

# Parallel Molecular Dynamics

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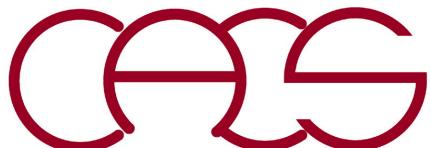
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Parallel-computing basics using MD as an example



# Parallel Computing

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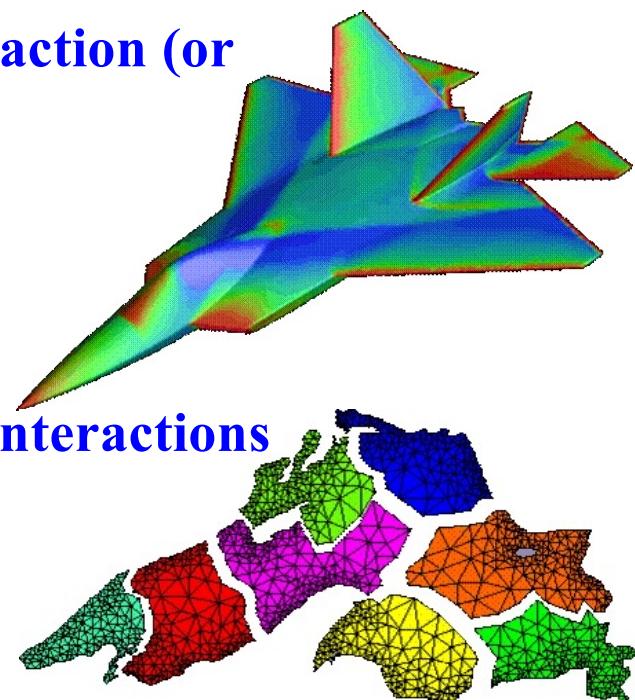
## Glossary

- **Parallel algorithm design = decomposition (who does what?)**
  - **Task:** Units of computation into which the main computation is subdivided
  - **Decomposition:** Dividing a computation into subsets of tasks that may be executed in parallel
- **Goal of parallel algorithm design = maximize concurrency & minimize task dependency/interaction**
  - **Concurrency:** The maximum number of tasks that can be executed simultaneously in parallel (limited by task dependency/interaction)
  - **Task dependency:** A task depends on another task, if the former uses data produced by the latter; represented by a directed acyclic graph called **task-dependency graph**
  - **Task interaction:** Tasks share inputs, outputs or intermediate data
- **Granularity:** Size of decomposed tasks: **fine-grained** = a large number of small tasks; **coarse-grained** = a small number of large tasks
- **Mapping:** Assign tasks (or processes = running programs to perform the tasks) to processors

A. Grama, A. Gupta, G. Karypis, & V. Kumar,  
*Introduction to Parallel Computing, 2nd Ed.* (Addison-Wesley, '03) Chap. 3

# Parallel Algorithm Design

- **Decomposition** (example: molecular dynamics)
  - Spatial decomposition ( $\approx$  domain decomposition)—coarse-grained
  - Particle decomposition—single-instruction multiple-data (SIMD) computers
  - Force decomposition—fine-grained
- **Maximal-concurrency algorithm:** Expose data locality in the problem (e.g., divide-&-conquer)
- **Scalability:** Achieve a large fraction of perfect speed-up (= number of processors) on a large number of processors
- **Load balancing:** Keep all processors equally busy
- **Optimization:** Optimal mapping to minimize task interaction (or communication between processes)
  - Owner-computes rule
  - Minimize the volume & frequency of data exchanges
  - Computation-communication overlapping
  - Data & computation replication
- **Issues:** Regular vs. irregular & static vs. dynamic task interactions



# Parallel Supercomputers

| Rank | System  | Cores      | Rmax<br>(PFlop/s) | Rpeak<br>(PFlop/s) | Power<br>(kW) |
|------|---|------------|-------------------|--------------------|---------------|
| 1    | <b>El Capitan</b> - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States  | 11,039,616 | 1,742.00          | 2,746.38           | 29,581        |
| 2    | <b>Frontier</b> - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE DOE/SC/Oak Ridge National Laboratory United States     | 9,066,176  | 1,353.00          | 2,055.72           | 24,607        |
| 3    | <b>Aurora</b> - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States | 9,264,128  | 1,012.00          | 1,980.01           | 38,698        |
| 4    | <b>JUPITER Booster</b> - BullSequana XH3000, GH Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, RedHat Enterprise Linux, EVIDEN EuroHPC/FZJ Germany       | 4,801,344  | 793.40            | 930.00             | 13,088        |
| 5    | <b>Eagle</b> - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States  | 2,073,600  | 561.20            | 846.84             |               |

Measured performance  
(in Pflop/s)

Theoretical performance

<http://www.top500.org> (June '25)

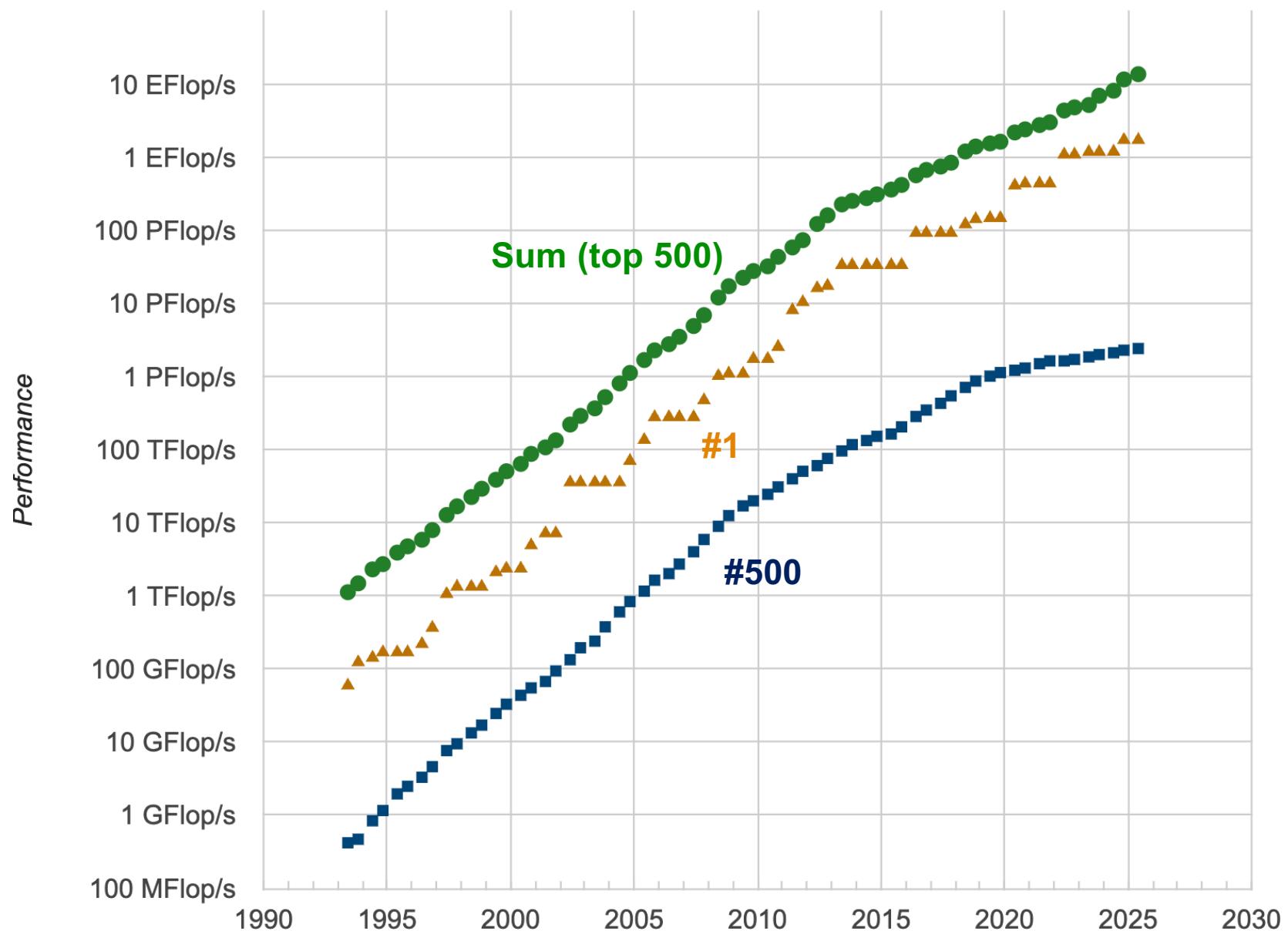
flop/s =  
floating-point  
operations/second

M (mega) =  $10^6$   
G (giga) =  $10^9$   
T (Tera) =  $10^{12}$   
P (Peta) =  $10^{15}$   
E (Exa) =  $10^{18}$   
Z (Zetta) =  $10^{21}$   
Y (Yotta) =  $10^{24}$



1.7 exaflop/s El Capitan

# Performance Development



# Message Passing Interface

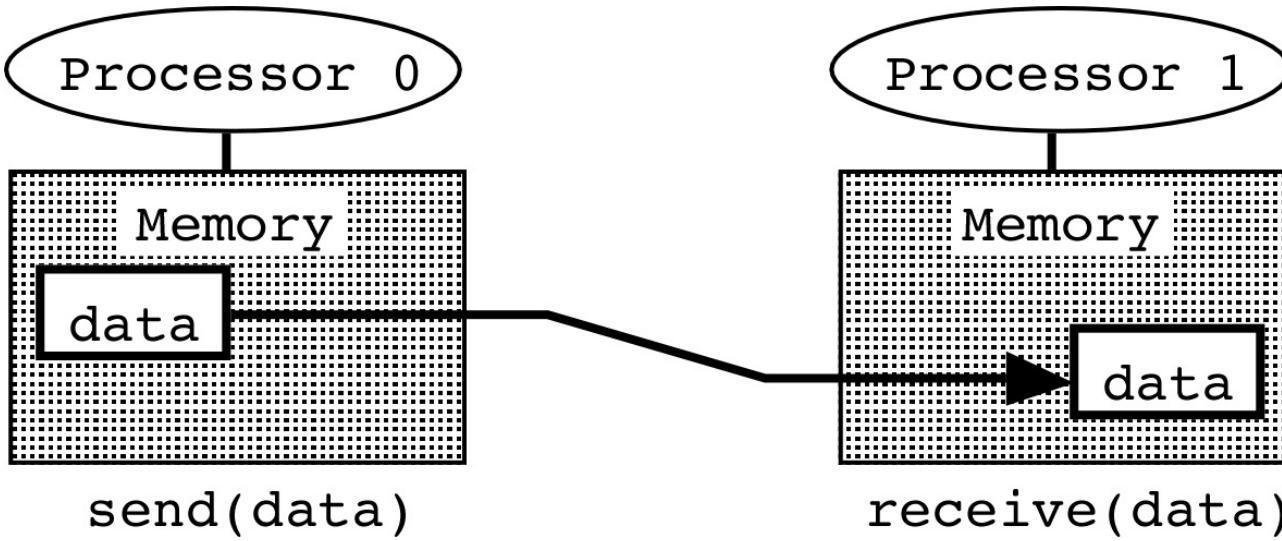
**MPI (Message Passing Interface): A standard message passing system that enables us to write & run applications on parallel computers (<http://www.mcs.anl.gov/mpi>).**

```
#include "mpi.h"
#include <stdio.h>
main(int argc, char *argv[ ]) {
    MPI_Status status;
    int myid;
    int n;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &myid);
    if (myid == 0) {
        n = 777;
        MPI_Send(&n, 1, MPI_INT, 1, 10, MPI_COMM_WORLD);
    } else {
        MPI_Recv(&n, 1, MPI_INT, 0, 10, MPI_COMM_WORLD, &status);
        printf("n = %d\n", n);
    }
    MPI_Finalize();
}
```

The diagram illustrates the MPI message exchange between two MPI ranks, P0 and P1. Rank P0 is shown at the top, and rank P1 is shown at the bottom. An arrow labeled "send to 1" points from P0 to P1, indicating the direction of the sent message. Another arrow labeled "recv from 0" points from P1 back to P0, indicating the direction of the received message. The MPI daemon is represented by an oval at the top, connected to both P0 and P1. The code annotations provide specific details about the MPI calls:

- MPI rank:** Points to the variable `&myid` in the `MPI_Comm_rank` call.
- Matching message labels:** Points to the argument `10` in the `MPI_Send` and `MPI_Recv` calls.
- Data triplet:** Points to the arguments `&n`, `1`, and `MPI_INT` in the `MPI_Send` call.
- To/from whom:** Points to the argument `1` in the `MPI_Send` call and the argument `0` in the `MPI_Recv` call.

# Single Program Multiple Data (SPMD)



## Process 0

```
if (myid == 0) {  
    n = 777;  
    MPI_Send(&n,...);  
}  
else {  
    MPI_Recv(&n,...);  
    printf(...);  
}
```

## Process 1

```
if (myid == 0) {  
    n = 777;  
    MPI_Send(&n,...);  
}  
else {  
    MPI_Recv(&n,...);  
    printf(...);  
}
```

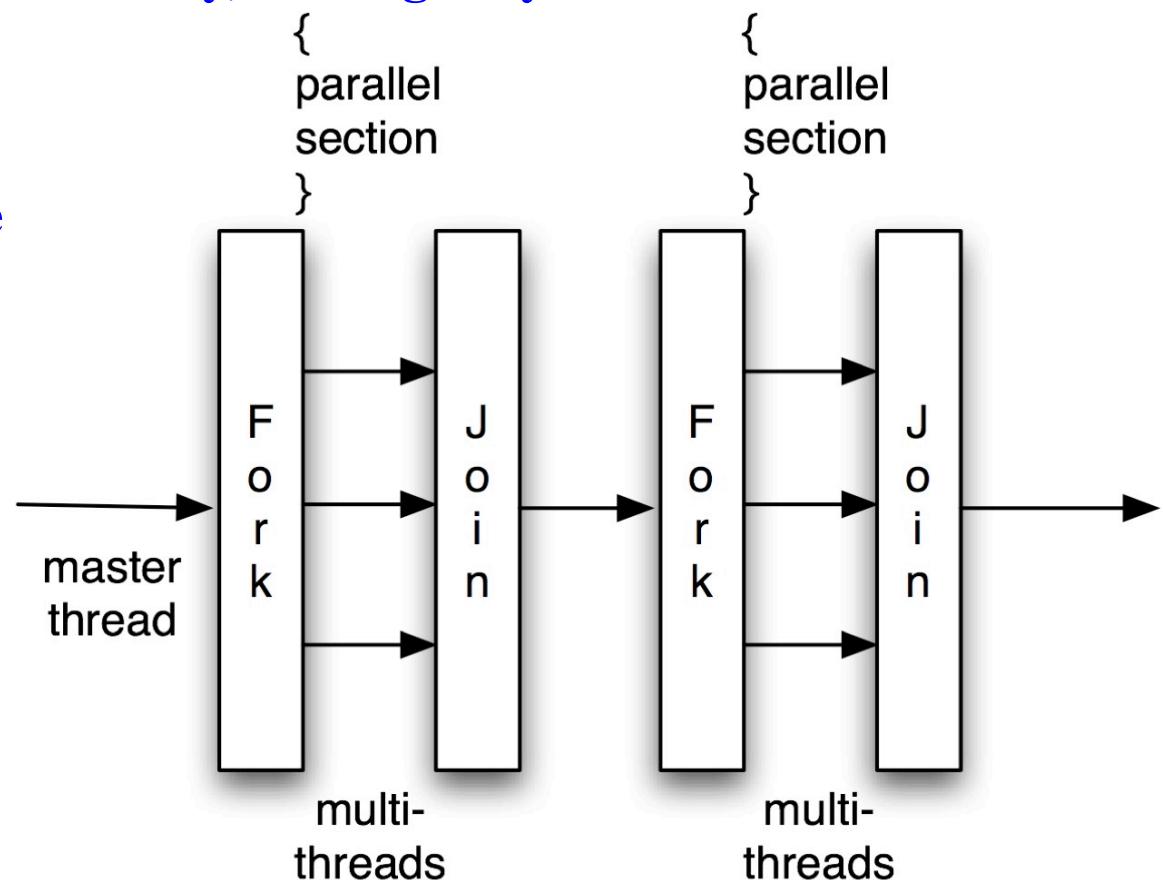
```
cSCI653_to_do()  
{  
    if (I == student)  
    {  
        do_assignment();  
        MPI_Send(...);  
    }  
    else if (I == teacher)  
    {  
        MPI_Recv(...);  
        grade();  
    }  
}
```

Parallel programming = choreography of “who does what”?

# OpenMP

- OpenMP (Open specifications for Multi Processing): Portable application program interface (API) for shared-memory parallel programming based on multi-threading by compiler directives (<http://www.openmp.org>)
- Fork-join parallelism:
  - > Fork: Master thread spawns a team of threads as needed
  - > Join: When the team of threads complete the statements in the parallel section, they terminate synchronously, leaving only the master thread
- OpenMP is typically used to parallelize loops
- OpenMP threads communicate by sharing variables

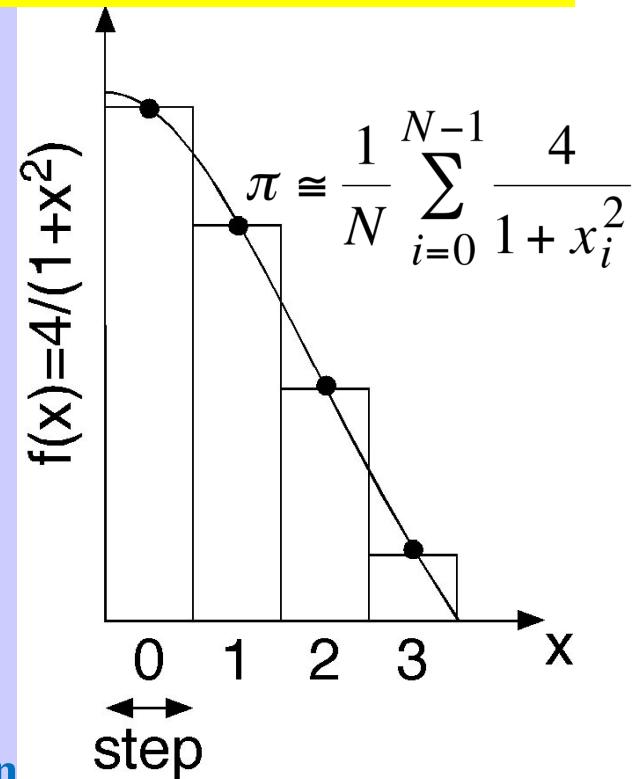
On Discovery, compile as  
> cc ... -fopenmp  
> mpicc ... -fopenmp



# OpenMP Programming

```
#include <stdio.h>
#include <omp.h>
#define NBIN 100000
#define MAX_THREADS 8
void main() {
    int nthreads,tid;
    double step,sum[MAX_THREADS]={0.0},pi=0.0;
    step = 1.0/NBIN;
#pragma omp parallel private(tid)
{
    int i;
    double x;
    nthreads = omp_get_num_threads();
    tid = omp_get_thread_num();
    for (i=tid; i<NBIN; i+=nthreads) {
        x = (i+0.5)*step;
        sum[tid] += 4.0/(1.0+x*x);}
    } data privatization to avoid race condition
    for(tid=0; tid<nthreads; tid++) pi += sum[tid]*step;
    printf("PI = %f\n",pi);
}
```

Array of partial sums  
for multi-threads



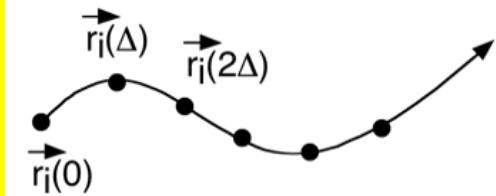
parallel section

- Obtain the number of threads & my thread ID
- By default, all variables are shared unless selectively changing storage attributes using private clauses

# Molecular Dynamics Algorithm

## Time discretization

$$\begin{cases} \vec{r}_i(t + \Delta) = \vec{r}_i(t) + \vec{v}_i(t)\Delta + \frac{1}{2}\vec{a}_i(t)\Delta^2 \\ \vec{v}_i(t + \Delta) = \vec{v}_i(t) + \frac{\vec{a}_i(t) + \vec{a}_i(t + \Delta)}{2}\Delta \end{cases} \quad \vec{a}_i = -\frac{1}{m}\frac{\partial V}{\partial \vec{r}_i}$$



## Time stepping: Velocity Verlet algorithm

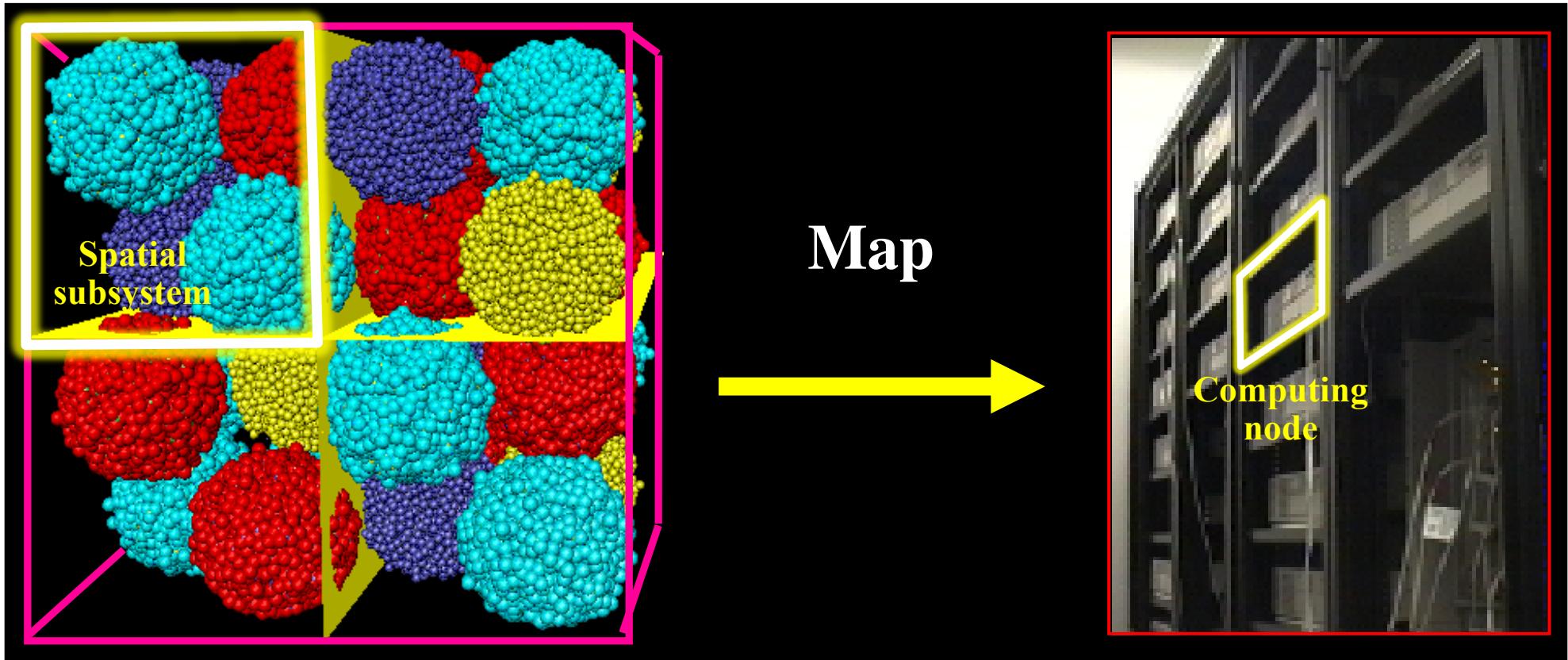
Given  $(\vec{r}_i(t), \vec{v}_i(t))$ ,

1. (Compute  $\vec{a}_i(t)$  as a function of  $\{\vec{r}_i(t)\}$ )
2.  $\vec{v}_i\left(t + \frac{\Delta}{2}\right) \leftarrow \vec{v}_i(t) + \frac{\Delta}{2}\vec{a}_i(t)$
3.  $\vec{r}_i(t + \Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i\left(t + \frac{\Delta}{2}\right)\Delta$
4. Compute  $\vec{a}_i(t + \Delta)$  as a function of  $\{\vec{r}_i(t + \Delta)\}$
5.  $\vec{v}_i(t + \Delta) \leftarrow \vec{v}_i\left(t + \frac{\Delta}{2}\right) + \frac{\Delta}{2}\vec{a}_i(t + \Delta)$

# Parallel Molecular Dynamics

Spatial decomposition (short ranged):

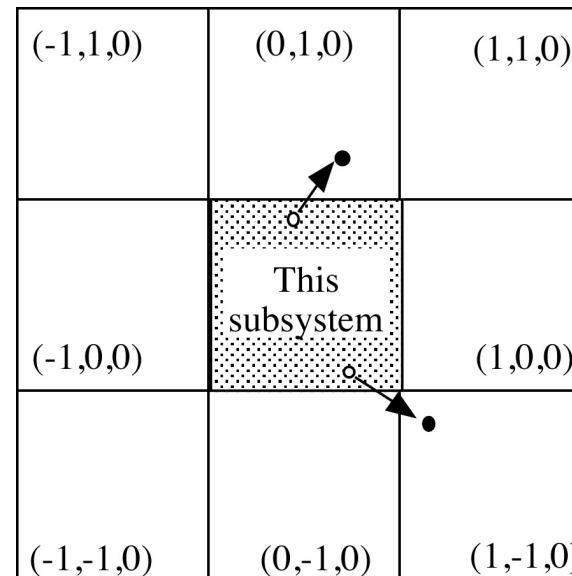
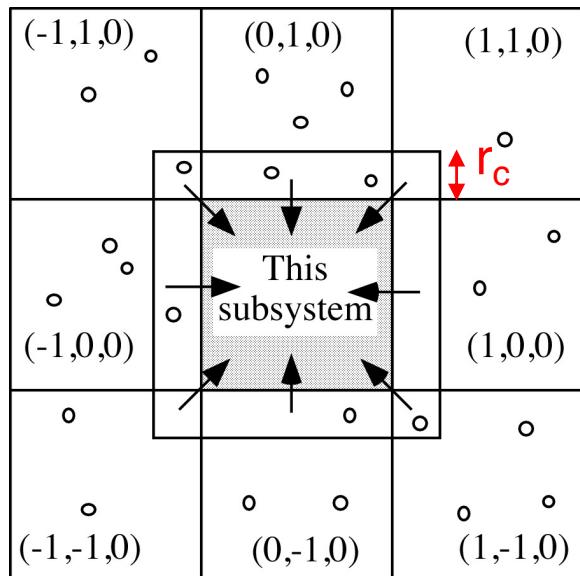
1. Divide the physical space into subspaces of equal volume
  2. Assign each subspace to a compute node (more generally, to a process) in a parallel computer
  3. Each node computes forces on the atoms in its subspace & updates their positions & velocities
- Who does what  
or MPI rank



# Parallel MD Algorithm

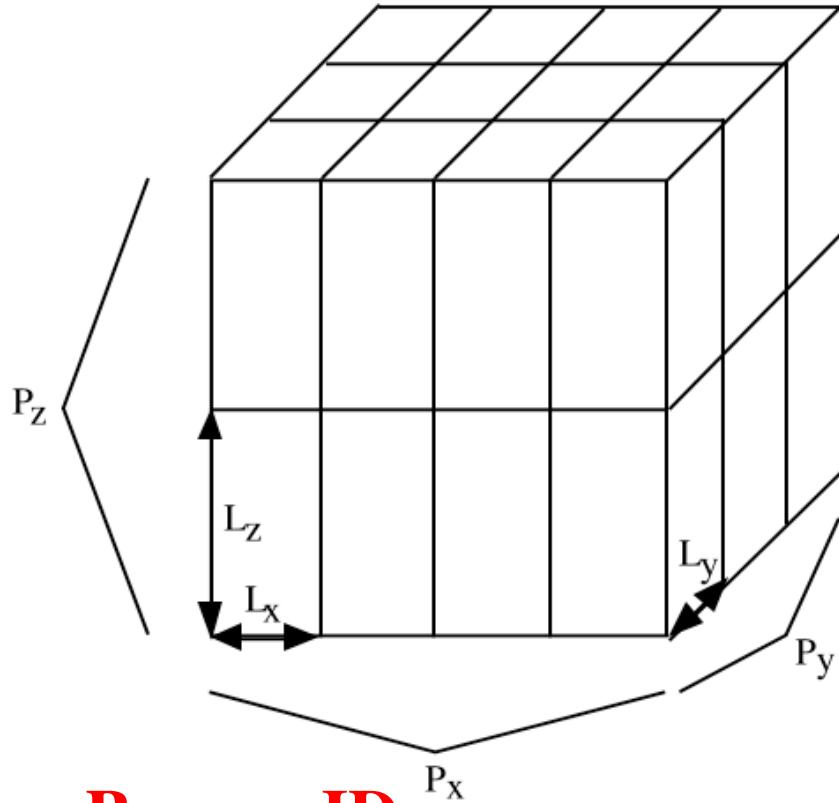
1.  $\vec{v}_i\left(t + \frac{\Delta}{2}\right) \leftarrow \vec{v}_i(t) + \frac{\Delta}{2} \vec{a}_i(t)$
2.  $\vec{r}_i(t + \Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i\left(t + \frac{\Delta}{2}\right) \Delta$
3. `atom_move()` // migrate moved-out atoms
4. `atom_copy()` // cache surface atoms
5. Compute  $\vec{a}_i(t + \Delta)$  as a function of  $\{\vec{r}_i(t + \Delta)\}$
6.  $\vec{v}_i(t + \Delta) \leftarrow \vec{v}_i\left(t + \frac{\Delta}{2}\right) + \frac{\Delta}{2} \vec{a}_i(t + \Delta)$

**atom\_copy()**

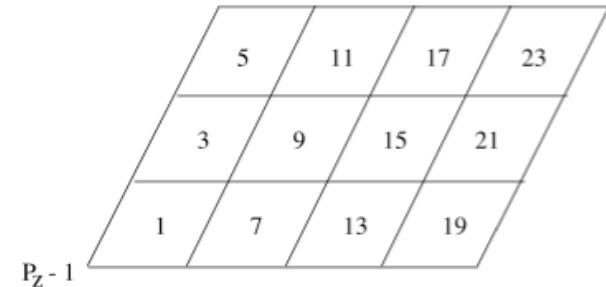


**atom\_move()**

# Spatial Decomposition



*Map a spatial subsystem to a process!*



- Process ID

*Vector*

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

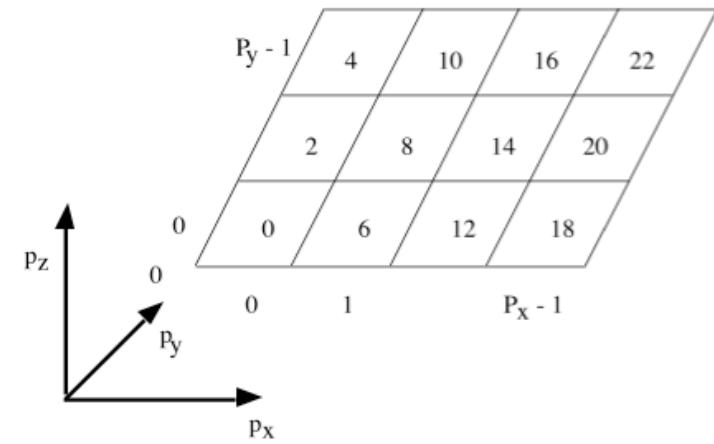
$$p_y = (p / P_z) \bmod P_y$$

$$p_z = p \bmod P_z$$

*Scalar*

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

Which 3D  
subspace?



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

In **pmd.h**

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

In **pmd.c**

```
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

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

$$p'(\kappa) = p'_x(\kappa) \times P_y P_z + p'_y(\kappa) \times P_z + p'_z(\kappa)$$

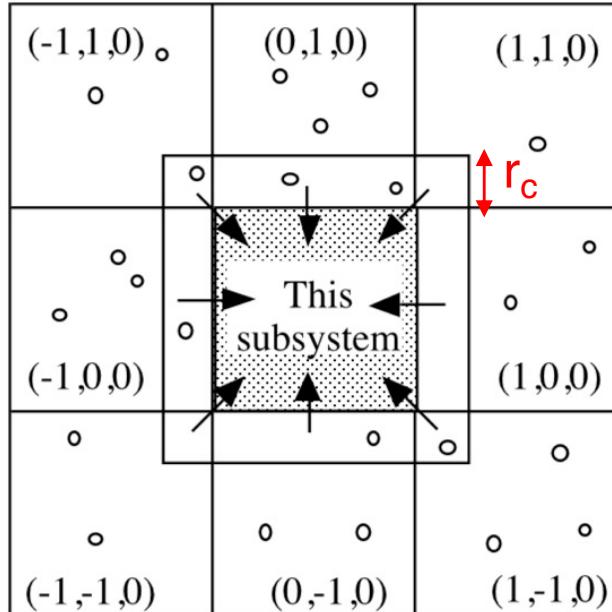
| Neighbor ID, $\kappa$ | $\vec{\delta} = (\delta_x, \delta_y, \delta_z)$ | $\vec{\Delta} = (\Delta_x, \Delta_y, \Delta_z)$ |
|-----------------------|---|---|
| 0 (east)              | (-1, 0, 0)                                      | ( $-L_x$ , 0, 0)                                |
| 1 (west)              | (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

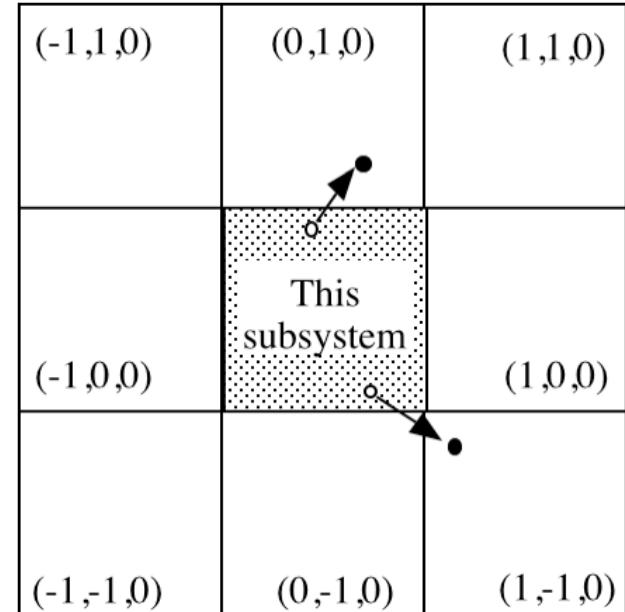
## In pmd.c

# Parallel MD Concepts

## Atom caching

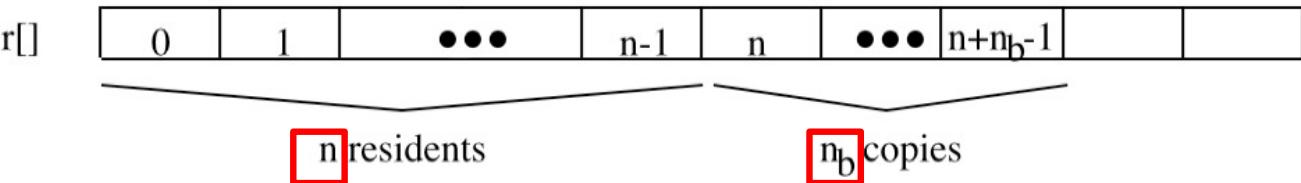


## Atom migration



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



# Parallel Interaction Computation

## SPMD: Who does what?

**Each process computes:**

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

```

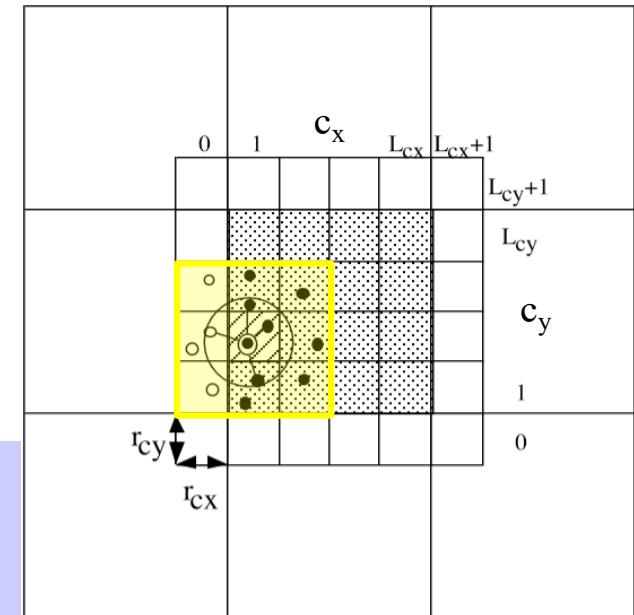
for resident cells, c {
    for neighbor (resident or cached) cells, c1 {
        scan atom i in cell c using c's linked list {
            scan atom j in cell c1 using c1's linked list {
                ...
                if (i < j &&  $r_{ij} < r_c^2$ ) {
                    compute pair force  $\mathbf{a}_{ij}$  & potential  $u(r_{ij})$ 
                    bintra = j < n; /* j is resident? */
                     $\mathbf{a}_i += \mathbf{a}_{ij}$ ; if (bintra)  $\mathbf{a}_j -= \mathbf{a}_{ij}$ ;
                    if (bintra) lpe += u( $r_{ij}$ ); else lpe += u( $r_{ij}$ )/2;
                }
            }
        }
    }
}

MPI Allreduce(&lpe, &potEnergy, ..., MPI SUM, ...);

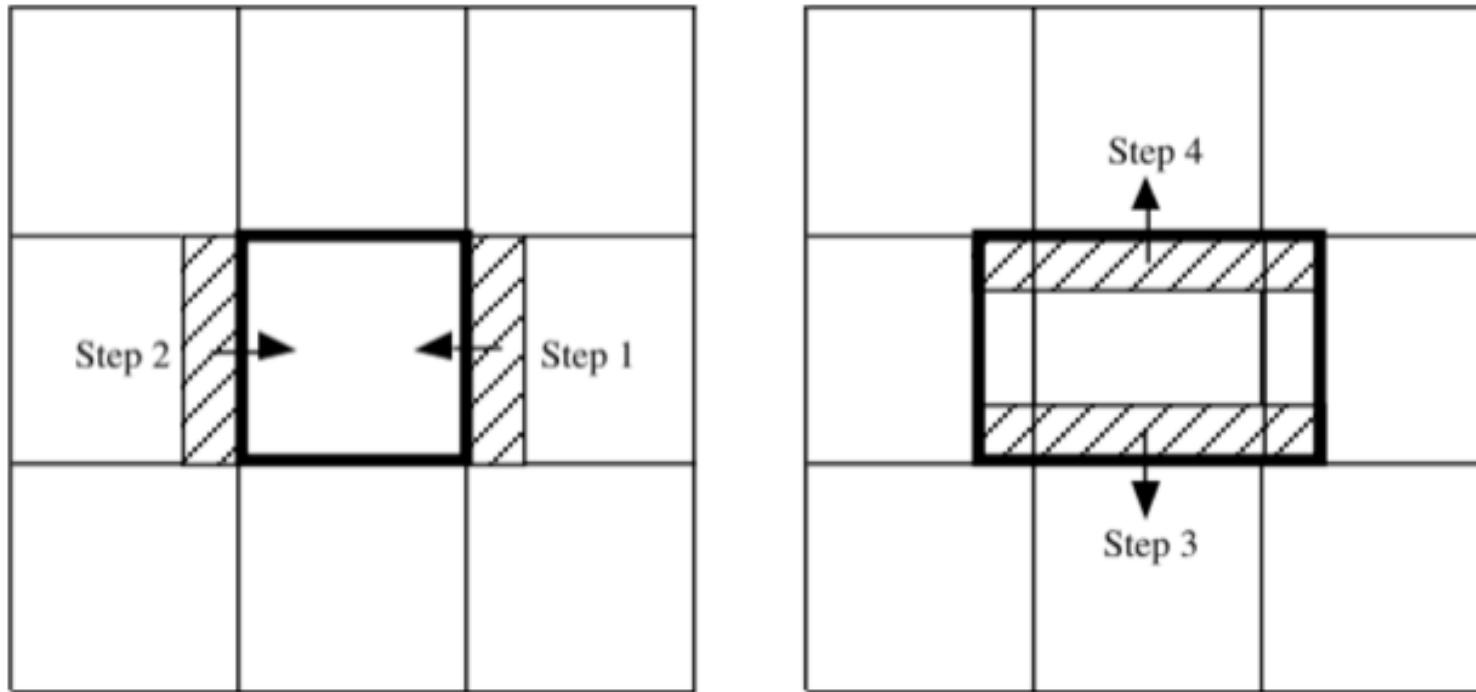
```

$j$        $bintra = (j < n)$   
 $r[]$        $0 \quad 1 \quad \dots \quad n-1 \quad n \quad \dots \quad n+n_b-1$   
 n residents      n<sub>b</sub> copies

**global reduction**



# Atom Caching: atom\_copy()



**26-step → 6-step communication by message 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**

  for lower and higher directions

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

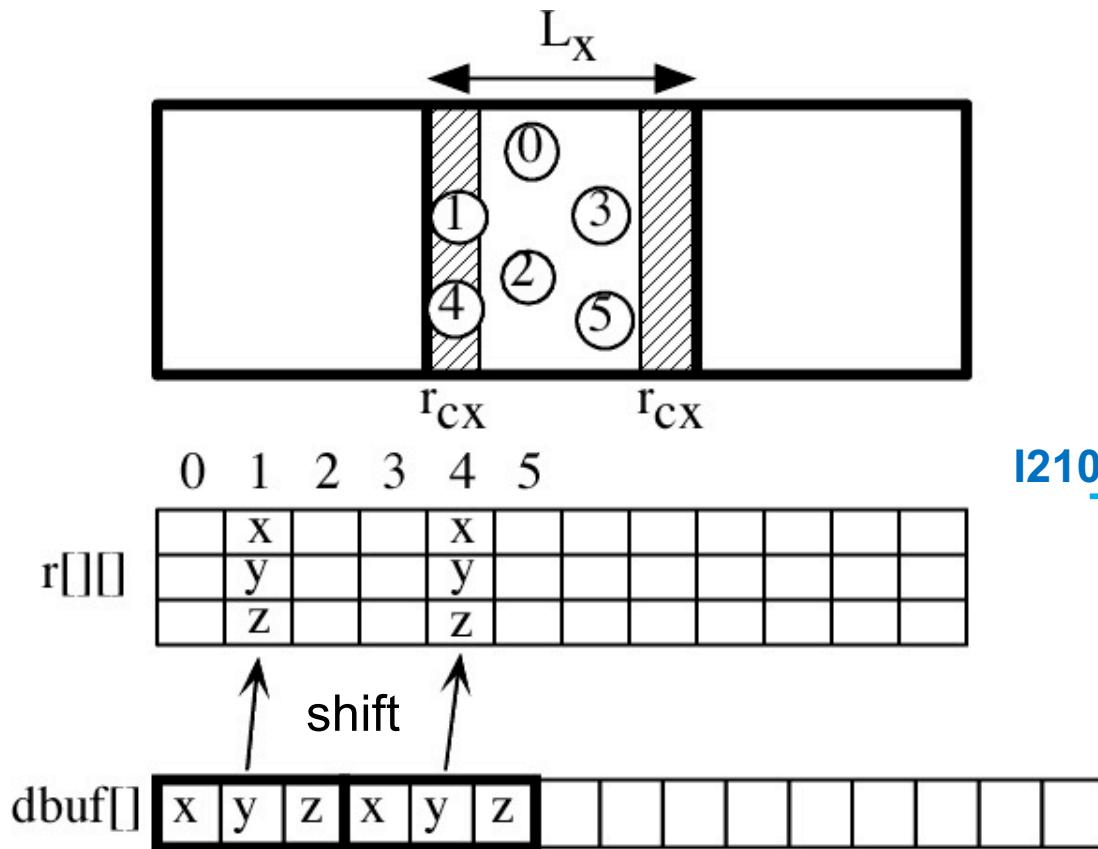
    Increment nbnew

  endfor

endfor

nb = nbnew

# Implementing Atom Caching

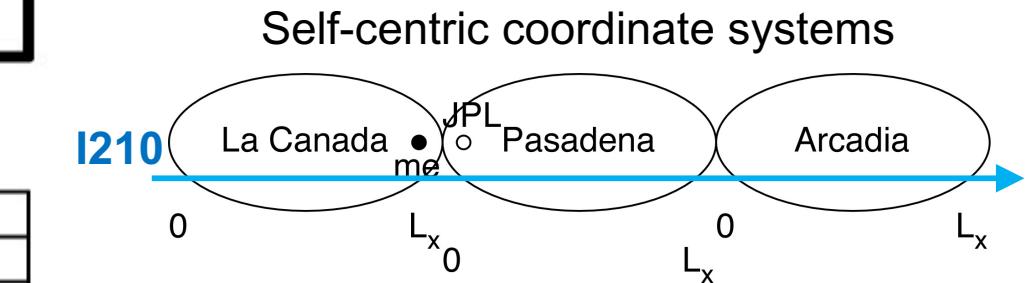


## Copying condition

```

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]
}

```

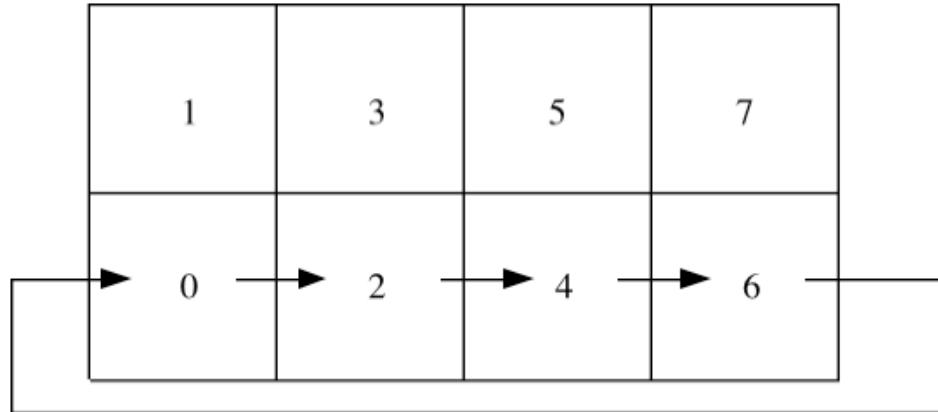


## 3 phases of message passing

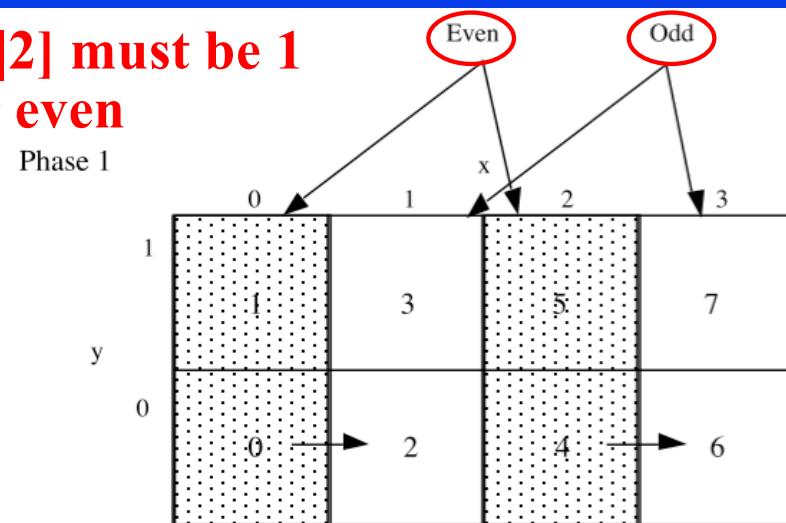
1. Message buffering:  $dbuf \leftarrow r\text{-sv (shift)}$ , gather
2. Message passing:  $dbuffr \leftarrow dbuf$   
Send dbuf  
Receive dbufr
3. Message storing:  $r \leftarrow dbufr$ , append after the residents

# Deadlock Avoidance

Cyclic dependence



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



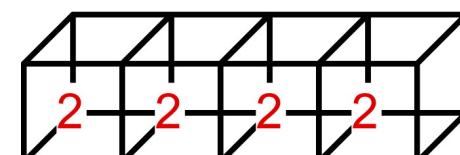
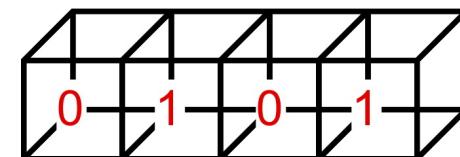
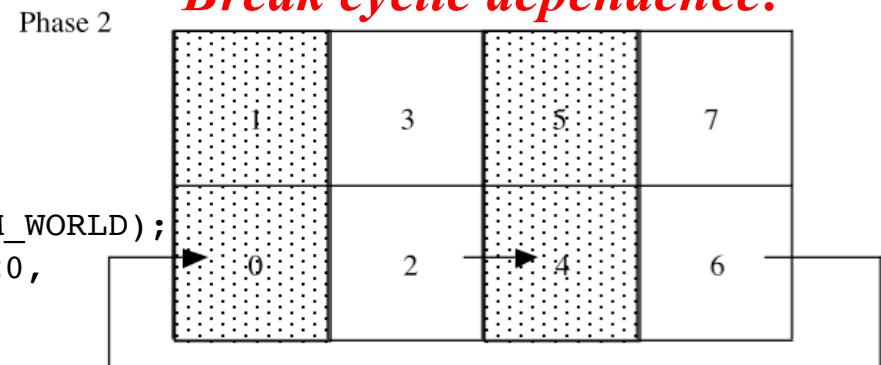
3-phase (deadlock-free) message passing

```

1. Message buffering: dbuf <- r, gather
2. Message passing: dbufr <- dbuf
/* Even node: send & recv, if not empty */
if (myparity[kd] == 0) {
    MPI_Send(dbufr, 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(dbufr, 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] = dbufr[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:

## Baseline 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 )
}
```

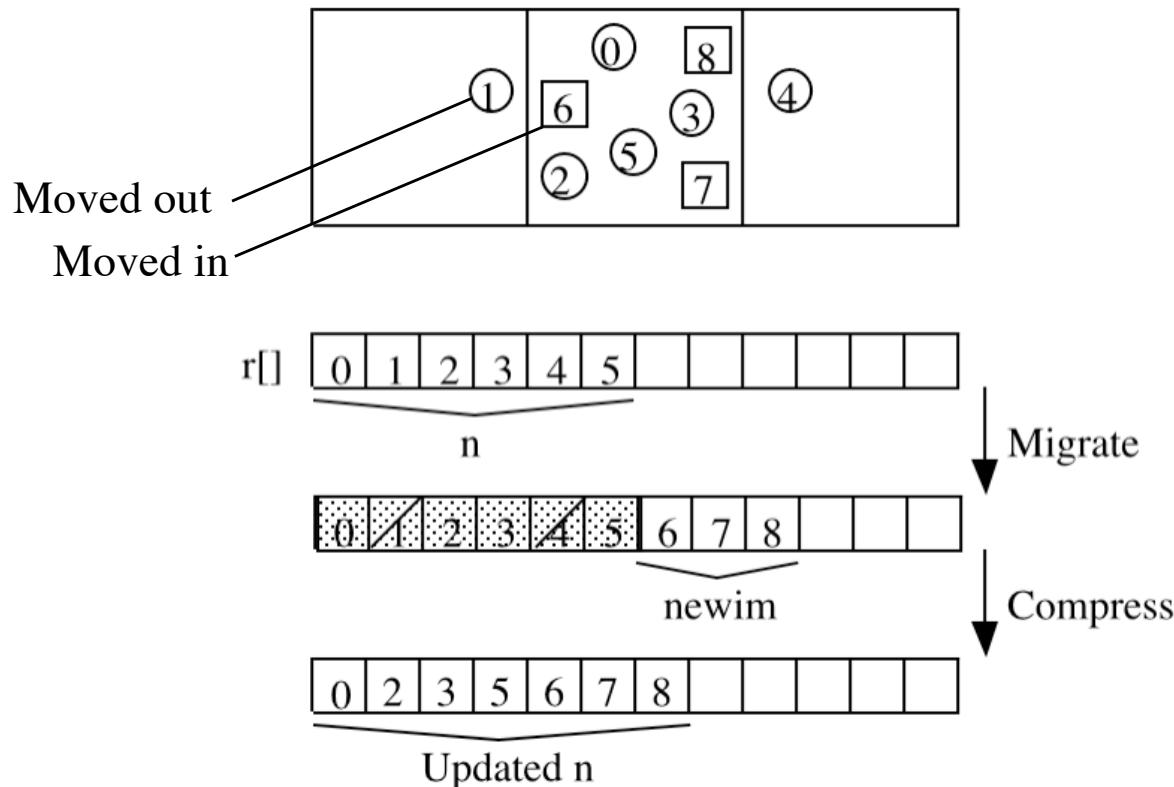
## CSCI 596 assignment

- Use non-blocking sends and receives instead



**MPI\_Irecv();**  
**MPI\_Send();**  
**MPI\_Wait();**

# 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

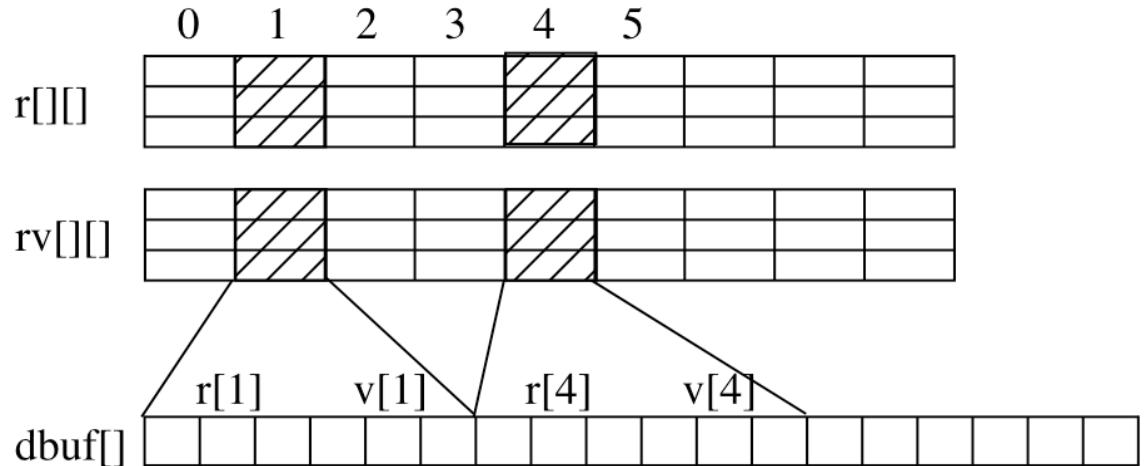
endfor

Compress the  $r$  array to eliminate the moved-out atoms

# Implementing Atom Migration

## Moving condition

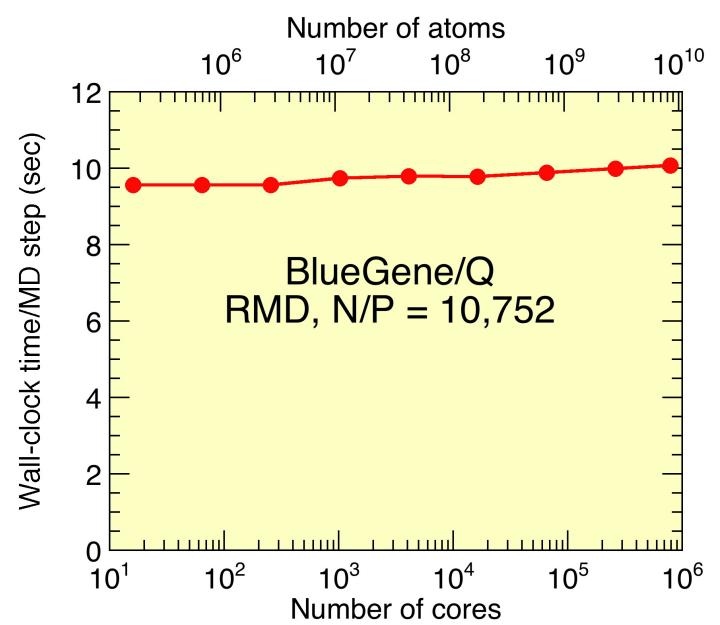
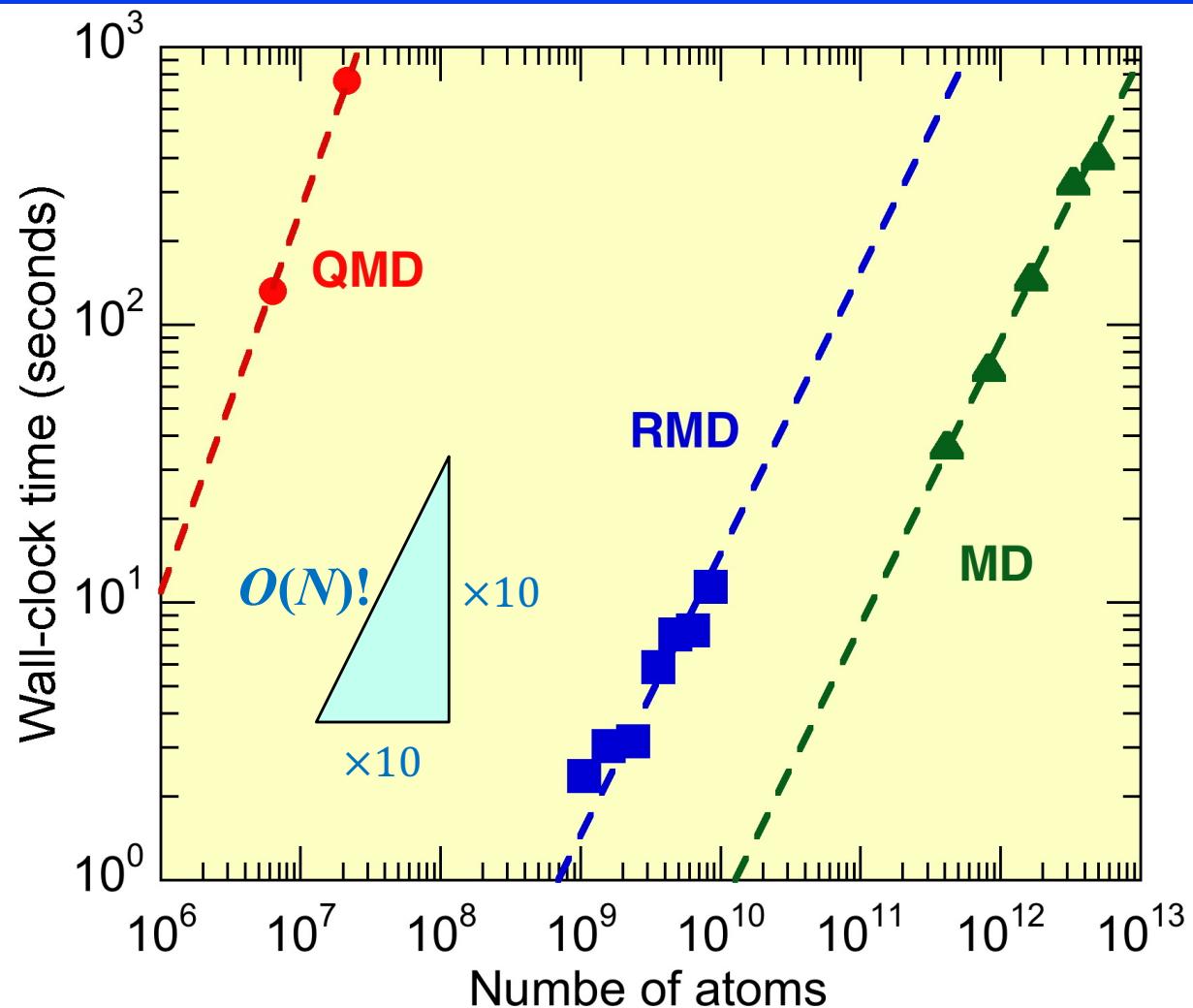
```
bmv(ri[],ku) {  
    kd = ku / 2 (= 0|1|2)  
    kdd = ku % 2 (= 0|1)  
    if (kdd == 0)  
        return ri[kd] < 0.0  
    else  
        return al[kd] < ri[kd]  
}
```



## 3 phases of message passing

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

# Spatial Decomposition Benchmark



**QMD (quantum molecular dynamics): DC-DFT**

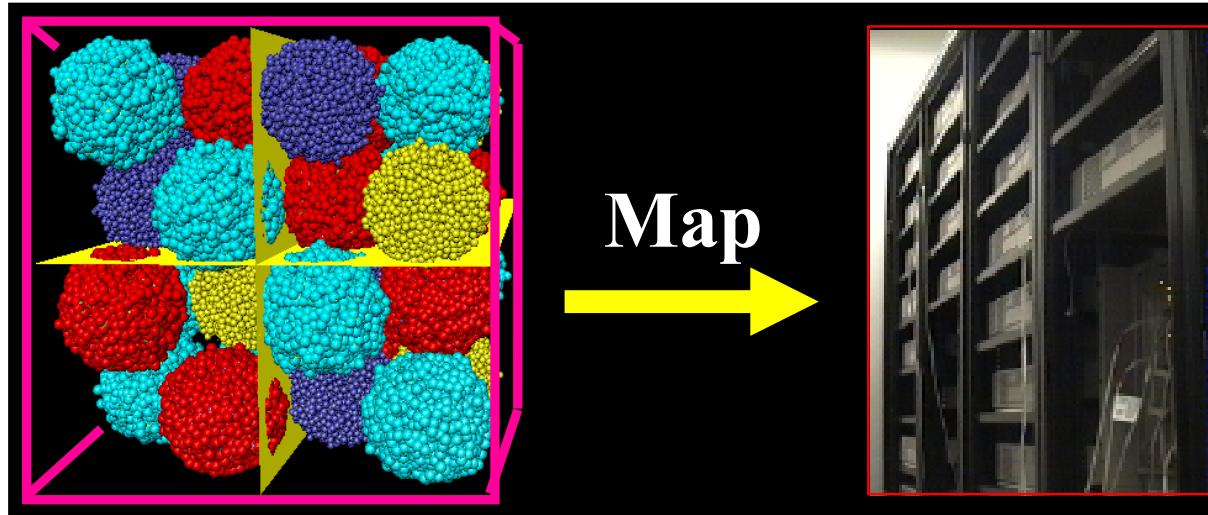
**RMD (reactive molecular dynamics): F-ReaxFF**

**MD (molecular dynamics): MRMD**

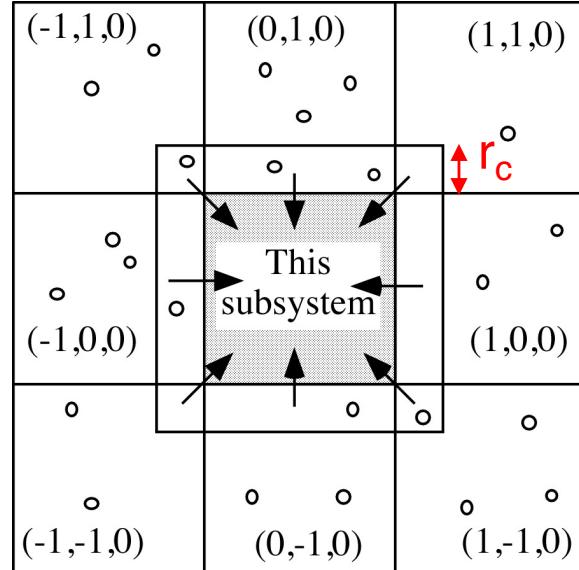
- 4.9 trillion-atom space-time multiresolution MD (MRMD) of  $\text{SiO}_2$
  - 8.5 billion-atom fast reactive force-field (F-ReaxFF) RMD of RDX
  - 1.9 trillion grid points (21.2 million-atom) DC-DFT QMD of SiC
- parallel efficiency 0.98 on 786,432 BlueGene/Q cores

# Cost of Spatial Decomposition MD

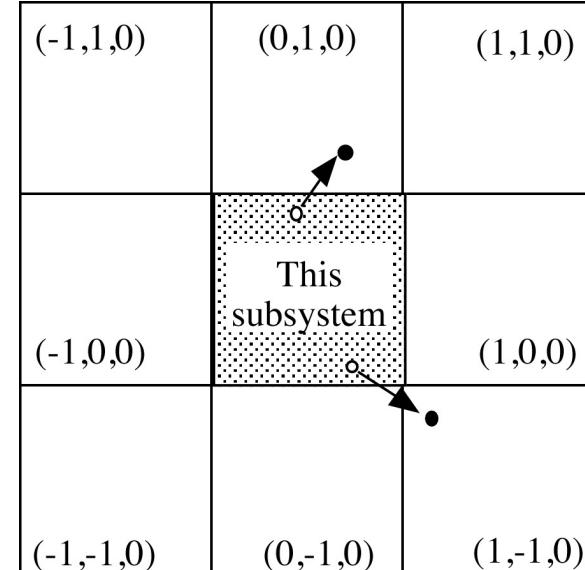
Spatial decomposition (short ranged):  $O(N/P)$  computation



Atom caching:  $O((N/P)^{2/3})$



Atom migration



Large overhead & lack of parallelism for small  $N/P$

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

See Grama'03, Chap. 5

- 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  $P$ ?

> Isognanular (weak) scaling:

$W_P = Pw$  ;  $w$  = constant workload per processor (granularity)

> Constant problem-size (strong) scaling:

$W_P = W$  — constant

# Analysis of Parallel MD

- Parallel execution time:

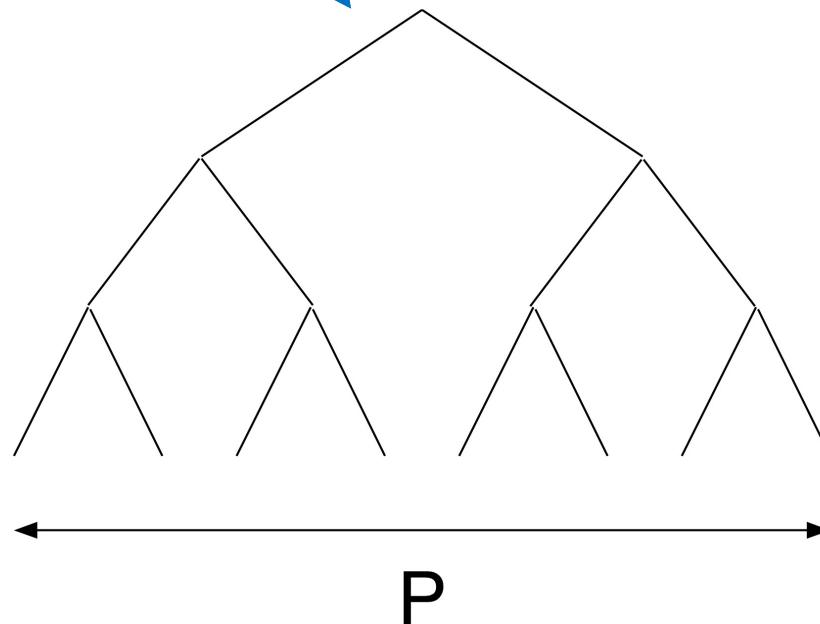
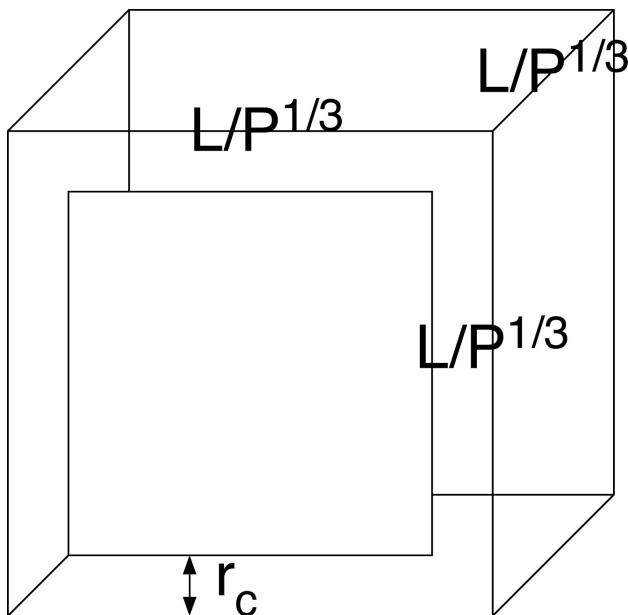
Workload  $\propto$  Number of atoms,  $N$  (linked-list cell algorithm)

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

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

`MPI_Allreduce()`

$$\begin{aligned} & \text{facets } \overbrace{6}^{\text{cached volume}} \quad \overbrace{\frac{L^2}{P^{2/3}} r_c}^{\text{atom density}} \\ & = 6r_c \frac{N^{2/3}/\rho^{2/3}}{P^{2/3}} \rho \\ & = 6r_c \rho^{1/3} \left( \frac{N}{P} \right)^{2/3} \end{aligned}$$



# Fixed Problem-Size Scaling

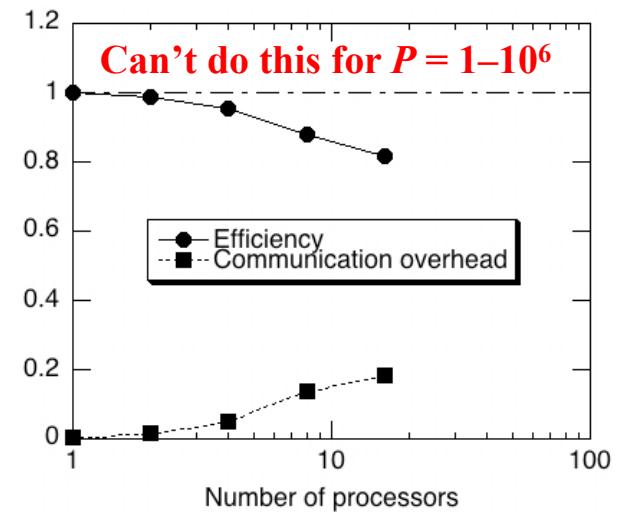
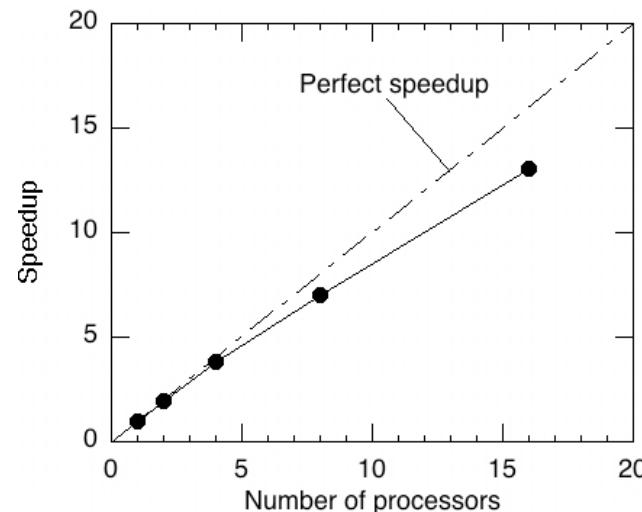
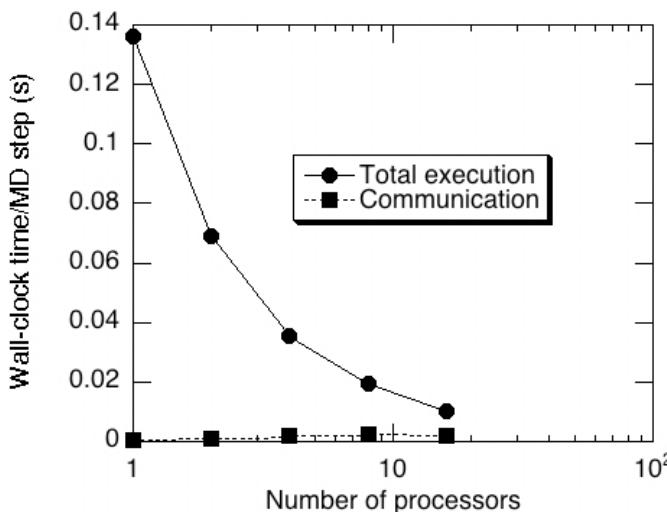
- Speedup:

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

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

- Efficiency:

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



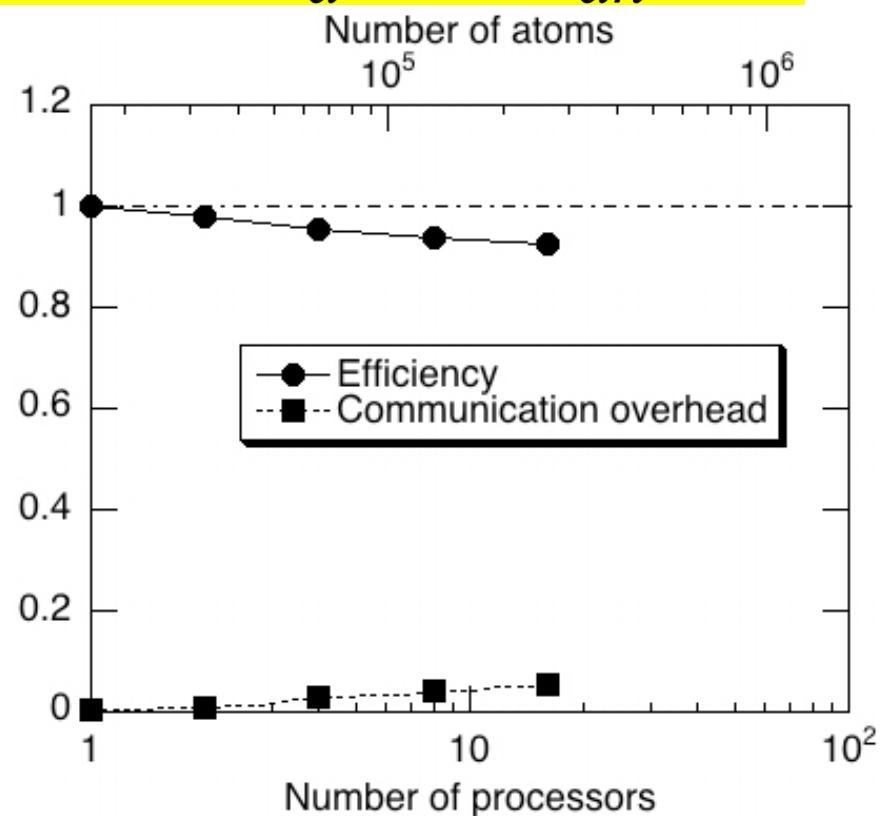
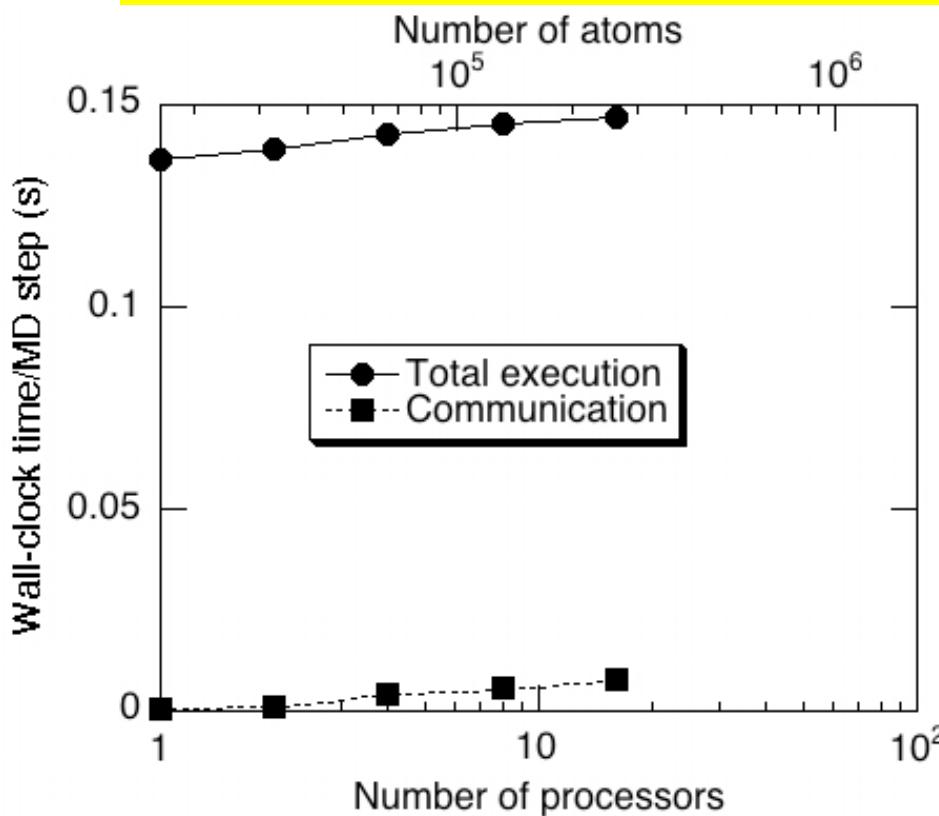
pmd.c:  $N = 16,384$ , on CARC

# Isogranular Scaling of Parallel MD

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

- Efficiency:

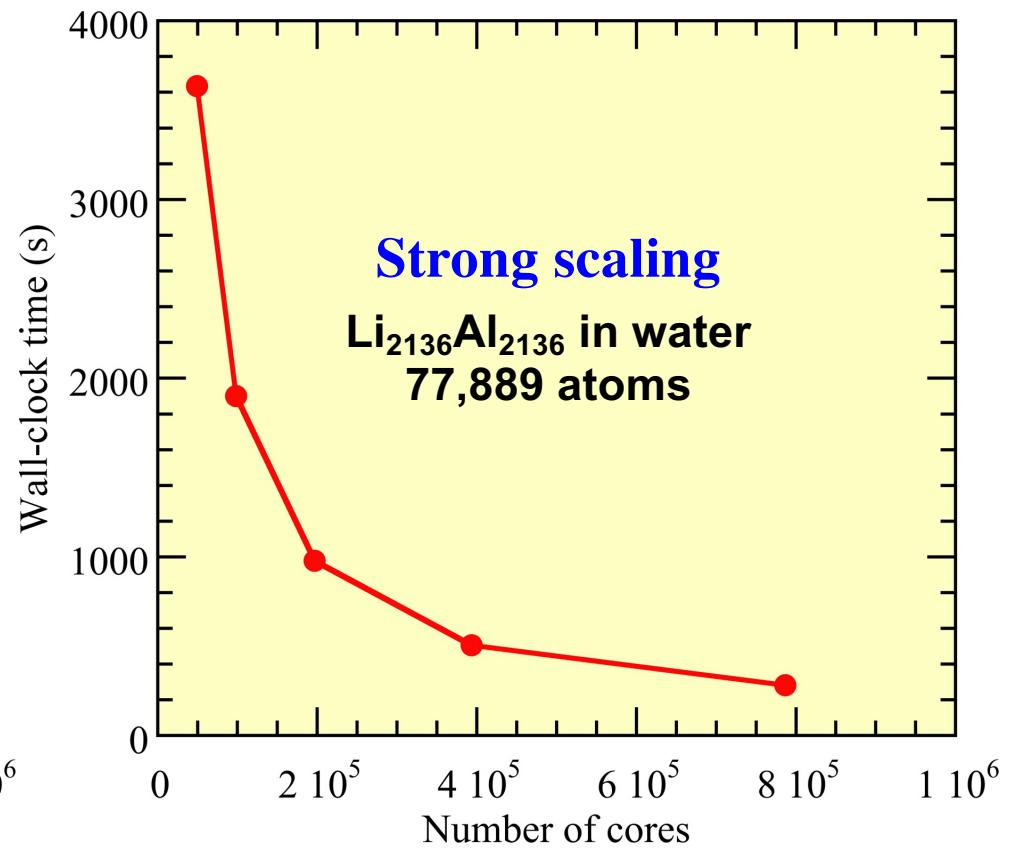
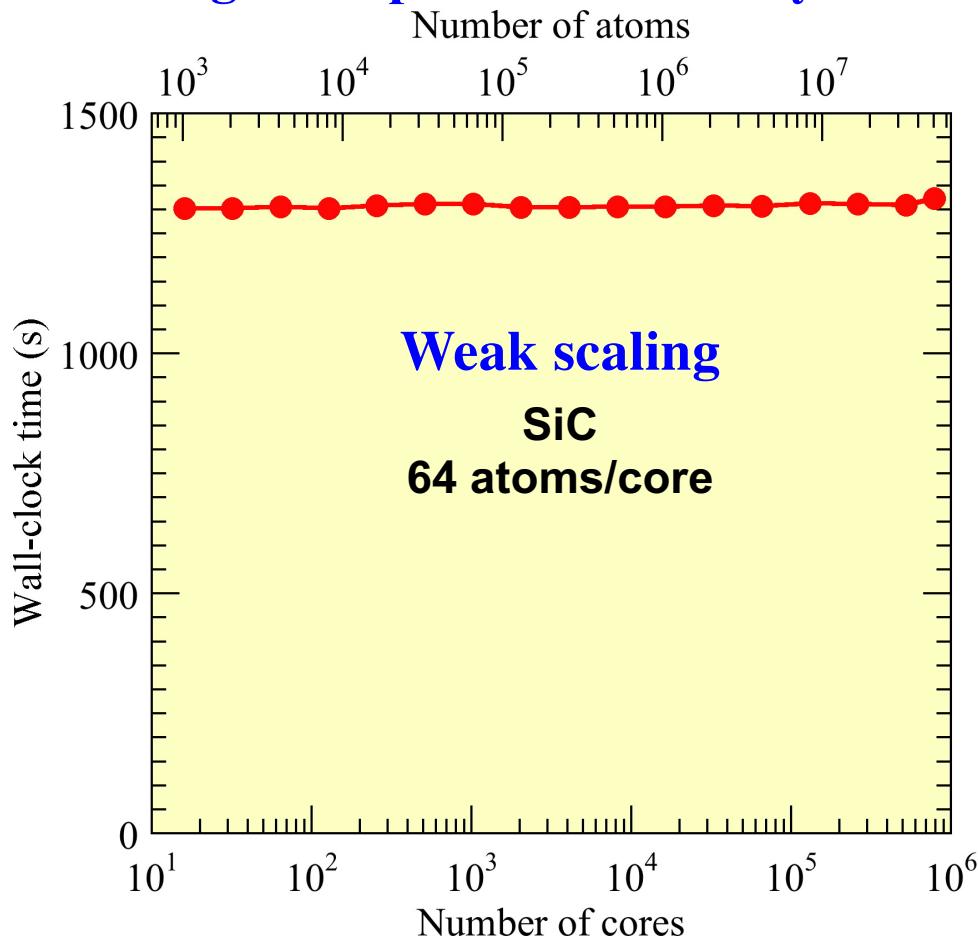
$$E_P = \frac{T(n,1)}{T(nP,P)} = \frac{an}{an + bn^{2/3} + c \log P} = \frac{1}{1 + \frac{b}{a} n^{-1/3} + \frac{c}{an} \log P}$$



pmd.c:  $N/P = 16,384$ , on CARC

# Parallel Performance of Quantum MD

- Weak-scaling parallel efficiency is 0.984 on 786,432 Blue Gene/Q cores for a 50,331,648-atom SiC system
- Strong-scale parallel efficiency is 0.803 on 786,432 Blue Gene/Q cores

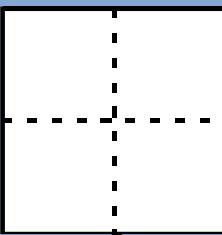


- 62-fold reduction of time-to-solution [441 s/SCF-step for 50.3M atoms] from the previous state-of-the-art [55 s/SCF-step for 102K atoms, Osei-Kuffuor *et al.*, PRL '14]

# Parallel Fast Multipole Method

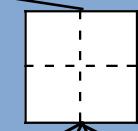
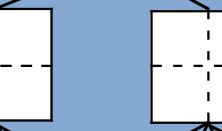
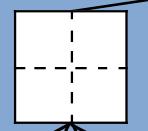
Level

$l = 1$



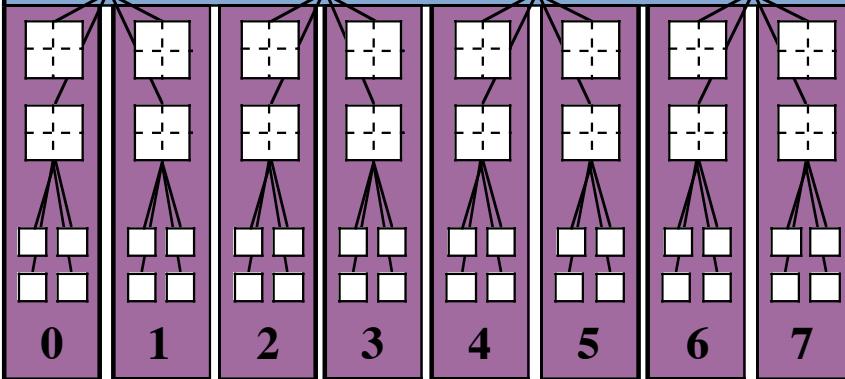
Upper levels:  
Global to all processors  
Overhead:  $O(\log P)$

$l = 2$



A. Nakano et al., *Comput. Phys. Commun.*  
83, 197 (1994)

$l = 3$

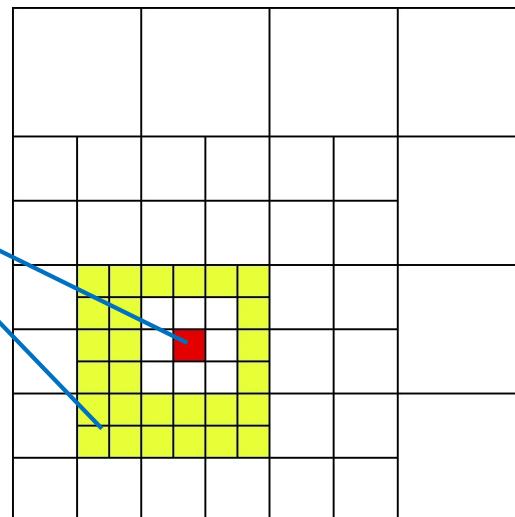


Lower levels:  
Spatial decomposition  
Computation:  $O(N/P)$

$l = 4$



Level-by-level  
short-ranged (M-to-L)  
interaction with cousins

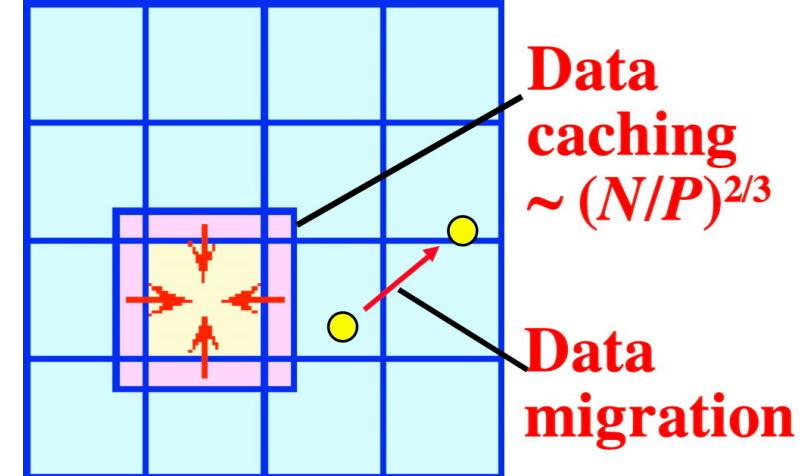


Coarse grain:

$N/P \sim 10^6; P \leq 10^3$

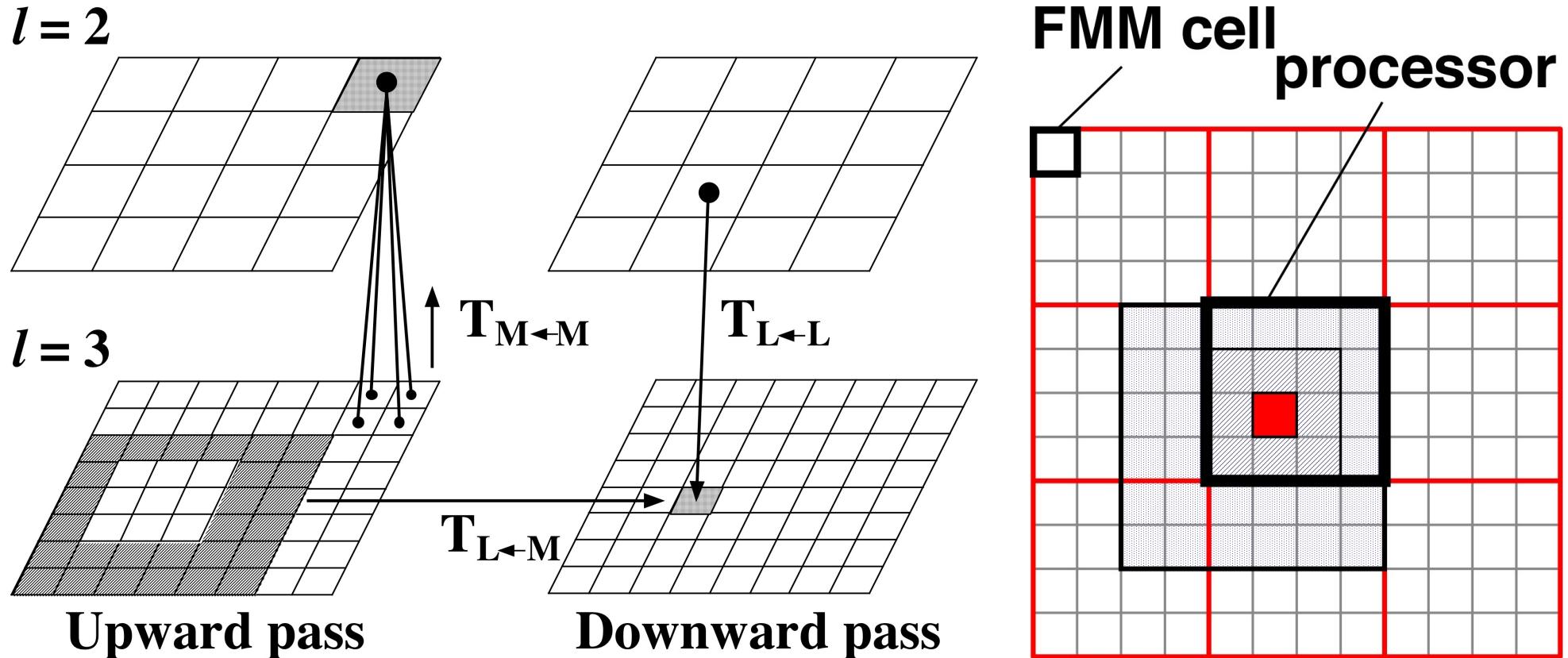


$N/P \gg \log P, (N/P)^{2/3}$



S. Ogata et al.,  
*Comput. Phys. Commun.*  
**153**, 445 ('03)

# Caching Interactive Cells



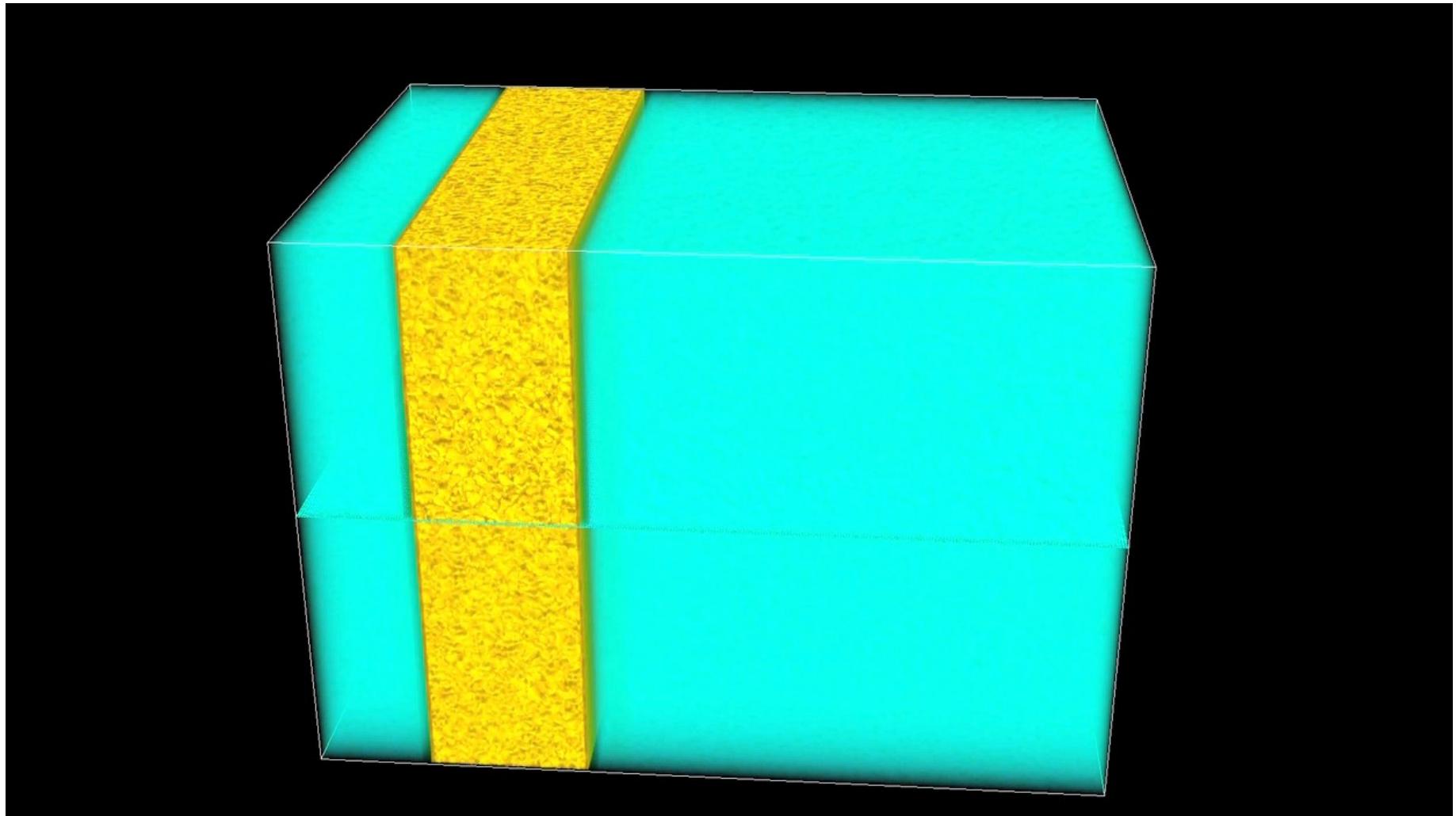
- $T_{M \leftarrow M}$  &  $T_{L \leftarrow L}$ : local at lower octree levels
- $T_{L \leftarrow M}$ : cache 2 boundary layers of cells at each level

See lecture note on “scalability analysis of parallel molecular-dynamics & fast-multipole-method algorithms”

<https://aiichironakano.github.io/cs653/02-2Scalability.pdf>

# Billion-Atom Molecular Dynamics

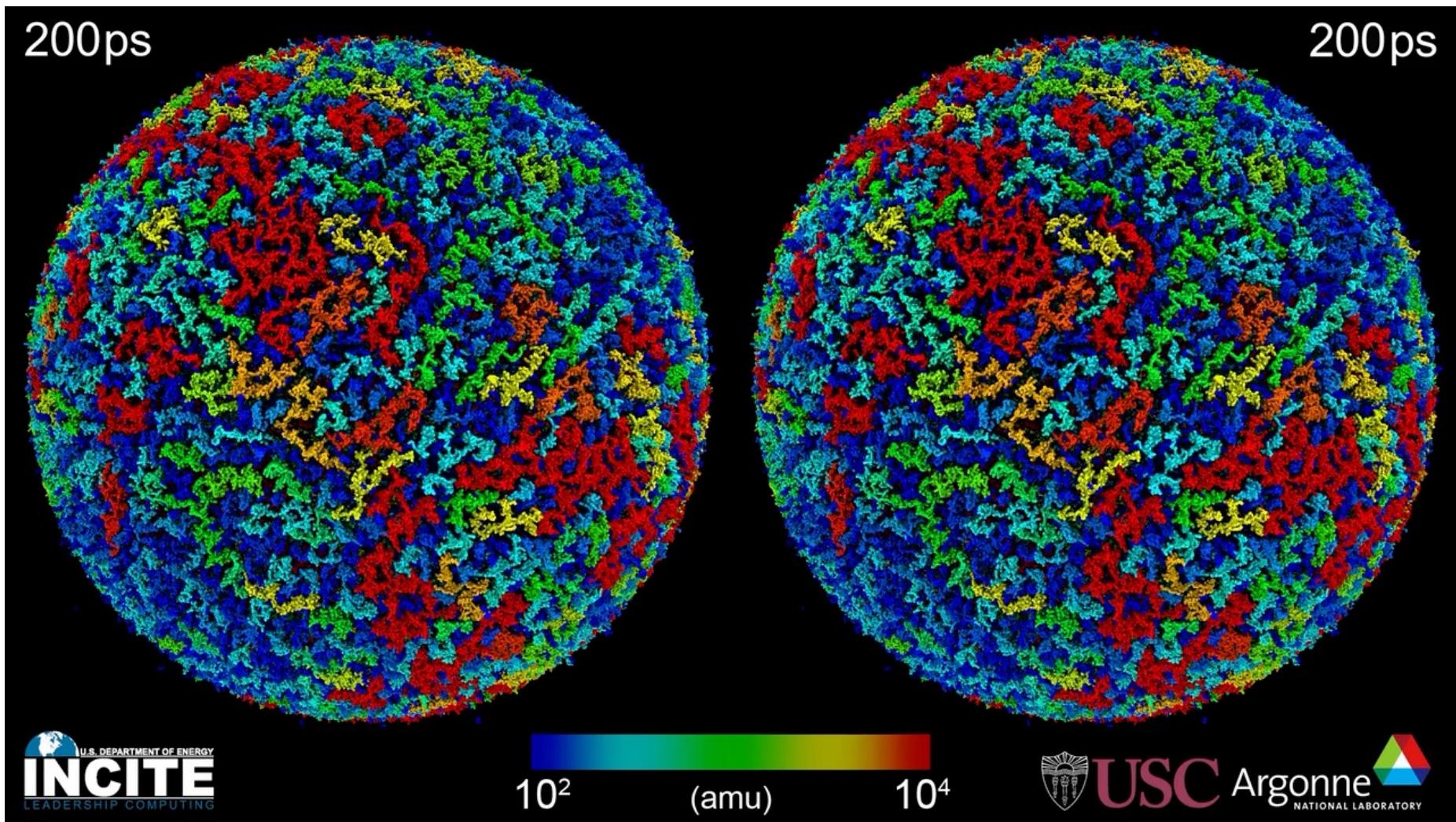
- Billion-atom MD simulation of shock-induced nanobubble collapse in water near silica surface (67 million core-hours on 163,840 Blue Gene/P cores)



- Water nanojet formation and its collision with silica surface

# 112 Million-Atom Reactive MD

- 112 million-atom reactive MD simulation to study nanocarbon synthesis by high-temperature oxidation of SiC nanoparticle (410 million core-hours on 786,432 Blue Gene/Q cores)



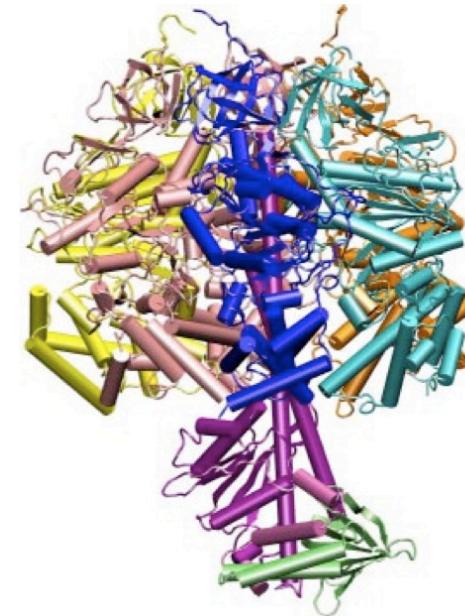
# Fine-Grained Parallel MD

## Pathways to a Protein Folding Intermediate Observed in a 1-Microsecond Simulation in Aqueous Solution

Yong Duan and Peter A. Kollman\*

An implementation of classical molecular dynamics on parallel computers of increased efficiency has enabled a simulation of protein folding with explicit representation of water for 1 microsecond, about two orders of magnitude longer than the longest simulation of a protein in water reported to date. Starting with an unfolded state of villin headpiece subdomain, hydrophobic collapse and helix formation occur in an initial phase, followed by conformational readjustments. A marginally stable state, which has a lifetime of about 150 nanoseconds, a favorable solvation free energy, and shows significant resemblance to the native structure, is observed; two pathways to this state have been found.

Science 282, 740 ('98)

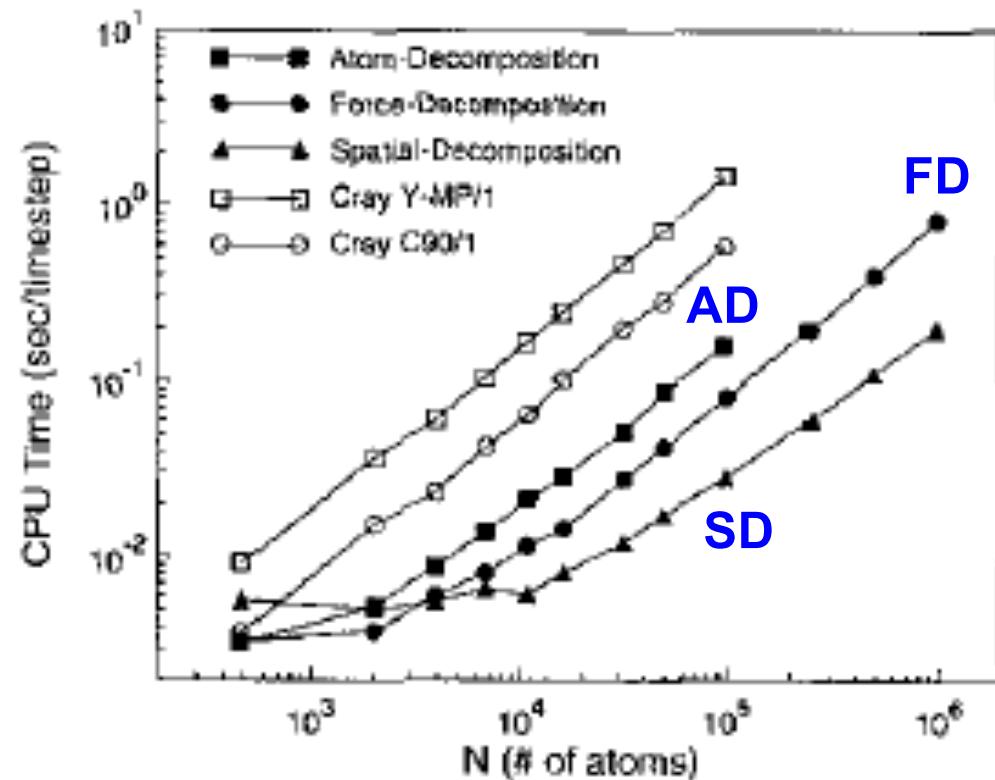
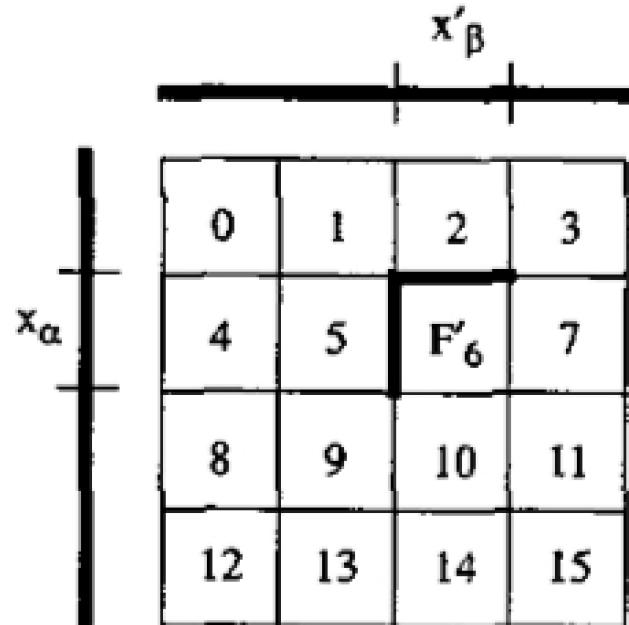


| Processors | Time/step |          | Speedup  |      | GFLOPS |       |
|------------|-----------|----------|----------|------|--------|-------|
|            | Total     | Per Node | MPI      | Elan | MPI    | Elan  |
| 1          | 1         | 28.08 s  | 28.08 s  | 1    | 1      | 0.480 |
| 128        | 4         | 248.3 ms | 234.6 ms | 113  | 119    | 54    |
| 256        | 4         | 135.2 ms | 121.9 ms | 207  | 230    | 99    |
| 512        | 4         | 65.8 ms  | 63.8 ms  | 426  | 440    | 204   |
| 510        | 3         | 65.7 ms  | 63.0 ms  | 427  | 445    | 205   |
| 1024       | 4         | 41.9 ms  | 36.1 ms  | 670  | 778    | 322   |
| 1023       | 3         | 35.1 ms  | 33.9 ms  | 799  | 829    | 383   |
| 1536       | 4         | 35.4 ms  | 32.9 ms  | 792  | 854    | 380   |
| 1536       | 3         | 26.7 ms  | 24.7 ms  | 1050 | 1137   | 504   |
| 2048       | 4         | 31.8 ms  | 25.9 ms  | 883  | 1083   | 423   |
| 1800       | 3         | 25.8 ms  | 22.3 ms  | 1087 | 1261   | 521   |
| 2250       | 3         | 19.7 ms  | 18.4 ms  | 1425 | 1527   | 684   |
| 2400       | 4         | 32.4 ms  | 27.2 ms  | 866  | 1032   | 416   |
| 2800       | 4         | 32.3 ms  | 32.1 ms  | 869  | 873    | 417   |
| 3000       | 4         | 32.5 ms  | 28.8 ms  | 862  | 973    | 414   |
|            |           |          |          |      |        | 467   |

J.C. Phillips, G. Zheng, S. Kumar, & L.V. Kale,  
in Proc. IEEE/ACM SC02

Table 1: NAMD performance on 327K atom ATPase benchmark system with multiple timestepping with PME every four steps for Charm++ based on MPI and Elan.

# Force Decomposition for Parallel MD

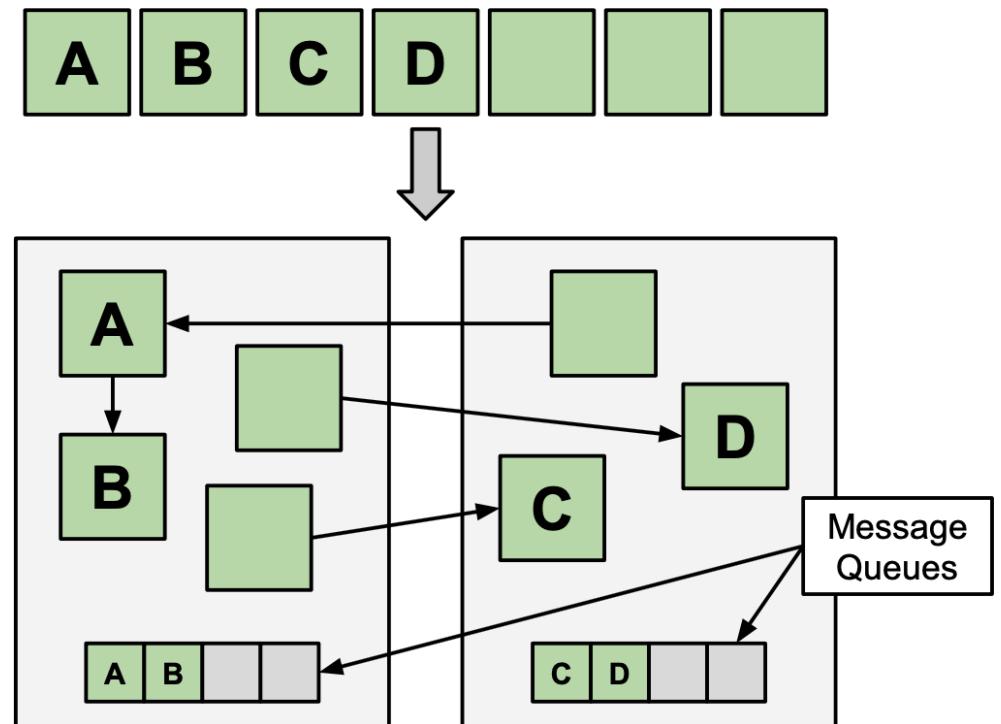
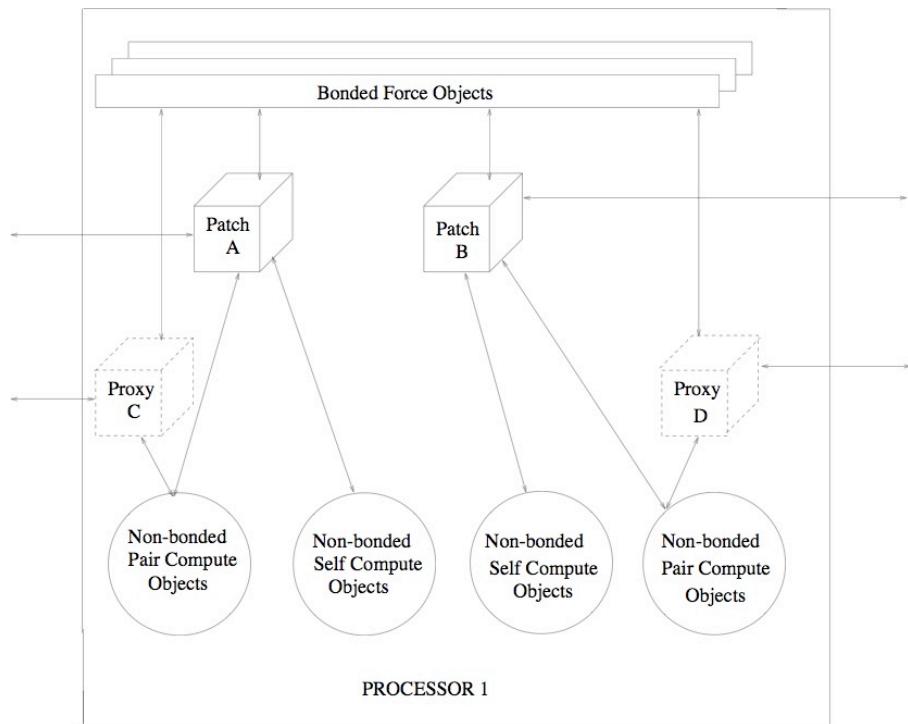


Runtime on 1,024-processor Intel Paragon

**FIG. 5.** The division of the permuted force matrix  $F'$  among 16 processors in the force-decomposition algorithm. Processor  $P_6$  is assigned a sub-block  $F'_6$  of size  $N/\sqrt{P}$  by  $N/\sqrt{P}$ . To compute its matrix elements it must know the corresponding  $N/\sqrt{P}$ -length pieces  $x_a$  and  $x'_\beta$  of the position vector  $x$  and permuted position vector  $x'$ .

# Hybrid Spatial+Force Decomposition

- Spatial decomposition of patches (localized spatial regions & atoms within)
- Inter-patch force computation objects assigned to any processor
- Message-driven object execution: computation-communication overlap



Kale *et al.*, *J. Comput. Phys.* **151**, 283 ('99); Phillips *et al.*, *SC02* (IEEE/ACM);  
Acun *et al.*, *SC14* (IEEE/ACM), Phillips *et al.*, *J. Chem. Phys.* **153**, 044130 ('20)

# Quantum MD@Scale

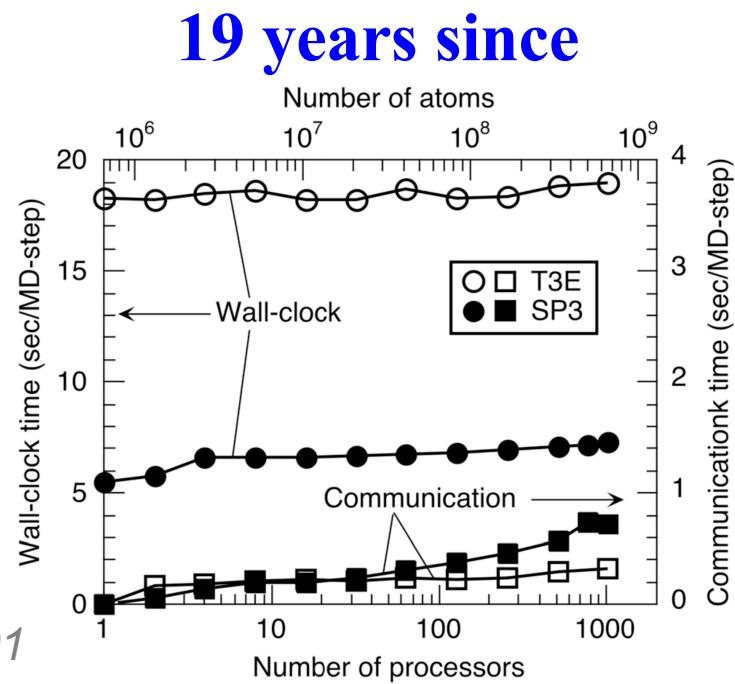
## Quantum dynamics at scale: ultrafast control of emergent functional materials

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 HPCAsia 2020*

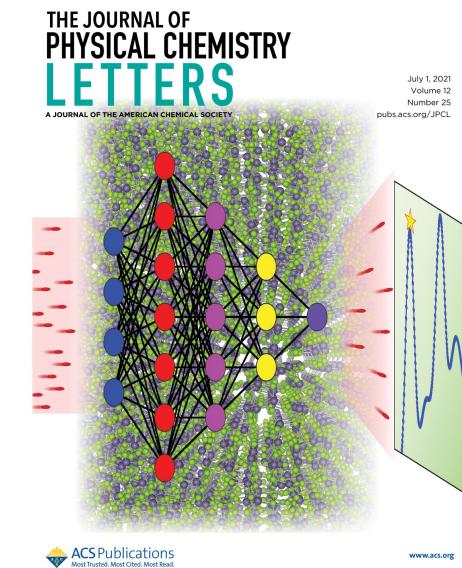
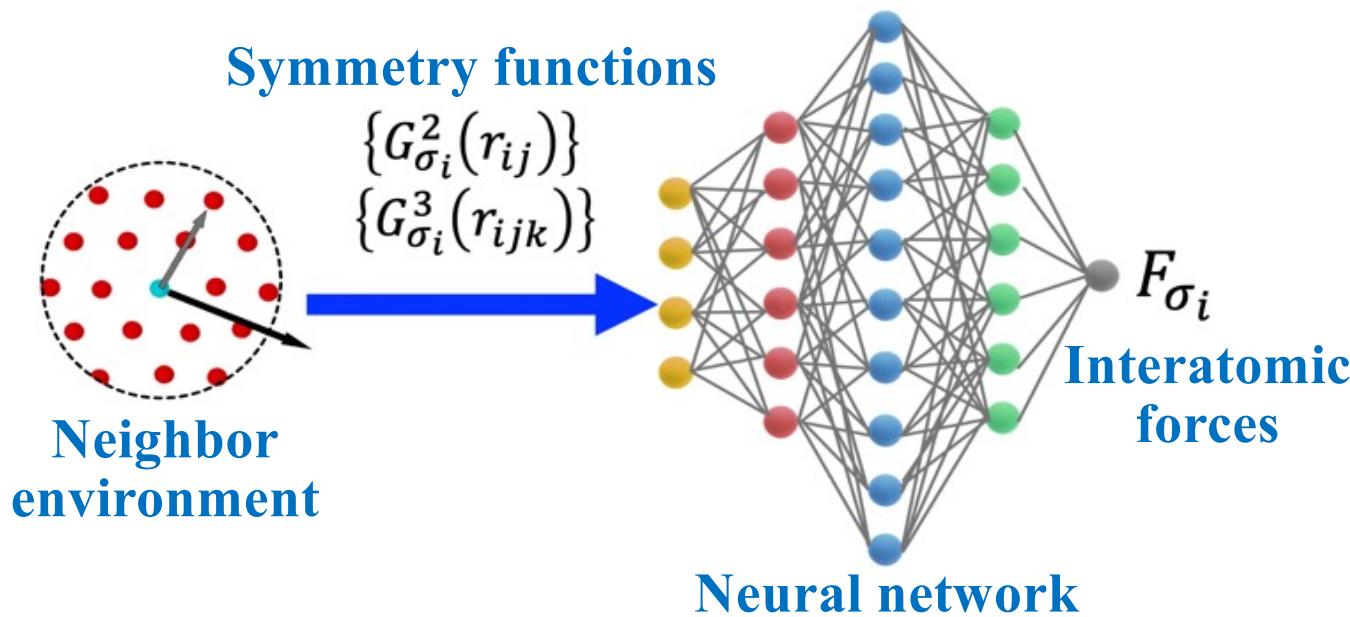


Scalable atomistic simulation algorithms  
for materials research, A. Nakano *et al.*,  
Best Paper, *IEEE/ACM Supercomputing 2001, SC01*



# 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 \('21\)](#)



[Allegro-Legato: scalable, fast, and robust neural-network quantum molecular dynamics via sharpness-aware minimization](#)

H. Ibayashi *et al.*, *ISC23—LNCS* **13948**, 223 ('23); *arXiv*: 2303.08169

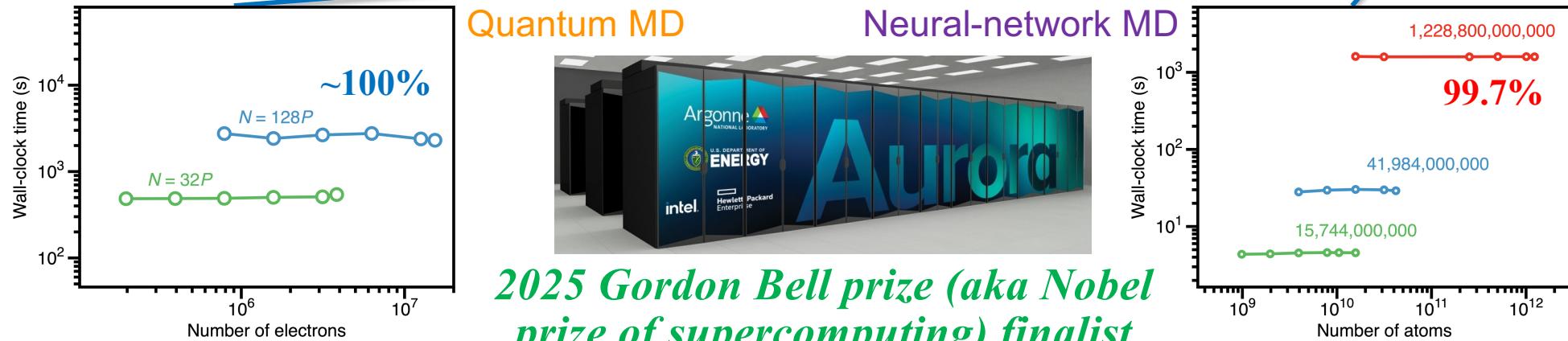
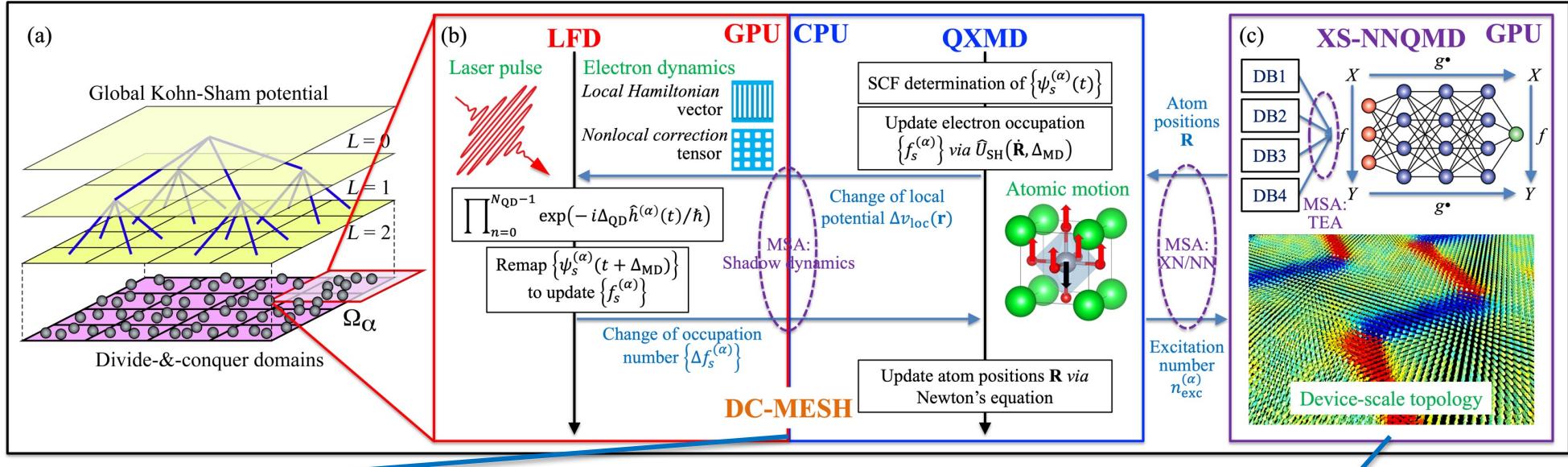
See also [Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning](#)

W. Jia *et al.*, *ACM/IEEE Supercomputing, SC20* (*Gordon Bell prize*)

# Quantum & Neural MD@Scale

## Multiscale light-matter dynamics in quantum materials: from electrons to topological superlattices

T. M. Razakh *et al.* <https://aiichironakano.github.io/cs653/Razakh-MLMD-GB25.pdf>



# What We Have Learned Here

---

- Single program multiple data (SPMD) parallel programming for multicomputers based on message passing interface (MPI), using molecular dynamics (MD) as a prototypical example.
- Parallel computing = decomposition (who does what).
- Data locality-exposing data structure like linked-list cells leads to straightforward parallelization.
- Spatial, particle, force & hybrid decompositions.
- Scalability analysis based on analytical models.