

Molecular Dynamics

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Objective: Basics of particle simulation

- Calculus (math) → simulation (science)
- Minimal knowledge to understand pmd.c



Why MD: Dynamic Irregular Dwarf

HPC 7 dwarfs

Dwarf	Description	Communication Pattern (Figure axes show processors 1 to 256, with black meaning no communication)	NAS Benchmark / Example HW	Dwarf	Description	Communication Pattern (Figure axes show processors 1 to 256, with black meaning no communication)	NAS Benchmark / Example HW
1. Dense Linear Algebra (e.g., BLAS [Blackford et al 2002], ScaLAPACK [Blackford et al 1996], or MATLAB [MathWorks 2006])	Data are dense matrices or vectors. (BLAS Level 1 = vector-vector; Level 2 = matrix-vector; and Level 3 = matrix-matrix.) Generally, such applications use unit-stride memory accesses to read data from rows, and strided accesses to read data from columns.		Block Triadiagonal Matrix, Lower Upper Symmetric Gauss-Seidel / Vector computers, Array computers	4. N-Body Methods (e.g., Barnes-Hut [Barnes and Hut 1986], Fast Multipole Method [Greengard and Rokhlin 1987])	Depends on interactions between many discrete points. Variations include particle-particle methods, where every point depends on all others, leading to an $O(N^2)$ calculation, and hierarchical particle methods, which combine forces or potentials from multiple points to reduce the computational complexity to $O(N \log N)$ or $O(N)$.		(no benchmark) / GRAPE [Tokyo 2006], MD-GRAPE [IBM 2006]
2. Sparse Linear Algebra (e.g., SpMV, OSKI [OSKI 2006], or SuperLU [Demmel et al 1999])	Data sets include many zero values. Data is usually stored in compressed matrices to reduce the storage and bandwidth requirements to access all of the nonzero values. One example is block compressed sparse row (BCSR). Because of the compressed formats, data is generally accessed with indexed loads and stores.		Conjugate Gradient / Vector computers with gather/scatter	5. Structured Grids (e.g., Cactus [Goodale et al 2003] or Lattice-Boltzmann Magnetohydrodynamics [LBMHD 2005])	Represented by a regular grid; points on grid are conceptually updated together. It has high spatial locality. Updates may be in place or between 2 versions of the grid. The grid may be subdivided into finer grids in areas of interest ("Adaptive Mesh Refinement"); and the transition between granularities may happen dynamically.		Multi-Grid, Scalar Penta-diagonal / QCDOC [Edinburg 2006], BlueGeneL
3. Spectral Methods (e.g., FFT [Cooley and Tukey 1965])	Data are in the frequency domain, as opposed to time or spatial domains. Typically, spectral methods use multiple butterfly stages, which combine multiply-add operations and a specific pattern of data permutation, with all-to-all communication for some stages and strictly local for others.		Fourier Transform / DSPs, Zalink PDSP [Zarlink 2006]	6. Unstructured Grids (e.g., ABAQUS [ABAQUS 2006] or FIDAP [FLUENT 2006])	An irregular grid where data locations are selected, usually by underlying characteristics of the application. Data point location and connectivity of neighboring points must be explicit. The points on the grid are conceptually updated together. Updates typically involve multiple levels of memory reference indirection, as an update to any point requires first determining a list of neighboring points, and then loading values from those neighboring points.		Unstructured Adaptive / Vector computers with gather/scatter, Tera Multi Threaded Architecture [Berry et al 2006]
				7. Monte Carlo (e.g., Quantum Monte Carlo [Aspuru-Guzik et al 2005])	Calculations depend on statistical results of repeated random trials. Considered embarrassingly parallel.	Communication is typically not dominant in Monte Carlo methods.	Embarrassingly Parallel / NSF Teragrid

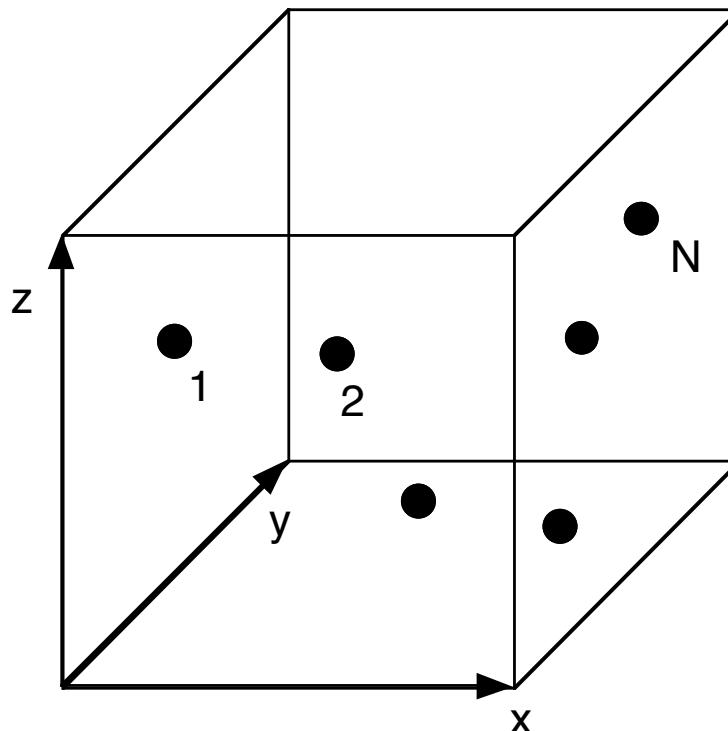
System: A Set of Point Atoms

$$\{\vec{r}_i = (x_i, y_i, z_i) \mid x_i, y_i, z_i \in \mathfrak{R}, i = 0, \dots, N - 1\}$$

int n: N , # of atoms

NMAX: Max # of atoms

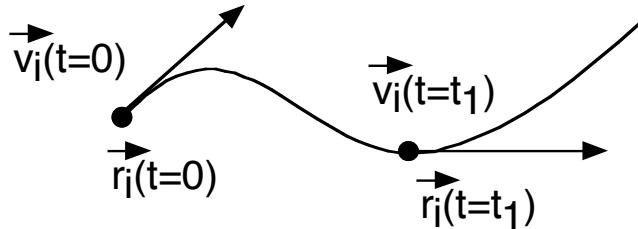
double r[NMAX][3]: $r[i][0|1|2] = x_i|y_i|z_i$



[pmd.h on the class home page](#)

Trajectory → Snapshots

Trace of atom positions



Velocity

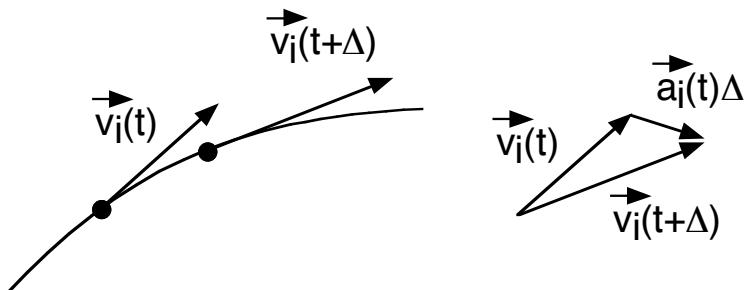
$$\vec{v}_i(t) = \dot{\vec{r}}_i(t) = \frac{d\vec{r}}{dt} \equiv \lim_{\Delta \rightarrow 0} \frac{\vec{r}_i(t + \Delta) - \vec{r}_i(t)}{\Delta}$$

double rv[NMAX][3]: rv[i][0|1|2] = $v_{ix}|v_{iy}|v_{iz}$

Acceleration

$$\vec{a}_i(t) = \ddot{\vec{r}}_i(t) = \frac{d^2\vec{r}}{dt^2} = \frac{d\vec{v}_i}{dt} \equiv \lim_{\Delta \rightarrow 0} \frac{\vec{v}_i(t + \Delta) - \vec{v}_i(t)}{\Delta}$$

double ra[NMAX][3]: ra[i][0|1|2] = $a_{ix}|a_{iy}|a_{iz}$



$$\begin{aligned} \vec{a}_i(t) &= \lim_{\Delta \rightarrow 0} \frac{\vec{v}_i(t + \Delta/2) - \vec{v}_i(t - \Delta/2)}{\Delta} \\ &= \lim_{\Delta \rightarrow 0} \frac{\frac{\vec{r}_i(t + \Delta) - \vec{r}_i(t)}{\Delta} - \frac{\vec{r}_i(t) - \vec{r}_i(t - \Delta)}{\Delta}}{\Delta} \\ &= \lim_{\Delta \rightarrow 0} \frac{\vec{r}_i(t + \Delta) - 2\vec{r}_i(t) + \vec{r}_i(t - \Delta)}{\Delta^2} \end{aligned}$$

Newton's Equation of Motion



Newton's 2nd law:

$$m\ddot{\vec{r}}_i(t) = \vec{F}_i(t)$$

Initial value problem: Given initial particle positions & velocities, $\{(\vec{r}_i(0), \vec{v}_i(0))\}$
Obtain those at later times $\{(\vec{r}_i(t), \vec{v}_i(t)); t \geq 0\}$

Potential energy:

$$\vec{F}_k = -\frac{\partial}{\partial \vec{r}_k} V(\vec{r}^N) = -\left(\frac{\partial V}{\partial x_k}, \frac{\partial V}{\partial y_k}, \frac{\partial V}{\partial z_k}\right)$$

where the partial derivative is

$$\frac{\partial V}{\partial x_k} = \lim_{h \rightarrow 0} \frac{V(x_0, y_0, z_0, \dots, x_k + h, y_k, z_k, \dots, x_{N-1}, y_{N-1}, z_{N-1}) - V(x_0, y_0, z_0, \dots, x_k, y_k, z_k, \dots, x_{N-1}, y_{N-1}, z_{N-1})}{h}$$

Pair potential:

$$V(\vec{r}^N) = \sum_{i < j} u(r_{ij}) = \sum_{i=0}^{N-2} \sum_{j=i+1}^{N-1} u(|\vec{r}_{ij}|)$$

Molecular Dynamics Equations

Given initial atomic positions & velocities, $\{(\vec{r}_i(0), \vec{v}_i(0)) | i = 0, \dots, N - 1\}$, obtain those at later times, $\{(\vec{r}_i(t), \vec{v}_i(t)) | i = 0, \dots, N - 1; t \geq 0\}$, by integrating the ordinary differential equation,

$$\ddot{\vec{r}}_k(t) = \vec{a}_k(t) = -\frac{\partial}{\partial \vec{r}_k} \sum_{i < j} u(r_{ij}) = \sum_{i < j} \vec{r}_{ij}(t) \left(-\frac{1}{r} \frac{du}{dr} \right)_{r=r_{ij}(t)} (\delta_{ik} - \delta_{jk})$$

where

$$-\frac{1}{r} \frac{du}{dr} = \frac{48}{r^2} \left(\frac{1}{r^{12}} - \frac{1}{2r^6} \right) \quad \text{(for the Lennard-Jones potential in a dimensionless unit)}$$

Force calculation algorithm— $O(N^2)$:

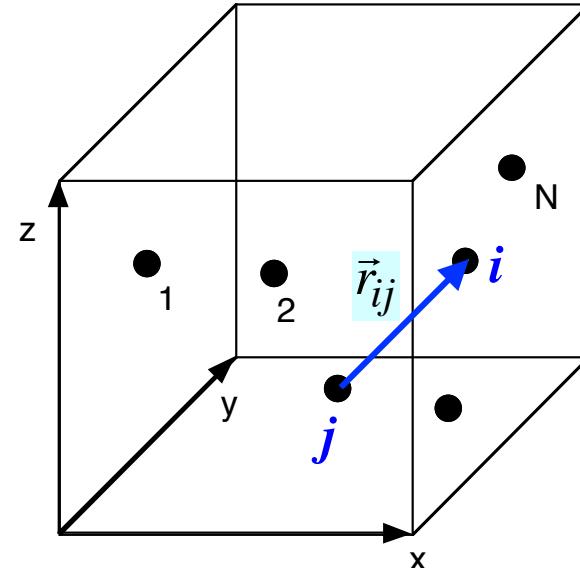
for $i = 0$ to $N-1$, $\vec{a}_i = 0$

for $i = 0$ to $N-2$

 for $j = i+1$ to $N-1$

 compute $\vec{\alpha} = \vec{r}_{ij} \left(-\frac{1}{r} \frac{du}{dr} \right)_{r=|\vec{r}_{ij}|}$
 $\vec{a}_i + = \vec{\alpha}$

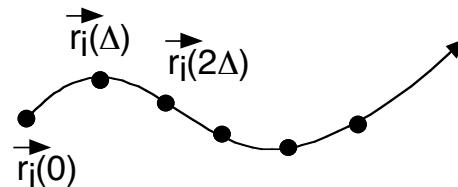
$\vec{a}_{j-} = \vec{\alpha}$



Time Discretization

Snapshots with time interval Δ : double DeltaT

$$(\vec{r}_i(0), \vec{v}_i(0)) \mapsto (\vec{r}_i(\Delta), \vec{v}_i(\Delta)) \mapsto (\vec{r}_i(2\Delta), \vec{v}_i(2\Delta)) \mapsto \dots$$



Question: How to predict the next state, $(\vec{r}_i(t + \Delta), \vec{v}_i(t + \Delta))$, from the current state, $(\vec{r}_i(t), \vec{v}_i(t))$?

Solution: Taylor expansion

$$f(x_0 + h) = \sum_{n=0}^{\infty} \frac{h^n}{n!} \frac{d^n f}{dx^n} \Big|_{x=x_0} = f(x_0) + h \frac{df}{dx} \Big|_{x=x_0} + \frac{h^2}{2} \frac{d^2 f}{dx^2} \Big|_{x=x_0} + \frac{h^3}{3!} \frac{d^3 f}{dx^3} \Big|_{x=x_0} + \dots$$

cf. <http://cacs.usc.edu/education/phys516/TaylorExpansion.pdf>

Verlet Discretization

Position:

$$\vec{r}_i(t + \Delta) = \vec{r}_i(t) + \vec{v}_i(t)\Delta + \frac{1}{2}\vec{a}_i(t)\Delta^2 + \frac{1}{6}\ddot{\vec{r}}_i(t)\Delta^3 + O(\Delta^4)$$

$$+ \quad \vec{r}_i(t - \Delta) = \vec{r}_i(t) - \vec{v}_i(t)\Delta + \frac{1}{2}\vec{a}_i(t)\Delta^2 - \frac{1}{6}\ddot{\vec{r}}_i(t)\Delta^3 + O(\Delta^4)$$

$$\vec{r}_i(t + \Delta) + \vec{r}_i(t - \Delta) = 2\vec{r}_i(t) + \vec{a}_i(t)\Delta^2 + O(\Delta^4)$$

$$\therefore \vec{r}_i(t + \Delta) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta) + \vec{a}_i(t)\Delta^2 + O(\Delta^4)$$

Velocity:

$$\vec{r}_i(t + \Delta) = \vec{r}_i(t) + \vec{v}_i(t)\Delta + \frac{1}{2}\vec{a}_i(t)\Delta^2 + \frac{1}{6}\ddot{\vec{r}}_i(t)\Delta^3 + O(\Delta^4)$$

$$- \quad \vec{r}_i(t - \Delta) = \vec{r}_i(t) - \vec{v}_i(t)\Delta + \frac{1}{2}\vec{a}_i(t)\Delta^2 - \frac{1}{6}\ddot{\vec{r}}_i(t)\Delta^3 + O(\Delta^4)$$

$$\vec{r}_i(t + \Delta) - \vec{r}_i(t - \Delta) = 2\vec{v}_i(t)\Delta + O(\Delta^3)$$

$$\therefore \vec{v}_i(t) = \frac{\vec{r}_i(t + \Delta) - \vec{r}_i(t - \Delta)}{2\Delta} + O(\Delta^2)$$

Verlet Algorithm

Verlet discretization:

$$\begin{cases} \vec{r}_i(t + \Delta) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta) + \vec{a}_i(t)\Delta^2 + O(\Delta^4) \\ \vec{v}_i(t) = \frac{\vec{r}_i(t + \Delta) - \vec{r}_i(t - \Delta)}{2\Delta} + O(\Delta^2) \end{cases}$$

Verlet algorithm:

Given $\vec{r}_i(t - \Delta)$ & $\vec{r}_i(t)$,

1. Compute $\vec{a}_i(t)$ as a function of $\{\vec{r}_i(t)\}$
2. $\vec{r}_i(t + \Delta) \leftarrow 2\vec{r}_i(t) - \vec{r}_i(t - \Delta) + \vec{a}_i(t)\Delta^2$
3. $\vec{v}_i(t) \leftarrow [\vec{r}_i(t + \Delta) - \vec{r}_i(t - \Delta)]/(2\Delta)$

Drawback: Positions & velocities are not simultaneously updated for the same time step

Velocity Verlet Algorithm

Theorem: The following algebraic equation gives the same sequence of states, $(\vec{r}_i(n\Delta), \vec{v}_i(n\Delta))$, as that obtained by the Verlet discretization.

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

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

Velocity Verlet Algorithm for StepLimit Steps

Initialize (\vec{r}_i, \vec{v}_i) for all i

Compute \vec{a}_i for all i as a function of $\{\vec{r}_i\}$ **function computeAccel()**

for stepCount = 1 to StepLimit

do the following **function singleStep()**

$\vec{v}_i \leftarrow \vec{v}_i + \vec{a}_i \Delta / 2$ for all i

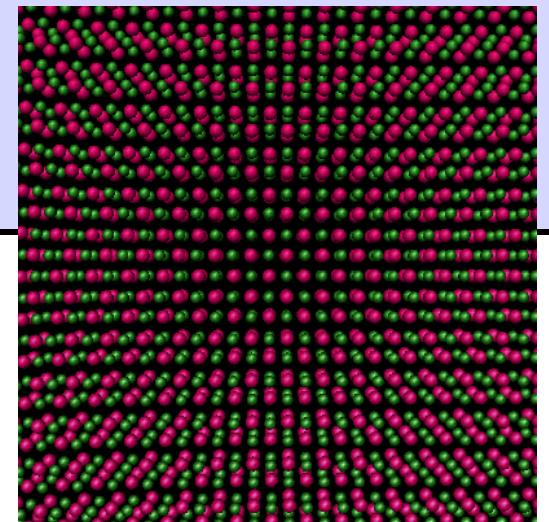
$\vec{r}_i \leftarrow \vec{r}_i + \vec{v}_i \Delta$ for all i

Compute \vec{a}_i for all i as a function of $\{\vec{r}_i\}$ **function computeAccel()**

$\vec{v}_i \leftarrow \vec{v}_i + \vec{a}_i \Delta / 2$ for all i

endfor

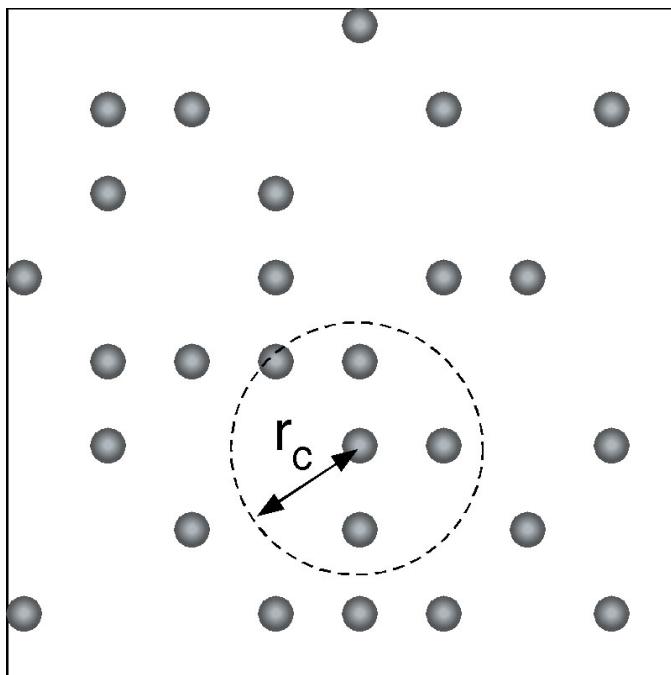
stepLimit+1 calls to function computeAccel()



Linked-List Cell Molecular Dynamics

- Computational complexity of `ComputeAccel()` in `md.c`:
 $\propto N(N-1)/2 = O(N^2)$
- Data locality (cut-off length, r_c) reduces the complexity to $O(N)$:
 $N \times (4\pi/3)r_c^3 \times (N/V)$
- $O(N)$ algorithm uses: (1) spatially localized cells; & (2) linked lists to keep track of atoms' cell membership

Data-local migration path to parallel MD



Prune the search space!

Cell Data Structures

Data-local spatial indexing scheme = cell + linked list

- Cell size

$$L_{ca} = \lfloor L_\alpha / r_c \rfloor \text{ (int lc[3])}$$

$$r_{ca} = L_\alpha / L_{ca} \text{ (\alpha = x, y, z) (double rc[3])}$$

where

L_α : simulation box length

(double Region[3])

r_c : Cut-off length (RCUT)

- Vector cell index, $0 \leq c_\alpha \leq L_{cx}-1$

- Serial cell index:

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

or

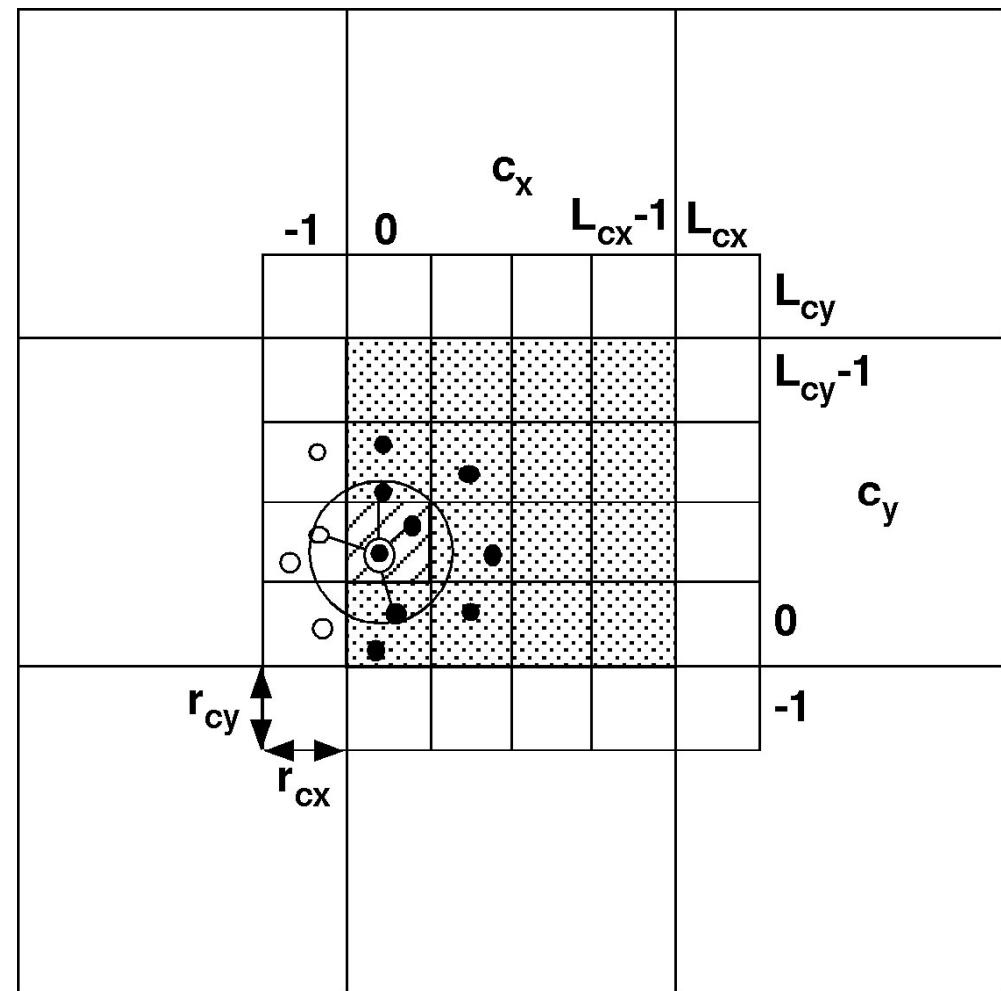
$$c_x = \lfloor c / (L_{cy} L_{cz}) \rfloor$$

$$c_y = \lfloor c / L_{cz} \rfloor \bmod L_{cy}$$

$$c_z = c \bmod L_{cz}$$

- Atom-to-cell mapping:

$$c_\alpha = \lfloor r_\alpha / r_{ca} \rfloor$$

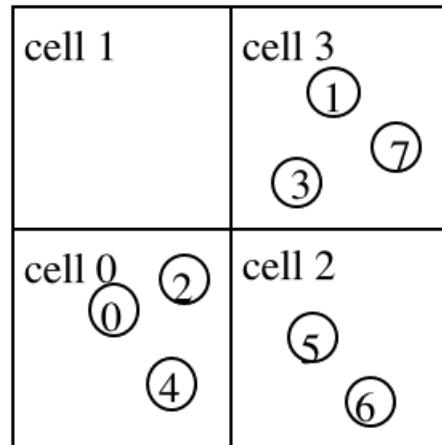


Linked Lists

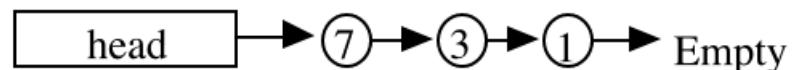
Data Structures:

`lscl[NMAX]`: Linked lists; `lscl[i]` holds the atom index to which the i -th atom points.

`head[NCLMAX]`: `head[c]` holds the index of the first atom in the c -th cell, or `head[c] = EMPTY (= -1)` if there is no atom in the cell.



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

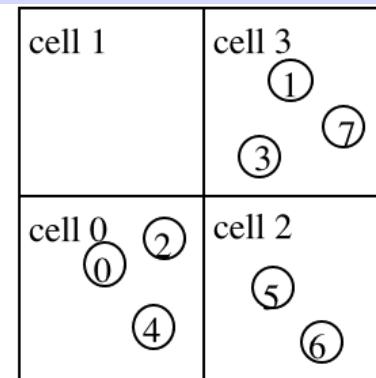


Linked List Construction Algorithm

```
/* Reset the headers, head */
for (c=0; c<lczxyz; c++) head[c] = EMPTY;
/* Scan atoms to construct headers, head, & linked lists, lscl */
for (i=0; i<nAtom; i++) {
    /* Vector cell index to which this atom belongs */
    for (a=0; a<3; a++) mc[a] = r[i][a]/rc[a];
    /* Translate the vector cell index, mc, to a scalar cell index */
    c = mc[0]*lcyz+mc[1]*lc[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;
}
```

where

$$\begin{aligned} lcyz &= lc[1]*lc[2] \\ lczxyz &= lcyz*lc[0] \end{aligned}$$



Single pass over atoms $\rightarrow O(N)!$

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



$O(N)$ Force Calculation Algorithm

```
for (mc[0]=0; mc[0]<lc[0]; (mc[0])++)  
for (mc[1]=0; mc[1]<lc[1]; (mc[1])++)  
for (mc[2]=0; mc[2]<lc[2]; (mc[2])++) { /* Scan inner cells */  
    O(N) c = mc[0]*lcyz+mc[1]*lc[2]+mc[2]; /* Calculate a scalar cell index */  
    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])++) { /* Scan neighbor cells */  
                O(1) for (a=0; a<3; a++) { /* Unwrapping the periodic boundary condition */  
                    if (mc1[a] < 0)  
                        rshift[a] = -Region[a];  
                    else if (mc1[a]>=lc[a])  
                        rshift[a] = Region[a];  
                    else  
                        rshift[a] = 0.0;  
                }  
                c1 = ((mc1[0]+lc[0])%lc[0])*lcyz  
                     +((mc1[1]+lc[1])%lc[1])*lc[2]  
                     +((mc1[2]+lc[2])%lc[2]); /* Scalar cell index of the neighbor cell */  
                i = head[c]; /* Scan atom i in cell c */  
                while (i != EMPTY) {  
                    j = head[c1]; /* Scan atom j in cell c1 */  
                    while (j != EMPTY) {  
                        if (i < j) { /* Avoid double counting of pair (i, j) */  
                            rij = ri-(rj+rshift); /* Image-corrected relative pair position */  
                            if (rij < rc2)  
                                Compute forces on pair (i, j)  
                        }  
                        j = lscl[j]; /* Follow the chain of linked atoms in neighbor cell */  
                    }  
                    i = lscl[i]; /* Follow the chain of linked atoms in central cell */  
                }  
            }  
        }  
    }  
}
```

Scaling of Linked-List Cell MD

