Algorithm 7 (The Radial Distribution Function)

```
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=0,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
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 to this algorithm:

1. *For efficiency reasons the sampling part of this algorithm is usually combined with the force calculation (for example, Algorithm 5).*
2. *The factor* `pi` *= 3.14159....*