Molecular Dynamics

Sandro Bottaro - SISSA

MHPC – April 2016

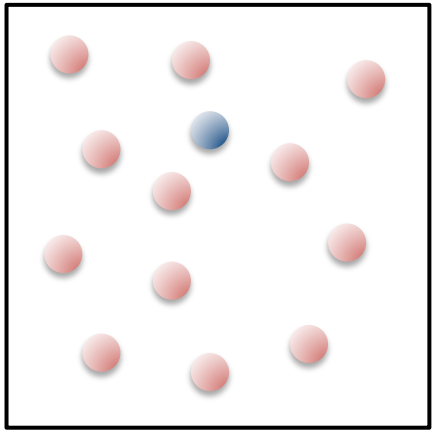
Cell list

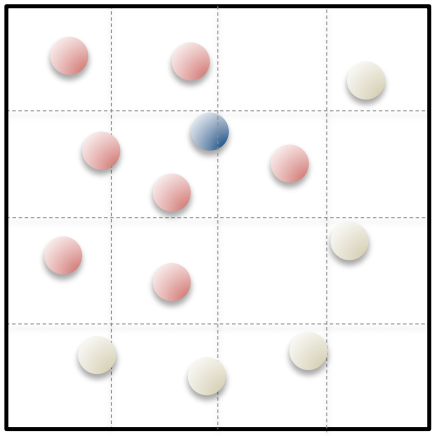
- Verlet list gives speed-up
- Energy/force calculation is O(N)
- List update is $O(N^2)$

Can we do better?

Cell lists

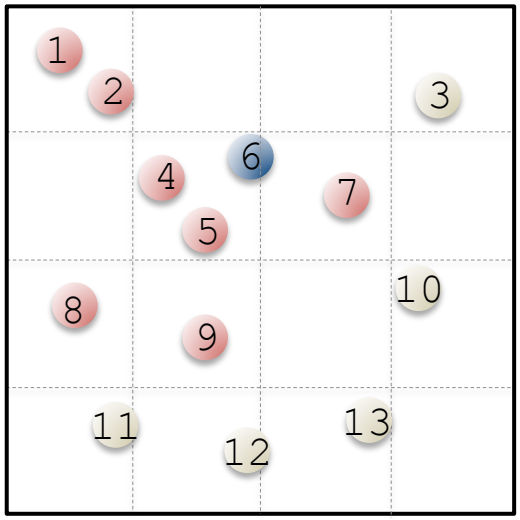
1. Divide unit cell in MxMxM cells (att! This has nothing to do with PBC!)
2. $l=L/M > r_c$
3. Search neighbors in adjacent cells only!
4. $N_c = N/M^3$
5. For each particle 27Nc neighbors instead of N-1





Implementation – naive

Construct a 2d array



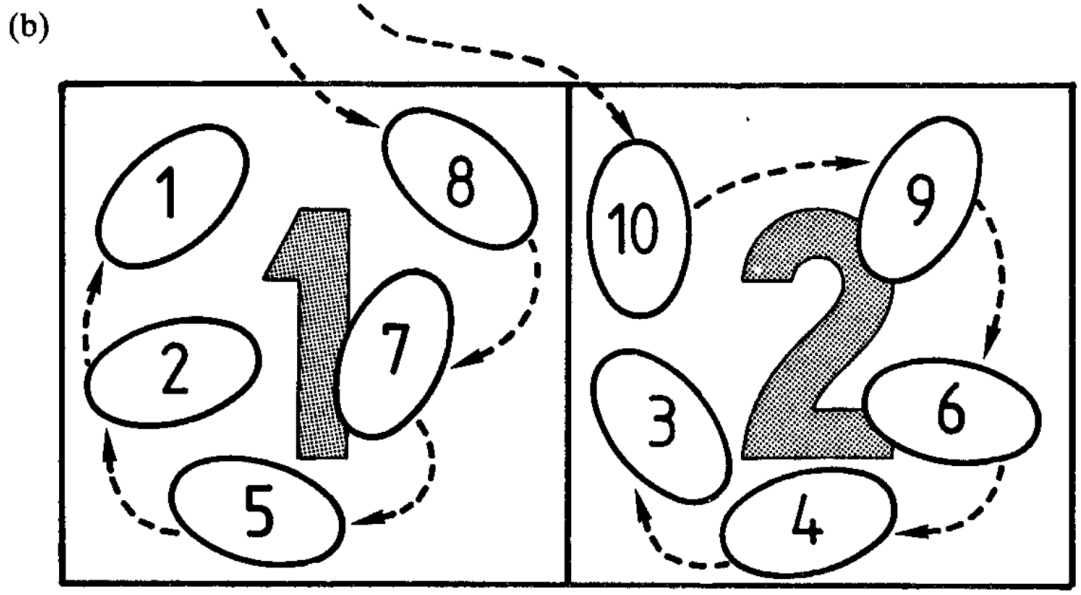
DOMAIN	PARTICLE
1	1 2
2	0
3	0
4	3
5	0
6	4 5 6
7	7
8	0
9	8
…	…

Implementation – linked cells

Construct 2 arrays:

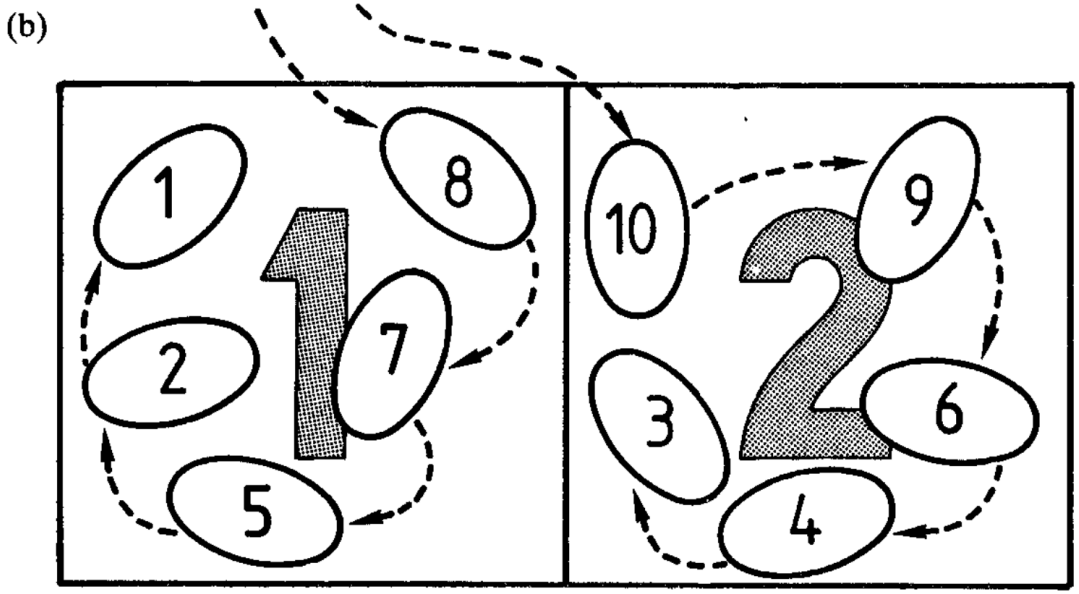
- HEAD length m^3 (number of cells)
  contains the index of one particle in that cell
  (none or 0 if there are no particles)
- LIST length n (number of atoms)
  contains the index of another particle in that cell

Implementation – linked cells



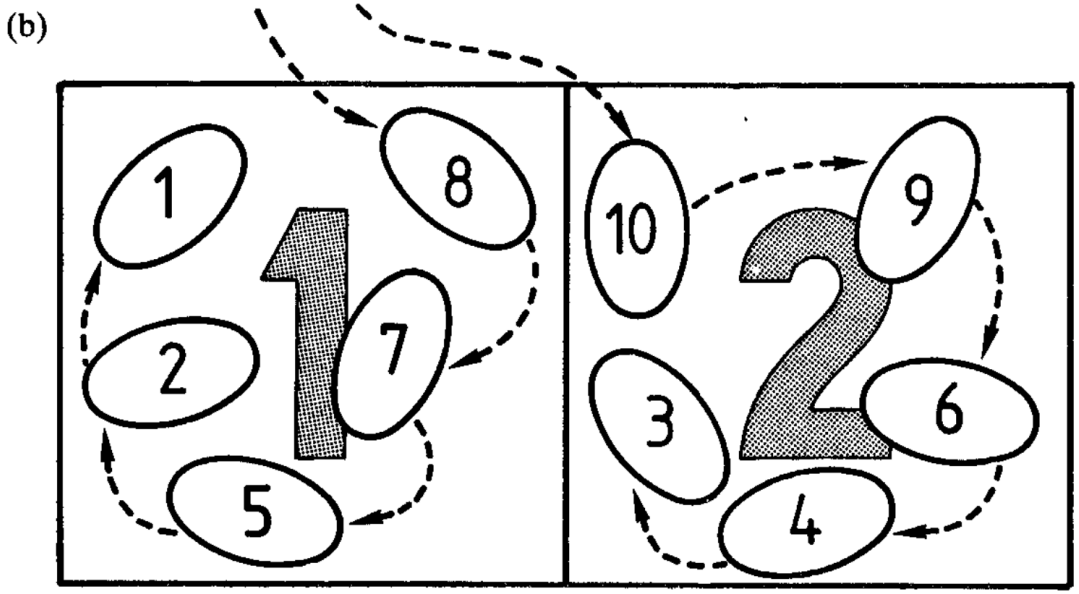
PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	8	10								
LIST	0	1	0	3	2	4	5	7	6	9

Implementation – linked cells



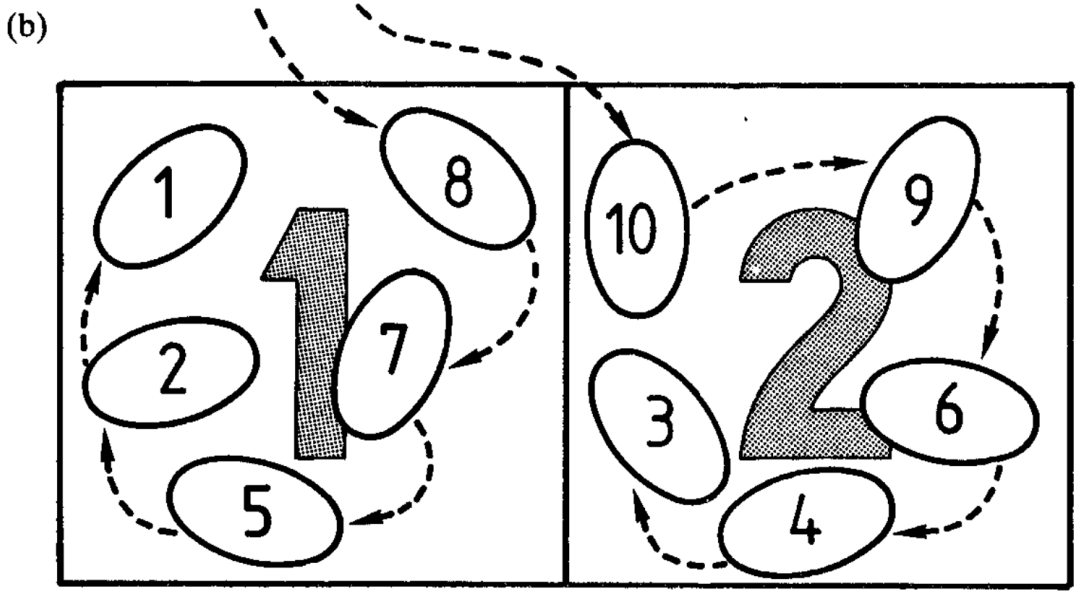
PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	8	10								
LIST	0	1	0	3	2	4	5	7	6	9

Implementation – linked cells



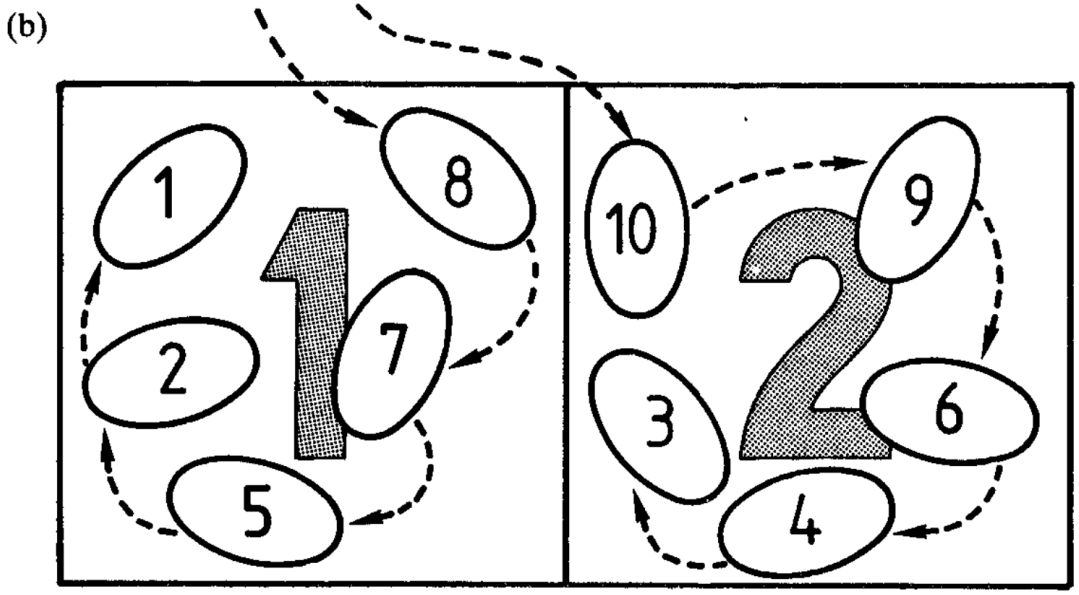
PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	**8**	10								
LIST	0	1	0	3	2	4	5	**7**	6	9

Implementation – linked cells



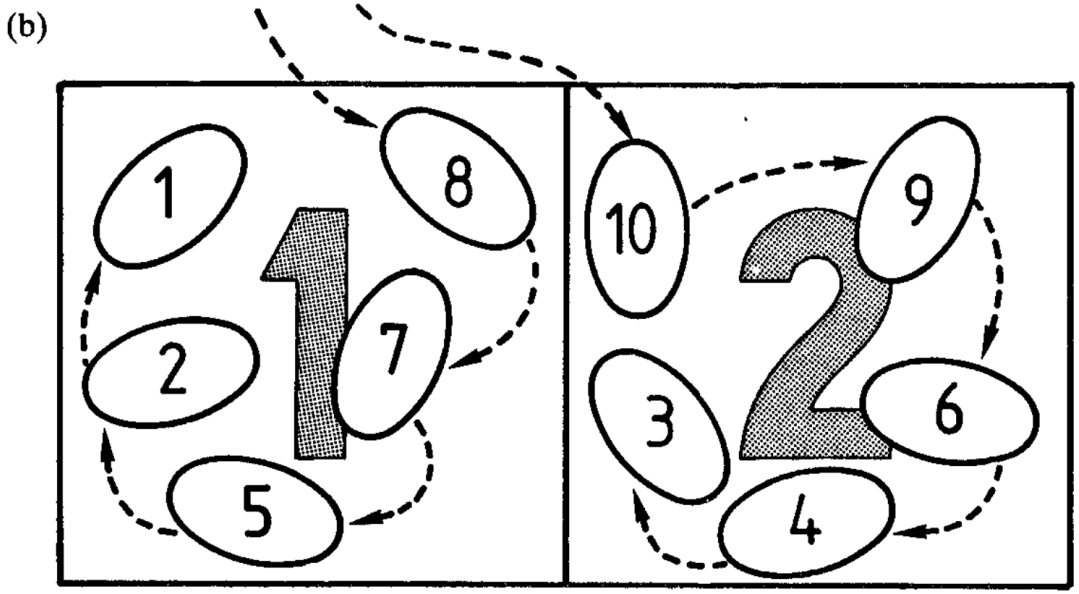
PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	8	10								
LIST	0	1	0	3	2	4	5	7	6	9

Implementation – linked cells



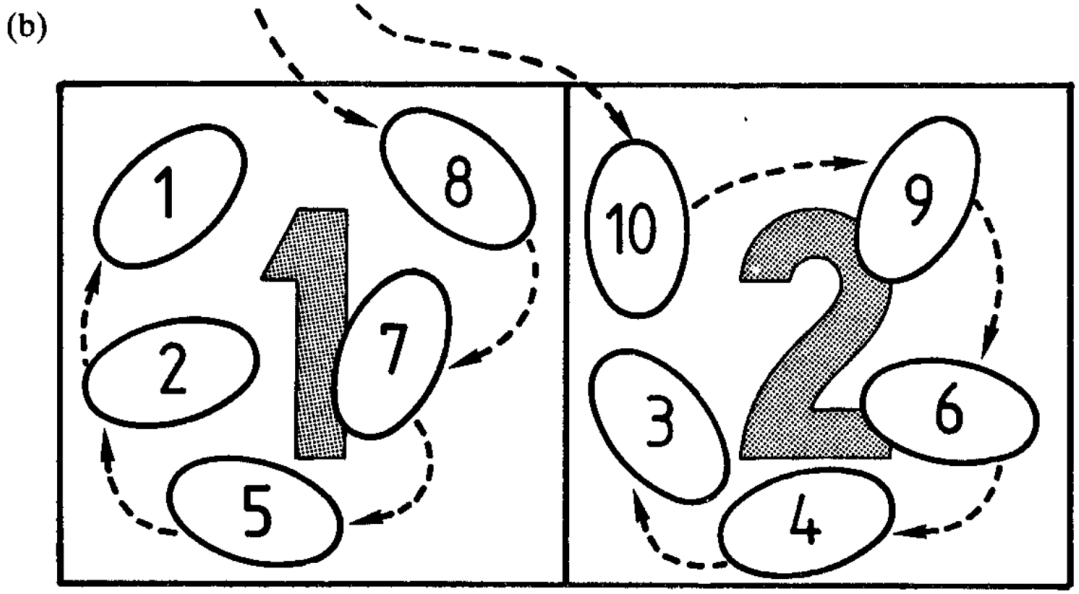
PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	**8**	10								
LIST	0	1	0	3	**2**	4	**5**	**7**	6	9

Implementation – linked cells



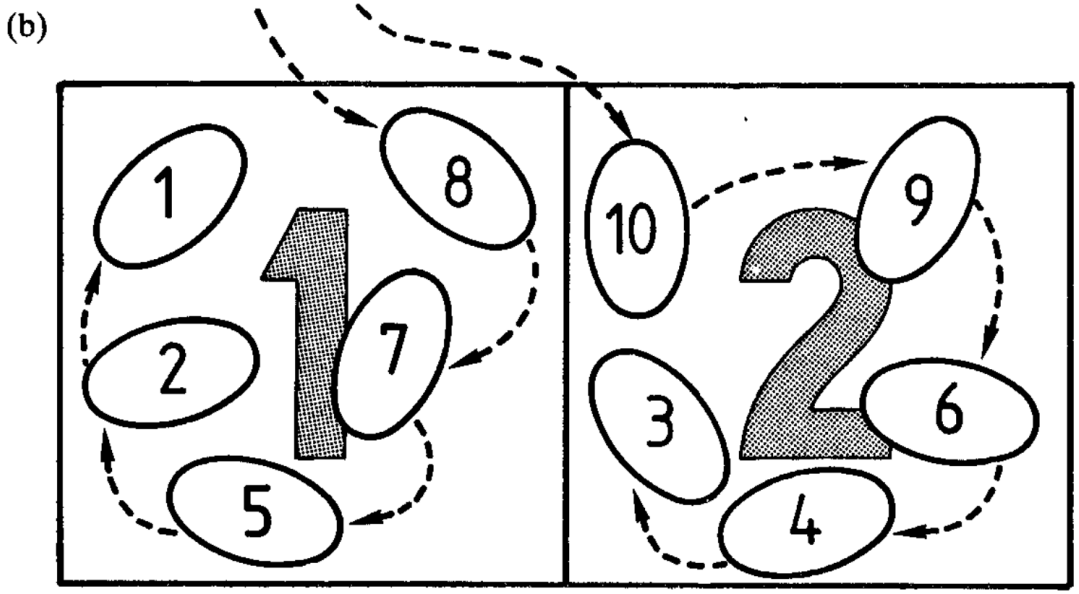
PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	**8**	10								
LIST	0	**1**	0	3	**2**	4	**5**	**7**	6	9

Implementation – linked cells



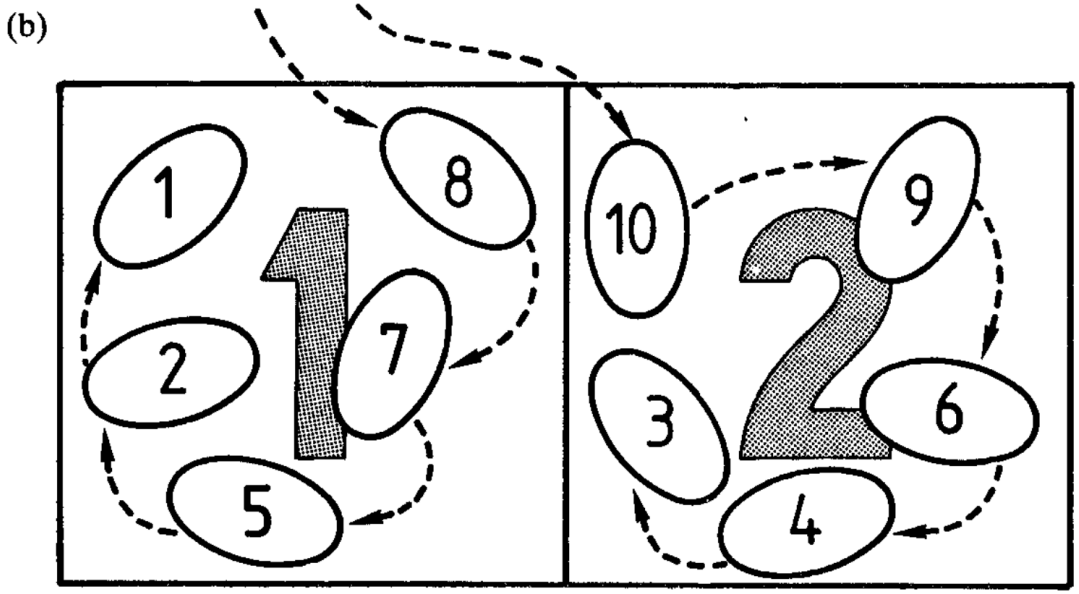
PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	**8**	10								
LIST	0	**1**	0	3	**2**	4	**5**	**7**	6	9

Implementation – linked cells



PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	**8**	10								
LIST	**0**	**1**	0	3	**2**	4	**5**	**7**	6	9

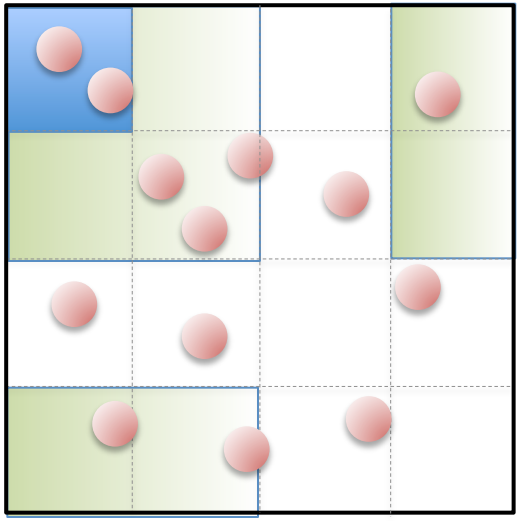
Implementation – linked cells



PARTICLE	1	2	3	4	5	6	7	8	9	10
HEAD	8	**10**								
LIST	0	1	**0**	**3**	2	**4**	5	7	**6**	**9**

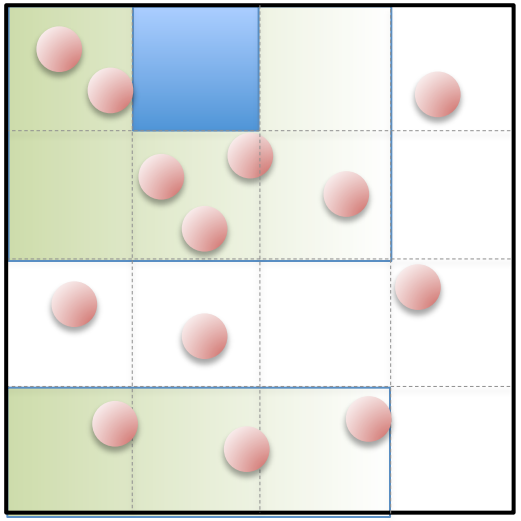
Implementation

Once list/linked cells are constructed loop over all cells and neighboring cells



Implementation

Once list/linked cells are constructed loop over all cells and neighboring cells



Implementation

Once list/linked cells are constructed loop over all cells and neighboring cells