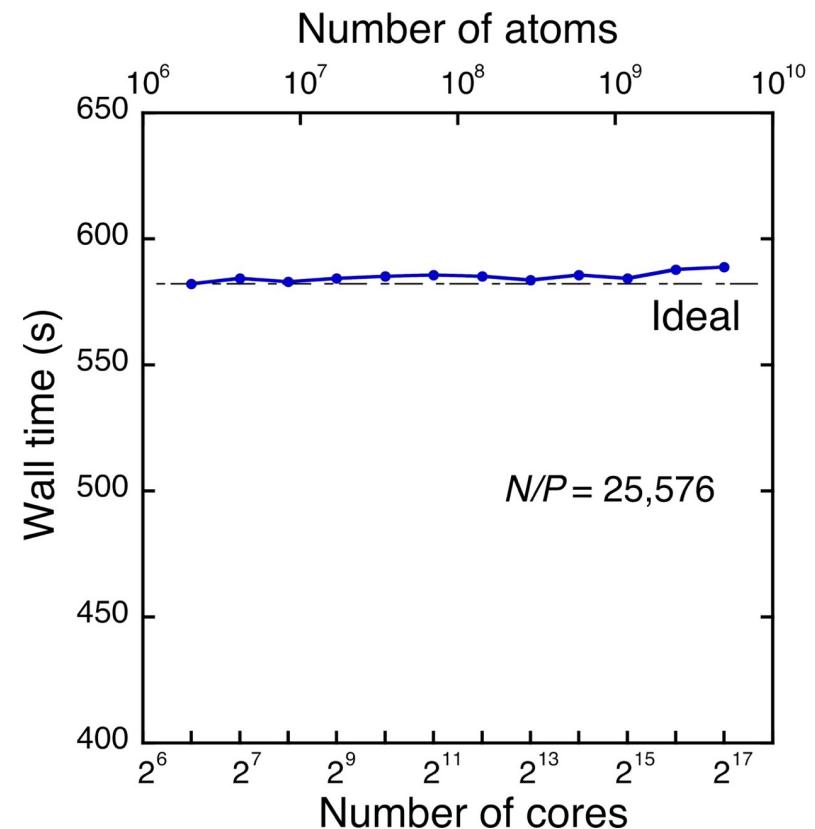
MD (molecular dynamics): MRMD

RMD (reactive molecular dynamics): F-ReaxFF

QMD (quantum molecular dynamics): DC-DFT

Portable Parallel Efficiency

- Weak-scaling parallel efficiency of 0.989 for a new generation of reactive molecular dynamics (RMD) on 131,072 Intel Knights Landing cores on Theta supercomputer at Argonne National Laboratory



K. Liu *et al.*, [Shift-collapse acceleration of generalized polarizable reactive molecular dynamics for machine learning-assisted computational synthesis of layered materials](#),
Proc. ScalA18 (IEEE, '18)

Quantum MD@Scale

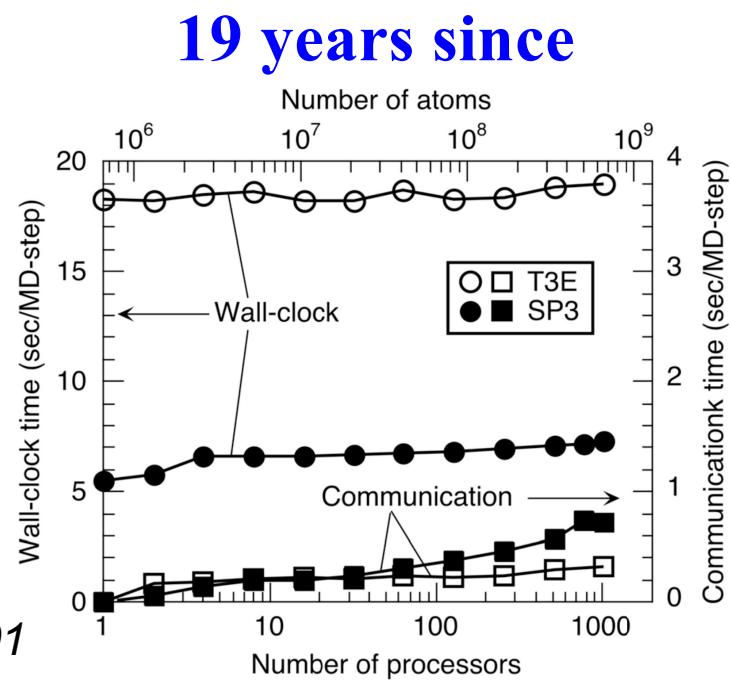
Quantum dynamics at scale: ultrafast control of emergent functional materials

S. C. Tiwari, P. Sakdhnagool, R. K. Kalia, A. Krishnamoorthy, M. Kunaseth,
A. Nakano, K. Nomura, P. Rajak, F. Shimojo, Y. Luo & P. Vashishta

Best Paper in *ACM HPC Asia 2020*

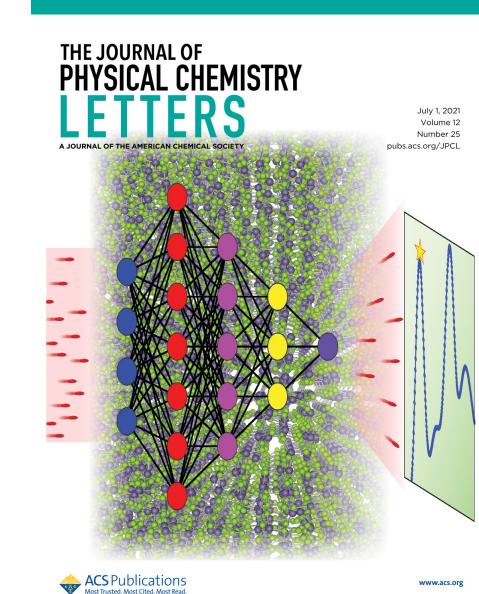
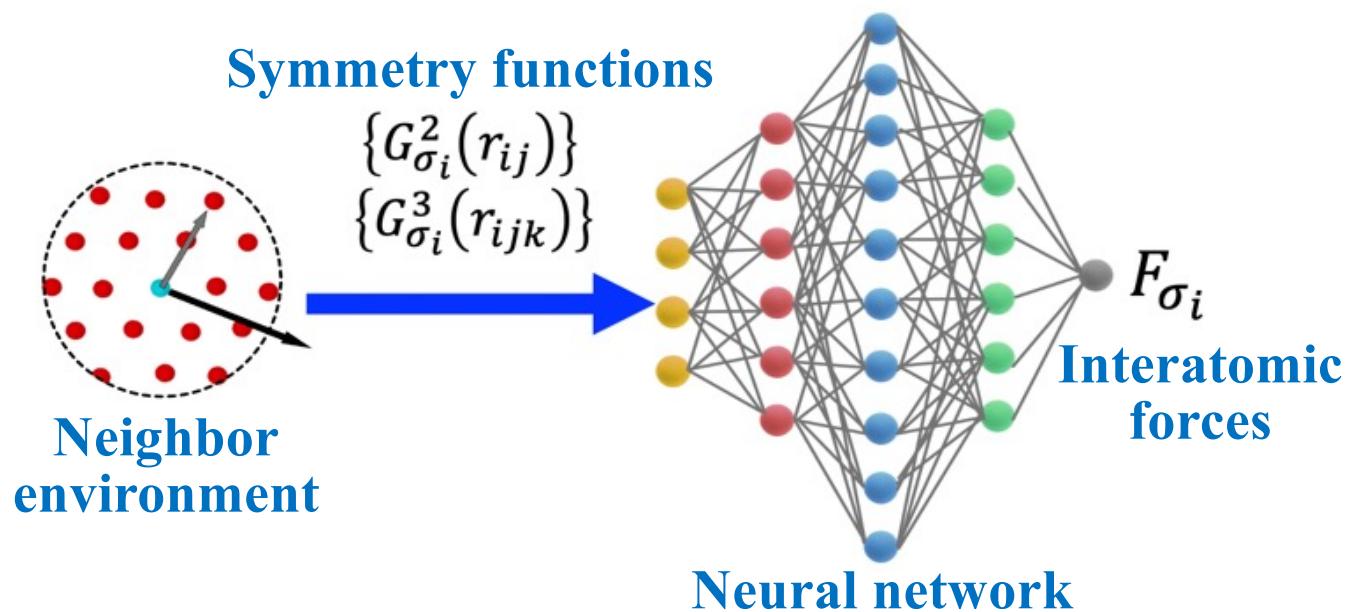


Scalable atomistic simulation algorithms
for materials research, A. Nakano *et al.*,
Best Paper, *IEEE/ACM Supercomputing 2001*, SC01



Neural MD@Scale

- Neural-network quantum molecular dynamics (NNQMD) could revolutionize atomistic modeling of materials, providing quantum-mechanical accuracy at a fraction of computational cost [*Phys. Rev. Lett.* **126**, 216403 ('21); *J. Phys. Chem. Lett.* **12**, 6020 ('21)]



Neural network molecular dynamics at scale & Ex-NNQMD: extreme-scale neural network quantum molecular dynamics,

P. Rajak *et al.*, *IEEE IPDPS ScaDL 20 & 21*

See also Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning

W. Jia *et al.*, *ACM/IEEE Supercomputing, SC20*

Fast, Robust & Scalable: Allegro-Legato

- **Allegro (fast) NNQMD:** State-of-the-art *accuracy & speed* founded on group-theoretical equivariance & local descriptors [Musaelian et al., *Nat. Commun.* **14**, 579 ('23)]
- **Fidelity-scaling problem:** On massively parallel computers, growing number of unphysical (adversarial) force predictions prohibits simulations involving larger numbers of atoms for longer times
- **Allegro-Legato (fast and “smooth”):** *Sharpness aware minimization (SAM)* enhances the *robustness* of Allegro through improved smoothness of loss landscape
 $w_* = \operatorname{argmin}_w [L(w) + \max_{\|\epsilon\|_2 \leq \rho} \{L(w + \epsilon) - L(w)\}]$ (L : loss; w : model parameters)
- **Elongated time-to-failure scaling, $t_{\text{failure}} = O(N^{-\beta})$,** without sacrificing accuracy or speed, thereby achieving spectroscopically stable long-time Hamiltonian trajectory

