

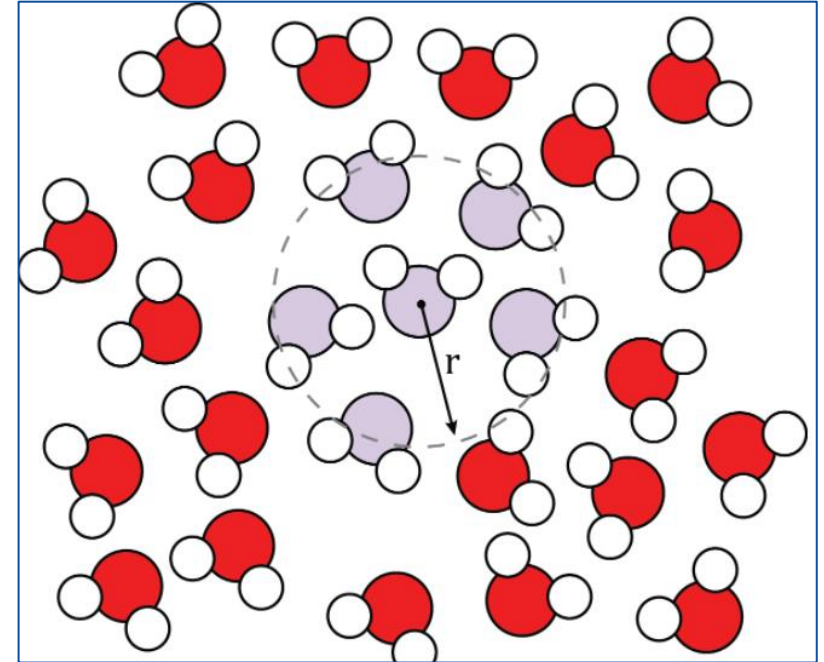
# Application

# APPLICATION

## Molecular Simulation

### RDF

The radial distribution function (RDF) denoted in equations by  $g(r)$  defines the probability of finding a particle at a distance  $r$  from another tagged particle.



# RDF

## Pseudo Code - C

```
for (int frame=0;frame<nconf;frame++){  
    for(int id1=0;id1<numatm;id1++){  
        {  
            for(int id2=0;id2<numatm;id2++){  
                {  
                    dx=d_x[id1]-d_x[id2];  
                    dy=d_y[id1]-d_y[id2];  
                    dz=d_z[id1]-d_z[id2];  
                    r=sqrtf(dx*dx+dy*dy+dz*dz);  
  
                    if (r<cut) {  
                        ig2=(int)(r/del);  
                        d_g2[ig2] = d_g2[ig2] +1 ;  
                    }  
                }  
            }  
        }  
    }  
}
```

- Across Frames
- Find Distance
- Reduction

# RDF

## Pseudo Code - Fortran

```
do iconf=1,nframes
  if (mod(iconf,1).eq.0) print*,iconf

  do i=1,natoms
    do j=1,natoms
      dx=x(iconf,i)-x(iconf,j)
      dy=y(iconf,i)-y(iconf,j)
      dz=z(iconf,i)-z(iconf,j)

      r=dsqrt(dx**2+dy**2+dz**2)
      if(r<cut)then
        g(ind)=g(ind)+1.0d0
      endif
    enddo
  enddo
enddo
```

- Across Frames
- Find Distance
- Reduction

# Acknowledgment

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