Treatment of long range potentials

The calculation of the energy and forces coming from long range electrostatic forces (monopole, dipole interaction etc) can be numerically expensive. Let us concentrate on the slowest decaying monopole interaction. The electrostatic problem is equivalent to a gravitational problem. Because the gravitational problem lends itself more easily to a pictorial description of the algorithm, we will consider the gravitational problem.

$$E = \sum_{i<j} \frac{m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Trivial algorithm

```
e=0.
do j=1,n
do i=1,j-1
  rij=sqrt( (x(i)-x(j))**2 + (y(i)-y(j))**2 + (z(i)-z(j))**2 )
  e=e+M(i)*M(j)/rij
enddo
enddo
```

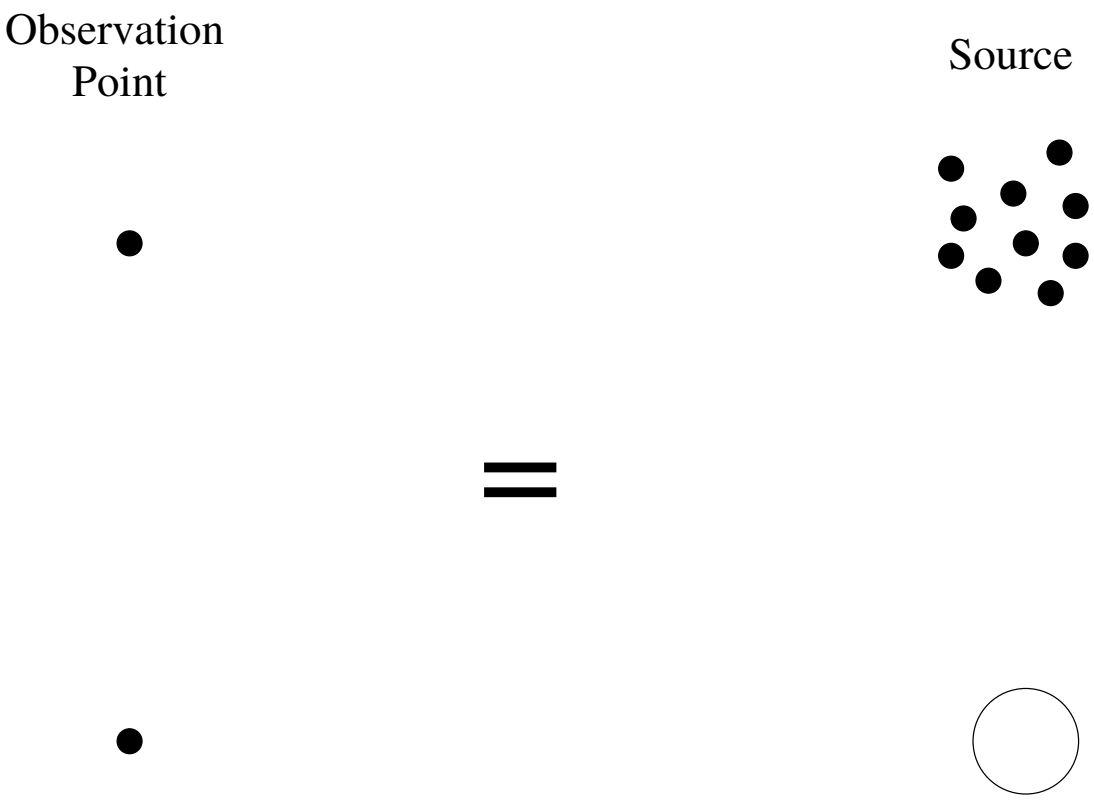
Quadratic scaling:

$$T_{CPU} \propto N^2$$

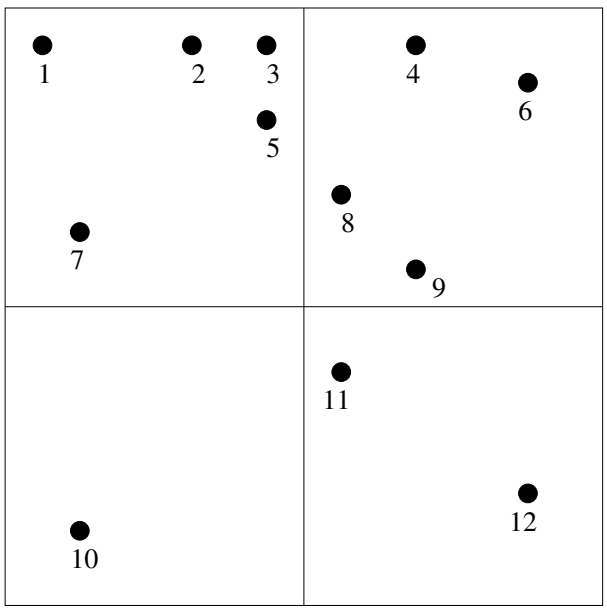
The Barnes Hut algorithm

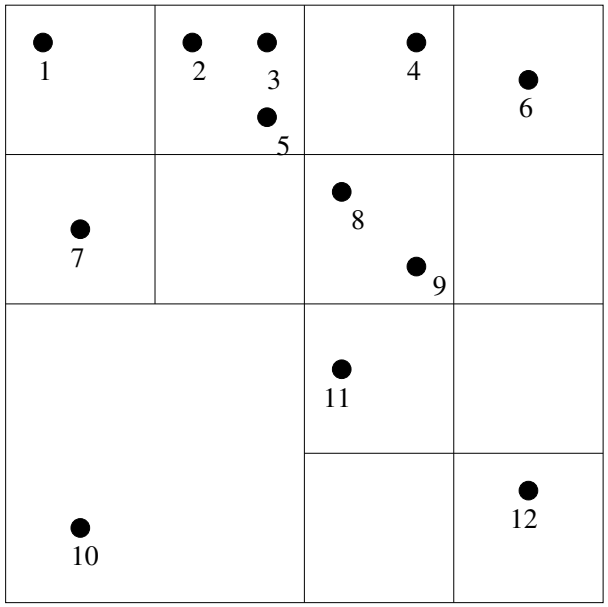
$$T_{CPU} \propto N \log(N)$$

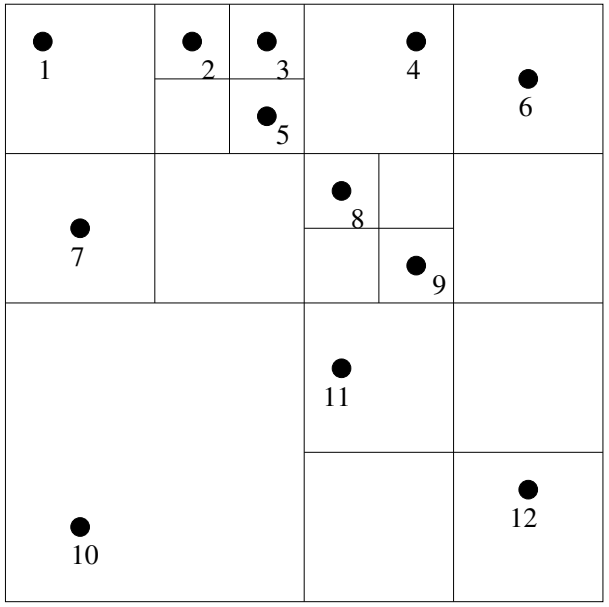
Central idea: *From far away, a bunch of stars looks like a single larger star*

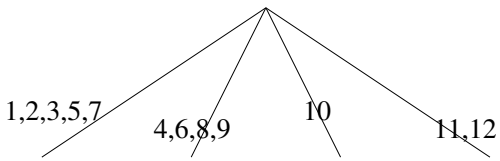


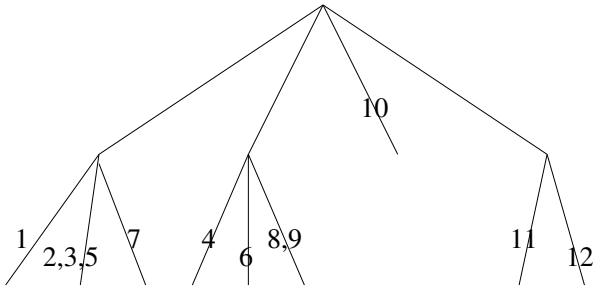
Step 1: Subdivide system and generate tree

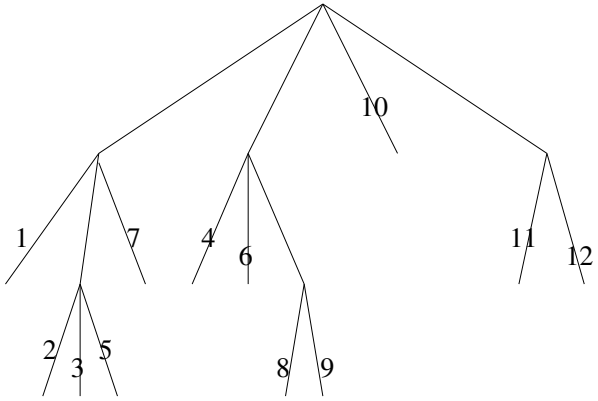






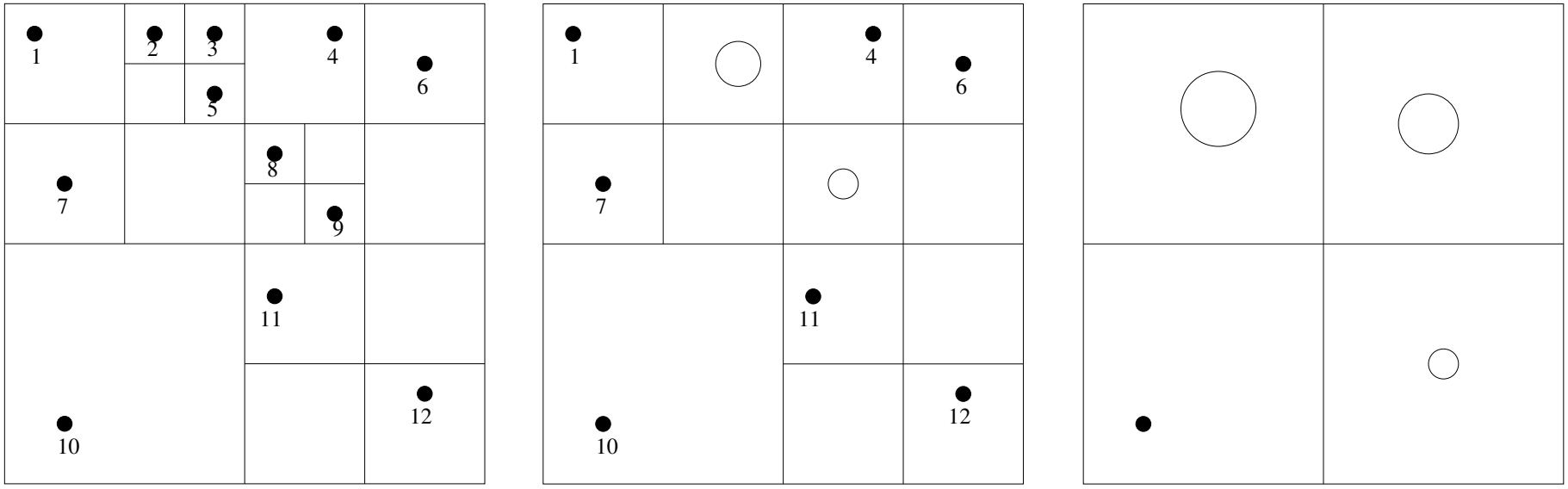






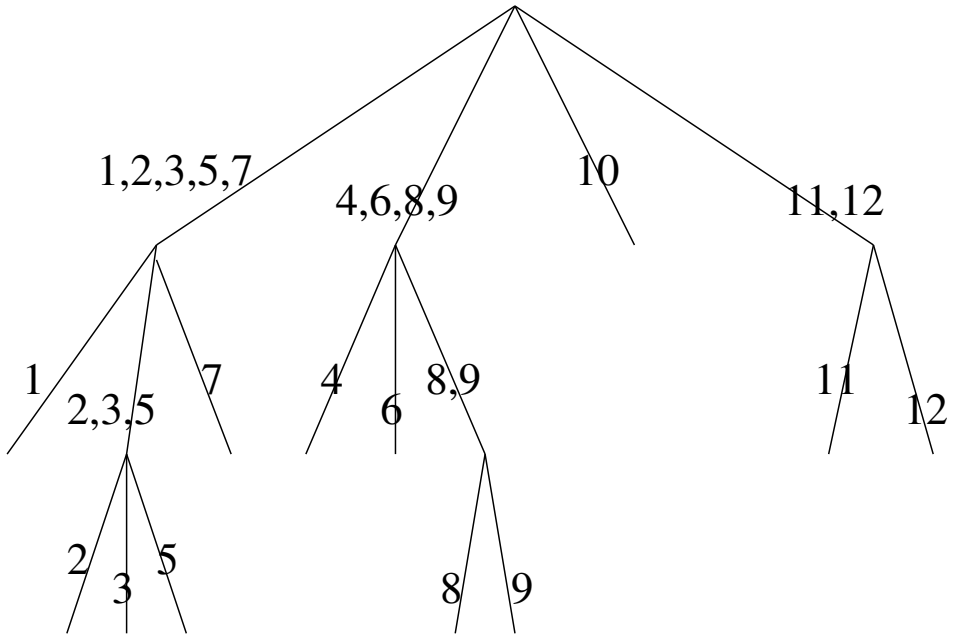
The initial box is chosen such that it contains the entire system. This initial box is then successively subdivided into sub-boxes, 4 in the 2-dim case, 8 in the 3-dim case. This subdivision is stopped when the sub-box contains a single star.

Step 2: Combine stars into super-stars, super-super-stars, ..., galaxies



Super-stars are formed out of individual stars contained in the boxes at the penultimate subdivision level. The mass of a super-star equals the sum of the masses of its constituent stars and it is centered at their center of mass. In the same way second order super-stars (super-super-stars) are formed out of super-stars, third order super-stars out of second order super-stars and so on.

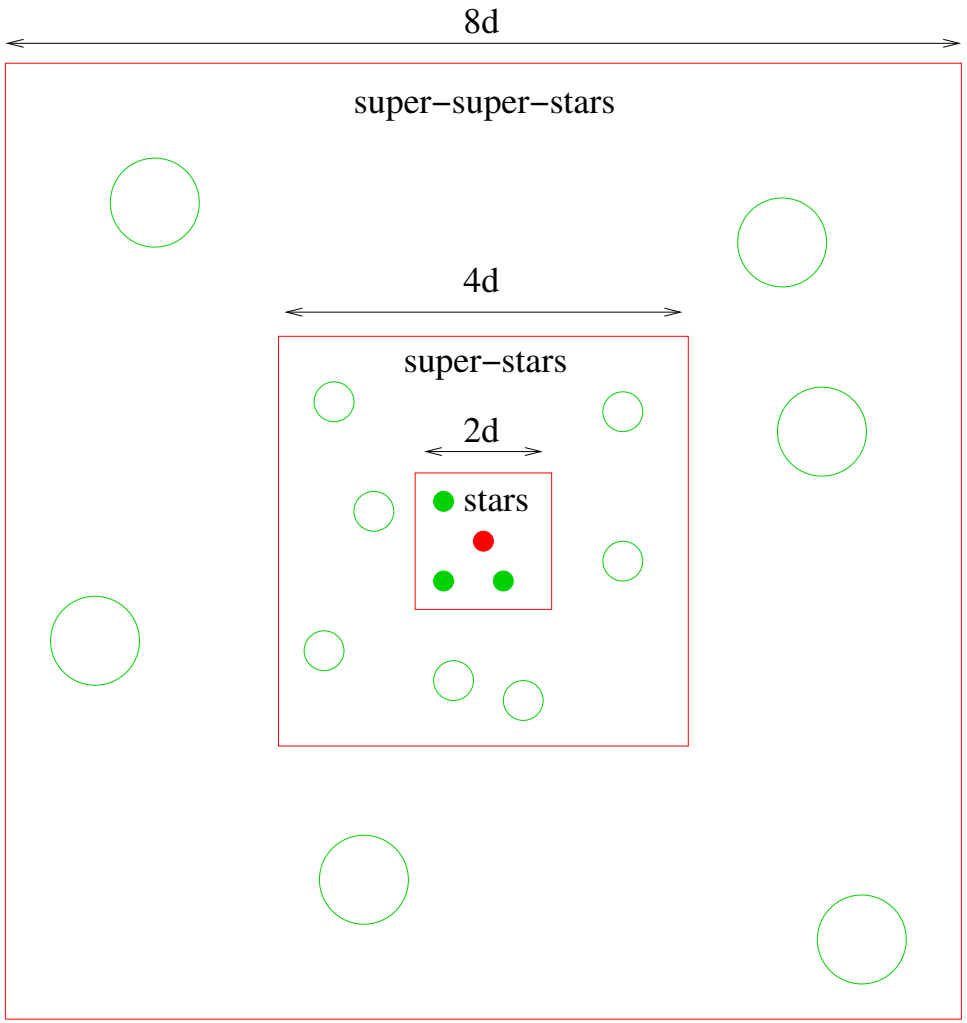
Final redundant data structure in tree form



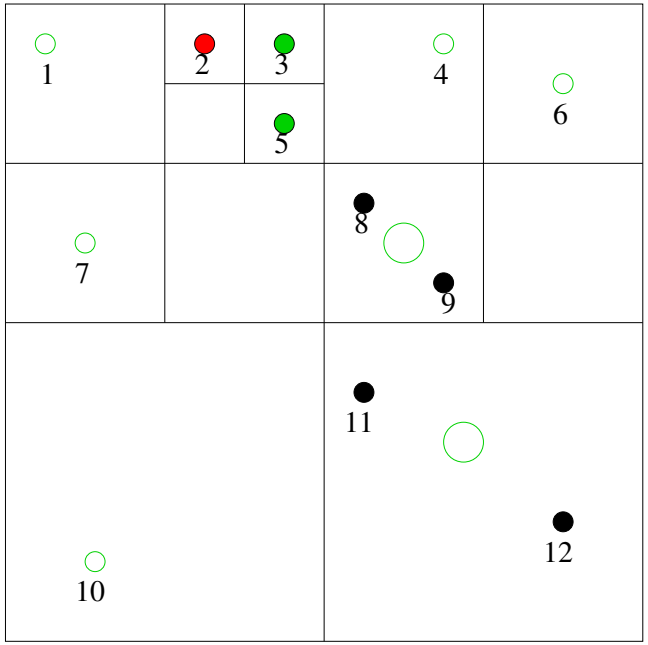
The final redundant data structure contains the positions and masses of the original stars as well as the positions and masses of all the super-stars of various order.

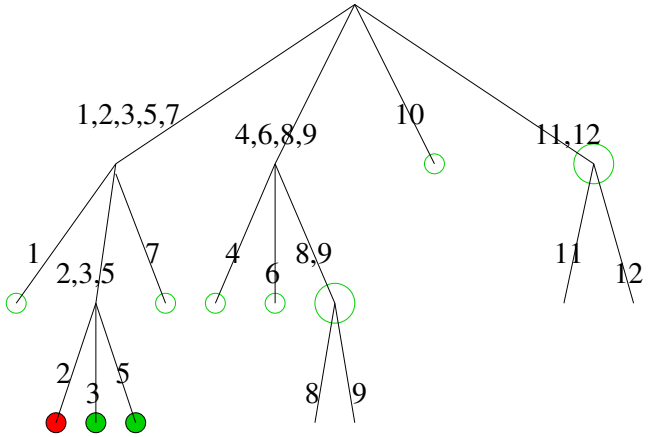
Step 3: Calculate forces

A distance d is introduced. The interaction of the red star with all the other green stars within a box of size $2d$ are calculated exactly. The interactions with the additional stars that are within a box of size $4d$ are not calculated exactly but are taken into account as interactions with the super-stars formed out of these additional stars. In the largest box shown below only the interactions of the red star with the second order super-stars are used.



Since the size of the boxes increases exponentially, there are of the order of $\log(n)$ types of interaction regions and each region contains a few super-stars of a certain order. Hence one has to sum $\log(n)$ terms to take into account the interaction of one fixed star with all the other $n-1$ stars. The total computational effort is consequently $c\,n\,\log(n)$, where c is the prefactor. The interaction to be considered for one particular (red) star of our previous example are shown below, both in real space and within the tree structure.

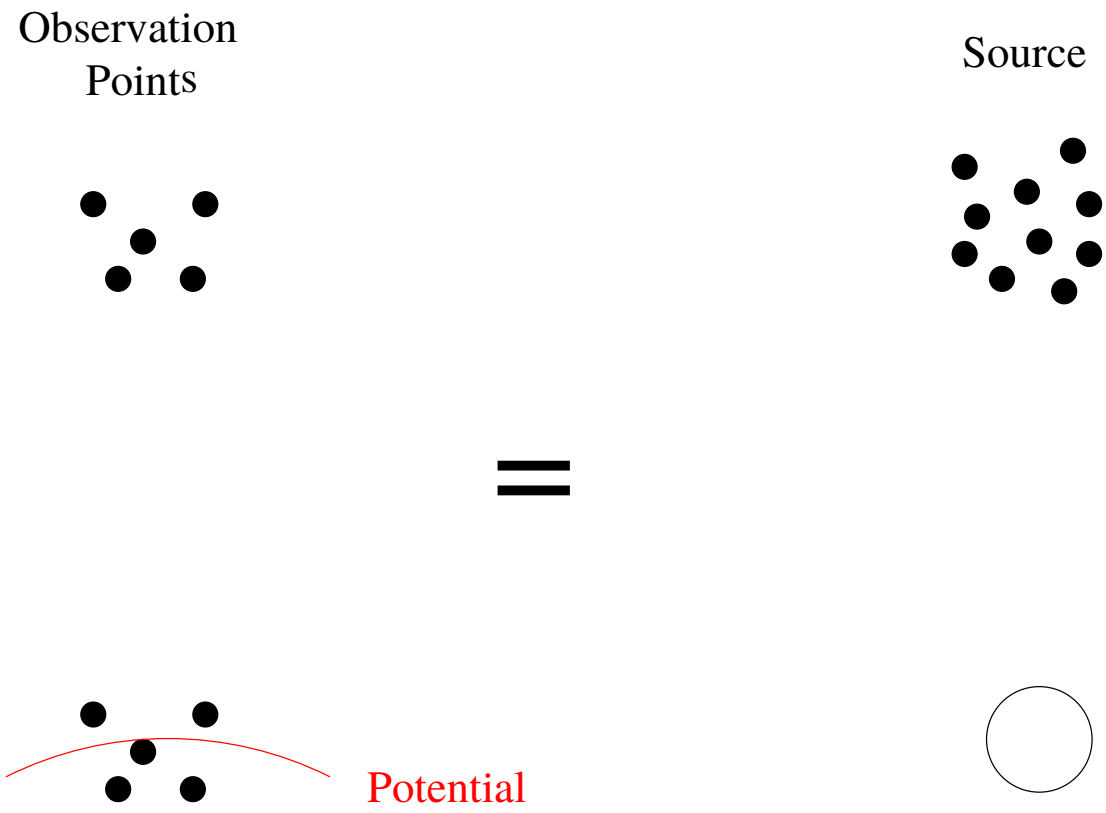




If one wants to obtain higher accuracy, one has to increase the distance d. This increases of course the prefactor c since more interactions will be calculated directly.

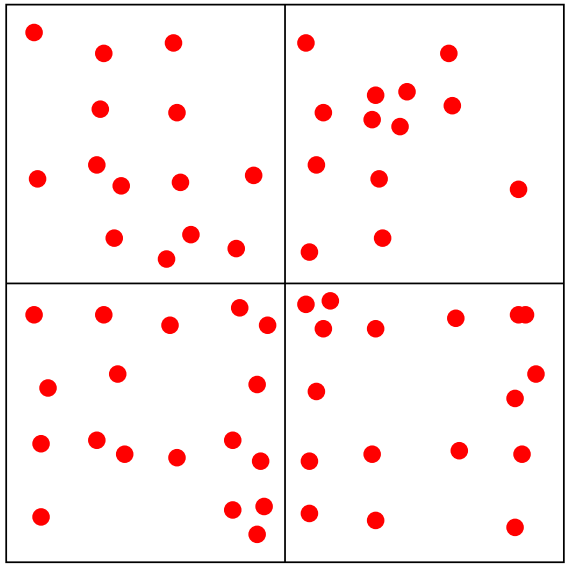
The fast multipole method

The fast multipole method (FMM) goes one step further than the Barnes Hut method. It uses not only the fact that the potential at an observation point does not depend on the details of a charge/mass source distribution far away, but also on the fact that the potential of such a charge/mass distribution is only slowly varying in the neighborhood of an observation point.

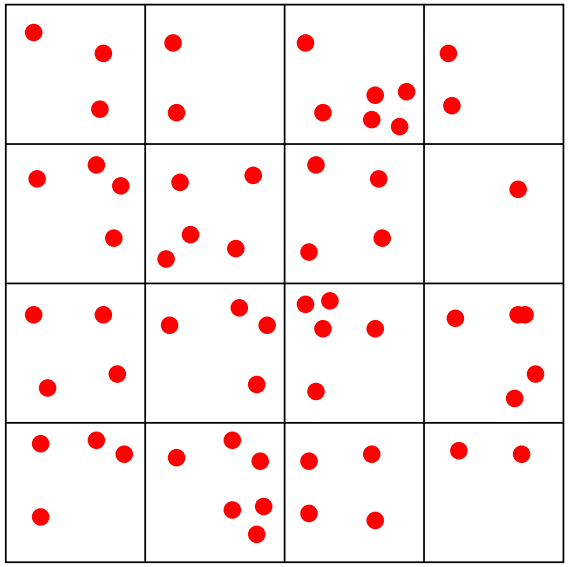


Even though both methods are hierarchical methods, there are differences. FMM is based on a hierarchy of cells that are combined into larger cells, whereas BH combines stars (particles) into super-stars, super-super-stars, etc. The FMM hierarchy is shown below. The cells at the highest (resolution) level (level 3 in the figure below) can contain more than 1 particle.

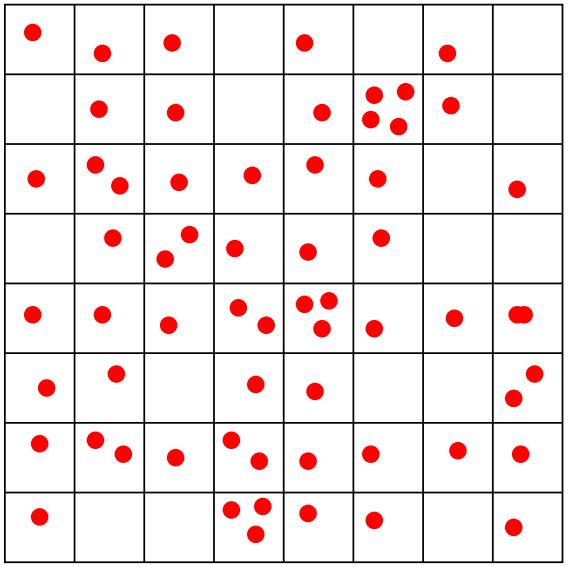
Level 1



Level 2



Level 3



FMM also uses redundant data structures. For each cell on any level of the hierarchy, the following 2 items are stored:

- The multipole coefficients $M_{l,m}$ of the charge distribution,

$$M_{l,m} = \sum_i m_i s_i^l Y_{l,m}^*(\hat{\mathbf{s}}) \tag{53}$$

where $\mathbf{s}$ is the position of the particle relative to the cell under consideration. How many multipoles are stored, depends on the precision that has to be achieved. The potential V is related to $M_{l,m}$ by

$$V_{multipole}(\mathbf{r}) = \sum_l \frac{4\pi}{(2l+1)\, r^{l+1}} \sum_{m=-l}^{m=l} M_{l,m}\, Y_{l,m}(\hat{\mathbf{r}})$$

- The coefficients $L_{l,m}$ of the local Taylor expansion of the potential

$$V_{Taylor}(\mathbf{r}) = \sum_l \sum_{m=-l}^{m=l} r^l L_{l,m}\, Y_{l,m}(\hat{\mathbf{r}})$$

The conventions of Jackson (1975) were used for the spherical harmonics and multipoles. FMM uses the following mathematical transformations. The origin is thereby always the center of the cell.

- COMBINE: 8 multipole coefficients $M^h_{l,m}$ from a high level are combined to obtain the multipole coefficient $M^{2h}_{l,m}$ of the parent cell. This requires to first shift the multipoles into the origin of the parent cell and then to add them. The shifted multipoles $M'^h_{l,m}$ are given by

$$M'^h_{l',m'} = \sum_{l,m} T^{MM}_{l',m',l,m} M^h_{l,m}$$

$$T^{MM}_{l',m',l,m} = 4\pi \frac{(-t)^{l'-1}(2l'+1)}{2(l+1)(2(l'-l)+1)} \frac{Y^*_{l-l',m-m'}(\hat{\mathbf{t}})\, a'_{l'-l,m'-m}\, a_{l,m}}{a_{l',m'}}$$

$$a_{l,m} = (-1)^{l+m} \frac{2\sqrt{l+1}}{\sqrt{4m\,(l+m)!\,(l-m)!}}$$

where $\mathbf{t}$ is the translation vector between the 2 origins.

$$M^{2h}_{l,m} = \sum_{\substack{8\ multipoles \\ from\ children}} M'^h_{l',m'}$$

- FLIP: The coefficients $M^h_{l,m}$ are transformed into the coefficients $L^h_{l,m}$

$$L^h_{l',m'} = \sum_{l,m} T^{LM}_{l',m',l,m} M^h_{l,m}$$

$$T^{LM}_{l',m',l,m} = 4\pi \frac{(-1)^{l+m} Y^*_{l+l',m-m'}(\hat{\mathbf{t}}) a_{l,m} a_{l',m'}}{t^{l'+l+1}(2l+1)(2l'+l) a_{l'+l,m'-m}}$$

where $\mathbf{t}$ is the position of the origin of the Taylor expansion relative to the origin of the multipole.

- SHIFT: The local Taylor expansion coefficients $L^h_{l,m}$ of 8 children are generated from the $L^{2h}_{l,m}$ of the parent cell.

$$L^h_{l',m'} = \sum_{l,m} T^{LL}_{l',m',l,m} L^{2h}_{l,m}$$

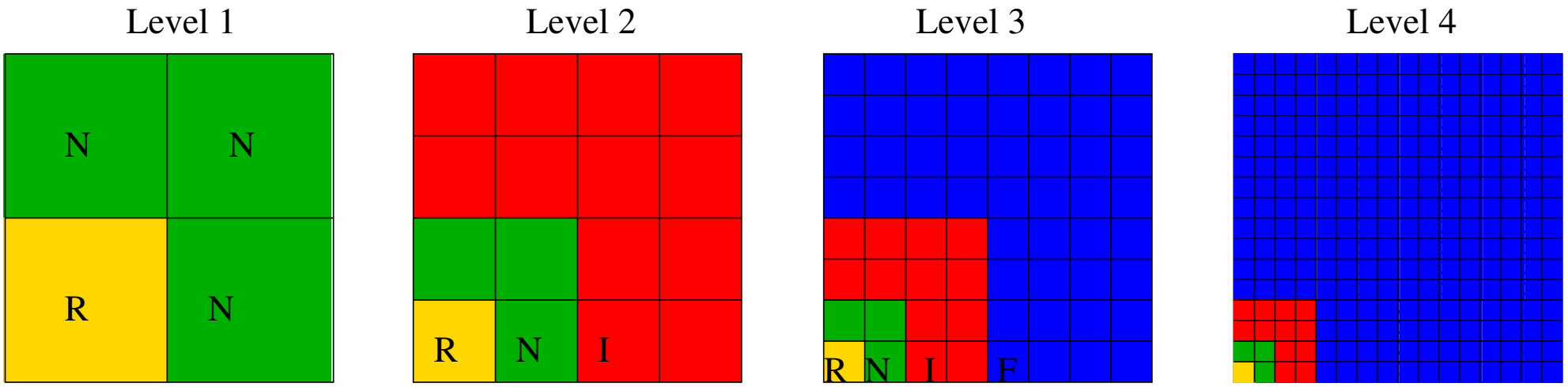
$$T^{LL}_{l',m',l,m} = 4\pi \frac{t^{l-l'} Y_{l-l',m'-m}(\hat{\mathbf{t}}) a_{l',m'} a_{l-l'',m-m'}}{(2l'+1)(2(l-l')+1) a_{l,m}}$$

$\mathbf{t}$ is again the translation vector between the 2 origins.

The FMM algorithm uses the following classification in the calculation of the interactions:

- A cell is near (N) to a reference cell (R) if it shares with this cell a side, edge or corner.
- A cell is interactive (I) to a reference cell (R) if both have parents that were near and if they are themselves not near
- A cell is far (F) in all other cases

The situation is illustrated below:

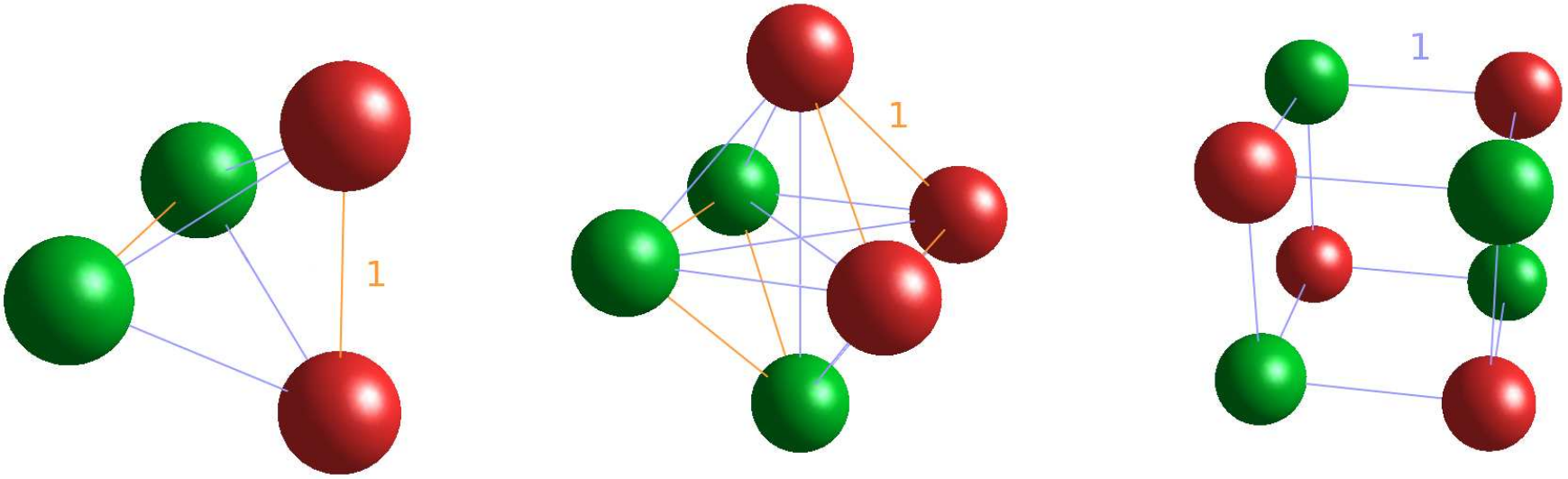


The FMM algorithm goes now as follows:

- Assign the particles to the cells at the finest level and calculate the multipole expansion coefficients $M_{l,m}$ on the finest level.
- Go from the finest level down to the coarsest level and use the COMBINE operation to generate the multipole expansion coefficients for all the bigger cells
- Go back from the coarsest level to the finest level. On each level calculate the coefficients $L_{l,m}$ that are due to interactions with INTERACTIVE cells using the FLIP operation. Use the SHIFT operation to obtain the $L_{l,m}$'s on the finer scales from the previously obtained $L_{l,m}$ on the coarser scales. The total $L_{l,m}$'s on the finest level are obtained by recursively summing both contributions from SHIFT and FLIP operations each level.
- Using the Taylor expansion, calculate on the finest level the potential/forces at the position of all the particles. This represents the potential/forces of all the particles in cells that are not NEAR cells on the finest level. The influence of the NEAR cells at the finest level is obtained by direct summation of the contributions of all the particles in the NEAR cells.

The most important workload is be done at the level of the finest cells. The work at the other levels is small compared to this one (e.g. $1/8$th at the second finest level). Hence the FMM algorithm exhibits linear scaling with respect to the number of the finest cells.

Exercise: *Calculate the monopole, dipole and quadrupole moments for the tetrahedral, octohedral and cubical arrangements of point charges shown below. Red spheres represent a positive charge of 1 and green spheres a negative charge of -1.*



Each polyhedron is centered at the origin and has an edge length of one. A tetrahedron can be obtained by filling four non-neighboring corners of a cube, and an octrahedron can be constructed by filling the six faces. The monopole and the dipole moments for a system of point charges are defined as,

$$Q = \sum_k q_k \; ; \; \mathbf{p} = \sum_k q_k \mathbf{r}_k$$

where q_k and $\mathbf{r}_k$ stand for the value and position of the k^{th} point charge, respectively. The quadrupole moment tensor is given by the following equation.

$$Q_{i,j} = \sum_k q_k \left(3r_{i,k}r_{j,k} - \delta_{i,j}|\mathbf{r}_k|\right)$$

The indices i and j run over the x, y and z components, so we can write for example the xx− or xy−element.

$$Q_{x,x} = \sum_k q_k \left(3x_k^2 - r_k^2\right) \; ; \; Q_{x,y} = \sum_k q_k \left(3x_k y_k\right)$$

These moments correspond to the multipole coefficients $M_{l,m}$ of equation 53 expressed with real-valued linear combinations of spherical harmonics.
Show that the value of the dipole is independent of the choice of the origin if the monopole of the system is zero.