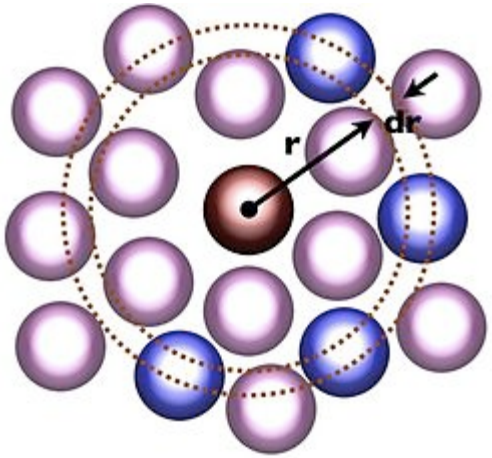
3. Simulating a system of N particles

- Structure: The radial distribution function (RDF)

- The radial distribution function (RDF) describes how density varies as a function of distance from a reference particle . It can be defined as

$$g(r) = \frac{1}{\rho}\frac{n(r)}{4\pi r^2 dr} = \frac{n(r)}{n_{id}(r)}$$



calculation of g(r)

$\rho = \frac{N}{V}$ average number density of particles

$n(r)$ Mean number of particles within a distance of r and r+dr away from a particle.

$n_{id}(r)$ Mean number of particles ….. for an ideal gas

- The RDF is usually determined by calculating the distance between all particle pairs and binning them into a histogram.

Algorithm for the calculation of the RDF

```
      subroutine gr (switch)                      radial distribution function
                                                  switch = 0 initialization,
                                                  = 1 sample, and =2 results
if (switch. eq.0) then                            initialization
     ngr = 0
     delg=box/(2*nhis)                            bin size
     do i = 1,nhis                                nhis = total number of bins
          g(i) = 0
     enddo
else if (switch.eq.1) then                        sample
     ngr = ngr + 1
     do i=1,npart-1
          do j=i+1,npart                          loop over all pairs
               xr = x(i)-x(j)               !!
               xr = xr-box*nint(xr/box)     !!    periodic boundary conditions
               r = sqrt(xr**2)              !!
               if (r.lt.box/2)  then              only within half the box length
                   ig = int(r/delg)
                   g(ig) = g(ig) +2               contribution for particle i and j
               endif
           enddo
      enddo
```

Algorithm for the calculation of the RDF *cont.*

```
else if (switch.eq.2) then                          determine g(r)
      do i=1,nhis
          r=delg*(i + 0.5)                          distance r
          vb = ((i+1)**3-i**3)*delg**3              volume between bin i+1 and i
          nid = (4/3)*pi*vb*rho                     number of ideal gas part . in vb
          g(i) =g(i) /(ngr*npart*nid)               normalize  g(r)
       enddo
    endif
    return
    end
```

Comments :

1. *The sampling part is usually combined with the force calculation*
2. *The factor pi=3.14159 ….*

From Frenkel&Smit book