Exercises Lecture XI
Classical fluids:
simulation with Metropolis Monte Carlo
(and with Molecular Dynamics)

1. **Monte Carlo Simulation of hard disks**

   Write a code for a Monte Carlo simulation of hard disks in 2D. One example is `hd-MC.f90`, which makes use of the *periodic boundary conditions* and the *minimum image convention* to calculate the minimum distance (function `separation`).
   If σ is the *diameter of the disks*, the highest possible density is ρ_{max}=$2/(\sqrt{3}\sigma^2)$. It is convenient to use σ as unit length and measure all lengths in terms of σ and use the *reduced density*, defined in general as $\rho^* = \rho\sigma^d$, where d is the dimensionality of the system. The highest possible *reduced density* is $\rho^*_{max} = \rho_{max}\sigma^2 = 1.1547$, corresponding to the maximum *packing fraction* $f = area_{occupied}/area_{available} = \pi/(2\sqrt{3}) = 0.9069$.

   (a) Start simulating the fluid with a density close to the maximum one. To this purpose, it is convenient to set the initial positions of the particles on a triangular lattice. Choose for instance $N = 16$ with the dimension of the box $L_x = 4.41\sigma$ and $L_y = 0.5\sqrt{3}L_x$. Calculate ρ^* and compare it with ρ^*_{max}. A reasonable first choice for the maximum random displacement in a Monte Carlo simulation is $dxmax = dymax = 0.1\sigma$. Calculate the corresponding *acceptance ratio*. Allow at least 500 MC steps for equilibration and average over $nmcs \geq 500$. Calculate $g(r)$. A reasonable choice for the bin width `dr` for the calculation of $g(r)$ is `dr`=0.1.

   (b) Reduce progressively ρ^*, saving the configuration of a run and using it as the input for the new run at lower ρ^*. Keeping the ratio L_x/L_y fixed, it is sufficient to rescale homogeneously all the positions. It may be convenient to vary progressively also $dxmax$ and $dymax$ in order to keep an *acceptance ratio* of the order of 50%. Calculate $g(r)$ for ρ^* =0.95, 0.92, 0.88, 0.85, 0.80, 0.70, 0.60, and 0.30 and compare the profiles (how many peaks? where? ...)

   (c) Take "snapshots" of the disks at intervals of about 10 to 20 MC steps per particle. Do you see any evidence of the solid becoming a fluid at lower densities?

2. **Monte Carlo simulation of a Lennard-Jones system**

Consider particles interacting with the Lennard-Jones potential:

$$v(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

It is convenient to use the adimensional quantities $E^* = E/\epsilon$, $T^* = k_B T/\epsilon$, $\rho^* = \rho\sigma^2$ for energy, temperature and density respectively. For numerical simulations use Periodic Boundary Conditions and the *minimum image convention*, with a *cutoff radius* for the potential consistent with the size of the simulation box. *(No draft code is given)*

(a) Start with $T^* = 0$ and calculate the energy E_0^* of the ground state of the system. Choose $N = 16$, $L_x = 4.5\sigma$, $L_y = (6\sqrt{3}/2)\sigma$, and the particles on a triangular lattice: the system is therefore close to the equilibrium, and a few MC steps are already enough to have a good estimate of E_0^*. Does the energy per particle change if you consider bigger systems at the same density?

(b) Increase the temperature $T^* = 3.5$ and calculate E^* and $g(r)$.

(c) Describe qualitatively $g(r)$ and compare it with the hard disks case.

(d) Repeat the calculations for a smaller density, expanding by a factor of 1.5 the dimensions of L_x and L_y. Compare with the previous results and with the hard disks case with the same density.

3. **Molecular dynamics of a Lennard-Jones system** *(Optional)*

The program `LJ-MD.f90`, from Gould-Tobochnick, considers a bidimensional Lennard-Jones system, and makes use of the *velocity-Verlet* algorithm for the numerical integration of the Newton equations of motion to perform a *molecular dynamics* simulation. In 1D (with obvious extension in higher dimensions) the algorithm is:

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n (\Delta t)^2$$

$$v_{n+1} = v_n + \frac{1}{2}(a_{n+1} + a_n)\Delta t$$

The new position x_{n+1} is used to find the new acceleration a_{n+1}, which is used together with a_n to obtain the new velocity v_{n+1}.

(a) Consider a system with $N = 16$ particles in a square box with $L = 6$. Choose $\Delta t = 0.01$ and test the program: follow the trajectories of the 16 particles making a plot, and check that the total energy is approximately conserved.

(b) Calculate the pair correlation function $g(r)$ for some of the cases with density and temperature proposed in the exercise with Monte Carlo simulation. Compare the results obtained with the two methods.

```
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
! program hdMC  -   MC simulation of hard disks in 2D with PBC
! unit length = diameter
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
implicit none
public :: initial,move,correl,output,save_config

integer, public :: N,nmcs,nbin,accept,nequil
real , dimension(:),allocatable, public :: x,y,gcum
real , public :: Lx,Ly, kx,ky, dr, dxmax,dymax, rho

contains

subroutine initial()
      integer :: Nx,Ny,m,i,j
      real  :: rmax,dx,dy,temp
      character(len=1) :: ans
      logical :: expr
      print*,' number of particles',&
           '(choose a number that can be factorized in two integers) >'
      read*,N
      rho = float(N)/(Lx*Ly)
      write(*,*)' reduced density (rho): ',rho
      print*,' number of columns Ny  (for which  N can be divided) >'
      read*,Ny
      temp = mod(N,Ny)
      if(mod(N,Ny) .ne. 0)call error('error in initial',' mod(N,Ny)',temp)
      Nx = N / Ny
      allocate(x(N),y(N))
      print*,' number of  MC steps per particle per equilibration>'
      read*,nequil
      print*,' number of  MC steps per particle per data production>'
      read*,nmcs
      rmax=min(Lx/2.0,Ly/2.0)
      print*,' number of bins for g(r) >'
      read*, nbin
      allocate(gcum(nbin))
      dr=rmax/nbin
      print*,' max trial displacement of a particle in x and y (dxmax=dymax) >'
      read*,dxmax
      dymax = dxmax
      kx = 2./Lx   ! parameter for PBC
      ky = 2./Ly
      print*,'N =',N,', Ny=',Ny,', Nx=',Nx,'nmcs=',nmcs
      print*,'nbin=',nbin,', rmax=',rmax,', Lx=',Lx,', Ly=',Ly
      print*,' start from old config. (y/n)? >'
```

```
      read(*,'(a)') ans
      if (ans=='y') then
         call read_config()
      else                    ! CREATES a new triangular lattice
         dx = Lx / float(Nx)        ;          dy = Ly / float(Ny)
! max. packing
! dx and dy must be separately .ge. sqrt(3)/2 (in units of sigma)
! and the product dx*dy .ge. sqrt(3)/2
         expr = ((dx<(sqrt(3.)/2)) .or. (dy<(sqrt(3.)/2) ) .or. & ((dx*dy)<(sqrt(3.)/2))
 if (expr) call error('error in initial','  dx*dy = ',dx*dy)
         m = 0
         do j = 1,Ny,2
            do i = 1,Nx
               m = m + 2
               if (m>N) call error('error in initial',' m>N! m = ',float(m))
               ! this should never occur! check!!!
               x(m-1) = (i-0.75)*dx
               y(m-1) = (j-0.5) *dy
               x(m)   = (i-0.25)*dx
               y(m)   = (j+0.5) *dy
             end do
         end do
      end if
  return
end subroutine

subroutine move()
! pick up a particle randomly, generates trial cocordinates,
! apply PBC, check overlap
      integer :: itrial,i
  real  :: xtrial,ytrial,r,ran1,xold,yold
  real , dimension(2) :: ran2
      do i=1,N
call random_number(ran1)
itrial = int(N*ran1 + 1)    ! choose a particle
if(itrial>N) then
        print*,'error generating ran1'
        stop
end if
                 xold=x(itrial)
 yold=y(itrial)
 call random_number(ran2)
 xtrial = x(itrial) + (2.*ran2(1)-1.)*dxmax
                 ytrial = y(itrial) + (2.*ran2(2)-1.)*dymax
         call cell(xtrial,ytrial)
         call overlap(itrial,xtrial,ytrial)
```

```
      end do
      return
end subroutine

subroutine cell(xtrial,ytrial)
! input  xtrial e ytrial,
! output : the same  but rescaled using PB (x in [0,Lx[ and y in [0,Ly[)
      real , intent(inout):: xtrial,ytrial
! floor(A) return the largest integer < or = A
! What follows is OK whatever xtrial and ytrial are
      xtrial = xtrial - Lx*floor(xtrial/Lx)
      ytrial = ytrial - Ly*floor(ytrial/Ly)
      if(xtrial<0 .or. xtrial>=Lx .or. ytrial<0 .or. ytrial>=Ly) &
call error('error   in  cell','  xtrial =',xtrial)
      return
end subroutine

subroutine separation(dx,dy)
! in input  distances dx and dy , which (being already rescaled)
!           are between 0 and L
! in output the same, but rescaled using minimum image convention
!           and therefore = or < L/2)
      real , intent(inout) :: dx,dy
      dx = dx - Lx*int(kx*dx)
      dy = dy - Ly*int(ky*dy)
      return
end subroutine

subroutine overlap(itrial,xtrial,ytrial)
! decide to accept or not after cheching overlap;
! in case, update arrays x,y
      integer, intent(in) :: itrial
      integer :: j
      real ,intent(in) :: xtrial,ytrial
      real :: r2,dx,dy
! disks overlap if distance < 1 (diameter)
  do j = 1,N
         if (itrial /= j) then
            dx = x(j) - xtrial
            dy = y(j) - ytrial
            call separation(dx,dy)    ! calculate true distances
            r2 = dx*dx + dy*dy
           if (r2<1.0) return                   ! overlap!
         end if
      end do
       accept = accept + 1
```

```
        x(itrial) = xtrial
        y(itrial) = ytrial
      return
end subroutine

subroutine correl()
! array gcum contains the number of particles at distance
! between r and r+dr from a given particle.
! gcum is calculated for N/2 particles (to count once each pair)
      integer :: ibin,i,j
      real :: r2,dx,dy
      do i=1,N-1
         do j=i+1,N
            dx = x(i) - x(j)
            dy = y(i) - y(j)
            call separation(dx,dy)
            r2 = dx*dx + dy*dy
            ibin = int(sqrt(r2)/dr)+1
            if (ibin<=nbin) then
gcum(ibin) = gcum(ibin) + 1
!ngcum=ngcum +1
            end if
          end do
      end do
     return
end subroutine

      subroutine output()
! calculate the normalized pair correlation function  g(r) ; this is done after each MC s
! dividing gcum for the number of samples, density, area 2\pi r dr
! of the circular strip from the referring particle. Divide by N/2
! because gcum has been calculated by summing over N/2 particles.
! Note: max. separation is max(Lx/2,Ly/2) (in PBC)
      integer :: ir
      real :: rmax,xnorm,r,g,area,pi,rho_max
      pi = 2*asin(1.)
      rho_max=2/sqrt(3.)
      rmax = nbin * dr
      write(*,fmt='(a23,1x,f6.2,a1)')' rho/rho_max=',rho/rho_max
      write(*,*)' acceptance ratio:',real(accept)/(N*nmcs)
      open(unit=3,file='g_of_r.dat',status='unknown')
      write(3,*)'# number of particles (even) =',N
      write(3,*)'# dimensions Lx, Ly  of the box =',Lx,Ly
      write(3,*)'# reduced density (rho)=',rho
      write(3,*)'# data production MC steps per particle (nmcs)=',nmcs
      write(3,*)'# bin dr for g(r) =',dr
```

```
      write(3,*)'# acceptance ratio =',float(accept)/(N*nmcs)
      write(3,*)'# rmax =',rmax
      xnorm = 2./(rho*nmcs*N)
      do ir = 1,nbin
            r    = ir*dr + 0.5*dr  ! r in the middle of the circular shell
            area = 2.0*pi*r*dr     ! area of the shell
            g    = gcum(ir)*xnorm/area
            write(3,*)r,g
      end do
      close(3)
         return
      endsubroutine


subroutine save_config()
!save config in a file
integer :: i
character(len=20) :: fileout
print*,' output filename to save config in a file  >'
read(*,'(a)')fileout
open(unit=3,file=fileout,status='replace',action='write')
write(3,*)Lx,Ly
do i=1,N
write(3,*)x(i),y(i)
enddo
return
endsubroutine

subroutine read_config()
real :: Lxold,Lyold,xscale,yscale
character(len=20) :: filein
integer :: i
print*,' filename old config. >'
         read(*,'(a)') filein
         open(unit=2,file=filein,status='unknown')
         read(2,*)Lxold,Lyold
         xscale = Lx / Lxold
         yscale = Ly / Lyold
         do i = 1,N
            read(2,*) x(i),y(i)
            x(i) = x(i) * xscale  ! uniformly rescale all x positions
            y(i) = y(i) * yscale  ! uniformly rescale all y positions
         enddo
         close(2)
endsubroutine
```

```
subroutine error(comment1,comment2,dummy)
character(len =16) :: comment1
character(len =10) :: comment2
real :: dummy
write(*,'(1x,a16,a10,1x,f10.4)')comment1,comment2,dummy
stop
return
endsubroutine

endmodule common

!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

   program hdMC
   use common
   implicit none
   integer :: imcs
   character(1) :: ans

   Lx=4.41*sqrt(0.9503/0.3)
   Ly=0.5*sqrt(3.)*Lx
   print*,'default values for Lx,Ly=',Lx,Ly
   print*,' change? (y/n)'
   read(*,'(a)')ans
   if(ans=='y')then
      print*,' insert Lx,Ly >'
      read(*,*)Lx,Ly
   end if

   call initial()

   do imcs = 1, nequil   !equilibration
       call move()
   enddo

   gcum = 0. ;   accept = 0
    do imcs = 1, nmcs
       call move()
       call correl()
    enddo

    call output()
    call save_config()
    deallocate(x,y,gcum)
    stop
endprogram hdMC
```

```
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
!
! hd-MD.f90 ;  simulation of 2D hard disks using MD - from Gould-Tobochnick
!
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

module periodic
public :: separation,pbc
integer, parameter, public  :: double = 2
contains

function separation(ds,L) result (separation_result)
   real (kind = double), intent (in) :: ds,L
   real (kind = double) :: separation_result
    if (ds > 0.5*L) then
        separation_result = ds - L
    else if (ds < -0.5*L) then
        separation_result = ds + L
    else
        separation_result = ds
    end if
end function separation

function pbc(pos,L) result (f_pbc)
   real (kind = double), intent (in) :: pos,L
   real (kind = double) :: f_pbc
    if (pos < 0.0) then
        f_pbc = pos + L
    else if (pos > L) then
        f_pbc = pos - L
    else
        f_pbc = pos
    end if
end function pbc

end module periodic

module common

use periodic
private

public :: minimum_collision_time,move,reset_list,check_overlap
public :: uplist,downlist,initial,check_momentum,kinetic_energy
public :: check_collision,contact,save_config,output
```

```
integer, public :: N
real (kind = double), public :: Lx,Ly,t,timebig
real(kind = double),public,dimension (:),allocatable :: x,y,vx,vy
real(kind = double),public,dimension (:),allocatable :: collision_time, partner

contains

subroutine initial(vsum,rho,area)
   real (kind = double), intent (out) :: vsum,rho,area
   real :: a_x,a_y,vmax,rnd
   integer :: i,nx,ny,row,col
   character(len = 20) :: start,file_name
   character(len = 100) :: dum
   t = 0.0
   print *, "read file (f) or lattice start (l) = "
   read *, start
   if (start == "f" .or. start == "f") then
      print *, "file name = "
      read *, file_name
      open (unit=7,file=file_name,status="old",action="read")
      read (unit=7,fmt = *) N
      read (unit=7,fmt = *) Lx,Ly
      allocate(x(N))
      allocate(y(N))
      allocate(vx(N))
      allocate(vy(N))
      read (unit=7,fmt = *) dum
      do i = 1,N
         read (unit=7,fmt = *) x(i),y(i)
         print *, x(i),y(i)
      end do
      read (unit=7,fmt = *) dum
      do i = 1, N
         read (unit=7,fmt = *) vx(i),vy(i)
      end do
      close(unit=7)
   else if (start == "l" .or. start == "l") then
      print *, "N (a square...)= "
      read *, N     ! assume that sqrt(N) is an integer
      allocate(x(N))
      allocate(y(N))
      allocate(vx(N))
      allocate(vy(N))
      print *, "Lx = "
      read *, Lx
      print *, "Ly = "
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```
      read *, Ly
      print *, "vmax = "
      read *, vmax
      nx = sqrt(real(N))
      ny = nx
       if (nx >= Lx .or. nx >= Ly) then
          print *, "box too small"
          stop
       end if
       a_x = Lx/nx             ! "lattice" spacing
       a_y = Ly/ny
       i = 0
       do col = 1,nx
           do row = 1,ny
               i = i + 1
               x(i) = (col - 0.5)*a_x
               y(i) = (row - 0.5)*a_y
               ! choose random positions and velocities
               call random_number(rnd)
               vx(i) = (2*rnd - 1)*vmax
               call random_number(rnd)
               vy(i) = (2*rnd - 1)*vmax
           end do
       end do
    end if
    call check_overlap()            ! check if two disks overlap
    call check_momentum()
    allocate(partner(N))
    allocate(collision_time(N))
    area = Lx*Ly
    rho = N/area
    timebig = 1.0e10
    vsum = 0                  ! virial sum
    do i = 1,N
        partner(i) = N
    end do
    collision_time(N) = timebig
    ! set up initial collision lists
    do i = 1,N
        call uplist(i)
    end do
end subroutine initial

subroutine check_momentum()
   real (kind = double) :: vxsum, vysum,vxcm,vycm
   !vxsum = 0.0
```

```
   !vysum = 0.0
   ! compute total center of mass velocity (momentum)
   vxsum = sum(vx)
   vysum = sum(vy)
   vxcm = vxsum/N
   vycm = vysum/N
   vx = vx - vxcm
   vy = vy - vycm
end subroutine check_momentum

subroutine minimum_collision_time(i,j,tij)

   real (kind = double), intent (out) :: tij
   integer, intent (out):: i,j

   integer :: k
   ! locate minimum collision time
   tij = timebig
   do k = 1, N
      if (collision_time(k) < tij) then
         tij = collision_time(k)
         i = k
      end if
   end do
   j = partner(i)
end subroutine minimum_collision_time

subroutine move(tij)
   real (kind = double), intent (in) :: tij
   integer :: k
   do k = 1,N
      collision_time(k) = collision_time(k) - tij
      x(k) = x(k) + vx(k)*tij
      y(k) = y(k) + vy(k)*tij
      x(k) = pbc(x(k),Lx)
      y(k) = pbc(y(k),Ly)
   end do
end subroutine move

subroutine reset_list(i,j)
   integer, intent (in) :: i,j
   integer :: k,test
    ! reset collision list for relevant particles
    do k = 1,N
        test = partner(k)
        if (k == i .or. test == i .or. k == j .or. test == j) then
```

```
            call uplist(k)
         end if
     end do
     call downlist(i)
     call downlist(j)
end subroutine reset_list

subroutine check_overlap()
   real (kind = double) :: tol,dx,dy,r2,r
   integer :: i,j
   tol = 1.0e-4
   do i = 1,N - 1
      do j = i + 1,N
         dx = separation(x(i) - x(j),Lx)
         dy = separation(y(i) - y(j),Ly)
         r2 = dx*dx + dy*dy
         if (r2 < 1.0) then
            r = sqrt(r2)
            if (1.0 - r > tol) then
               print *, "particles ",i," and ",j,"overlap"
               stop
            end if
         end if
      end do
   end do
end subroutine check_overlap

subroutine kinetic_energy(ke)
   real (kind = double), intent (out) :: ke
   integer :: i
   ke = 0.0
   do i = 1,N
      ke = ke + vx(i)*vx(i) + vy(i)*vy(i)
   end do
   ke = 0.5*ke
   print "(a,f13.6)", "kinetic energy =", ke/N
end subroutine kinetic_energy

subroutine uplist(i)
   integer, intent (in) :: i
   integer :: j
   ! look for collisions with particles j > i
   if (i == N) then
      return
   end if
   collision_time(i) = timebig
```

```
   do j = i + 1,N
      call check_collision(i,j)
   end do
end subroutine uplist

subroutine downlist(j)
   integer, intent (in) :: j
   integer :: i
   ! look for collisions with particles i < j
   if (j == 1) then
      return
   end if
   do i = 1,j - 1
      call check_collision(i,j)
   end do
end subroutine downlist

subroutine check_collision(i,j)
   integer, intent (in) :: i,j
   real (kind = double) :: dx,dy,dvx,dvy,bij,tij,r2,v2,discr
   integer :: xcell,ycell
   ! consider collisions between i and periodic images of j
   do xcell = -1,1
      do ycell = -1,1
         dx = x(i) - x(j) + xcell*Lx
         dy = y(i) - y(j) + ycell*Ly
         dvx = vx(i) - vx(j)
         dvy = vy(i) - vy(j)
         bij = dx*dvx + dy*dvy
            if (bij < 0) then
               r2 = dx*dx + dy*dy
               v2 = dvx*dvx + dvy*dvy
               discr = bij*bij - v2*(r2 - 1.0)
               if (discr > 0.0) then
                  tij = (-bij - sqrt(discr))/v2
                  if (tij < collision_time(i)) then
                     collision_time(i) = tij
                     partner(i) = j
               end if
            end if
         end if
      end do
   end do
end subroutine check_collision

subroutine contact(i,j,virial)
```

```
   real (kind = double), intent (out) :: virial
   integer, intent (in) :: i,j
   real (kind = double) :: dx,dy,dvx,dvy,factor,delvx,delvy
   ! compute collision dynamics for particles i and j at contact
   dx = separation(x(i) - x(j),Lx)
   dy = separation(y(i) - y(j),Ly)
   dvx = vx(i) - vx(j)
   dvy = vy(i) - vy(j)
   factor = dx*dvx + dy*dvy
   delvx = - factor*dx
   delvy = - factor*dy
   vx(i) = vx(i) + delvx
   vx(j) = vx(j) - delvx
   vy(i) = vy(i) + delvy
   vy(j) = vy(j) - delvy
   virial = delvx*dx + delvy*dy
end subroutine contact

subroutine output(collisions,temperature,vsum,rho,area)
   real (kind = double), intent (in) :: temperature,vsum,rho,area
   integer, intent (in) :: collisions
   real :: mean_virial,mean_pressure
   print "(a,i6)", "collisions =",collisions
   print "(a,f10.4)", "t =",t
   print *, ""
   mean_virial = vsum/(2.0*t)
   mean_pressure = rho*temperature + mean_virial/area
   print "(a,f10.4)", "P =", mean_pressure
end subroutine output

subroutine save_config(i,j,tij)
   real (kind = double), intent (inout) :: tij
   integer, intent (inout) :: i,j
   character(len = 32) :: config
   integer :: k
   ! move particles away from collision for final configuration
   call minimum_collision_time(i,j,tij)
   call move(0.5*tij)
   print *, "file name of configuration?"
   read *, config
   print *, config
   open (unit=1,file=config,status="replace",action="write")
   write (unit=1, fmt="(i4)") N
   write (unit=1, fmt="(2f13.6)") Lx,Ly
   write (unit=1,fmt="(t3,a,t20,a)") "x","y"
   do k = 1,N
```

```
      write (unit=1, fmt="(2f13.6)") x(k),y(k)
   end do
   write(unit=1, fmt="(t3,a,t20,a)") "vx","vy"
   do k = 1,N
      write(unit=1,fmt="(2f13.6)") vx(k),vy(k)
   end do
   close(unit=1)
end subroutine save_config

end module common

program hd
   ! dynamics of system of hard disks
   ! program based in part on fortran program of Allen and Tildesley
   use periodic
   use common

   real (kind = double) :: virial,temperature,vsum,rho,area,ke,tij
   integer :: collisions, i,j,nshow
   call initial(vsum,rho,area)
   call kinetic_energy(ke)
   temperature = ke/N
   collisions = 0                ! number of collisions
   nshow = 10       ! show output every nshow collisions
   do
      if (collisions > 100) then
         exit
      end if
      call minimum_collision_time(i,j,tij)
      ! move particles forward and reduce collision times by tij
      call move(tij)
      t = t + tij
      collisions = collisions + 1
      call contact(i,j,virial)       ! compute collision dynamics
      vsum = vsum + virial
      if (modulo(collisions,nshow) == 0) then
         call output(collisions,temperature,vsum,rho,area)
      end if
      ! reset collision list for relevant particles
      call reset_list(i,j)
      ! check for overlaps to debug program
      ! call check_overlap()
   end do
   call save_config(i,j,tij)
end program hd
```

```
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
!  LJ-MD.f90 (from Gould-Tobochnick)
!
!  simulate a 2D system of particles interacting via the
!  Lennard-Jones potential;
!  Use periodic boundary conditions and minimum imagee convention;
!  Use velocity-Verlet algorithm to integrate the equation of motion
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
module periodic
public :: separation,pbc
integer, public, parameter :: double = 8
contains

function separation(ds,L) result (separation_result)
! minimum image convention.
! NOTE that this implementation assumes that the max dist between
! particles is L in each direction, i.e. it is OK if called after
! the function pbd
   real (kind = double), intent (in) :: ds,L
   real (kind = double) :: separation_result
    if (ds > 0.5*L) then
        separation_result = ds - L
    else if (ds < -0.5*L) then
        separation_result = ds + L
    else
        separation_result = ds
    end if
end function separation

function pbc(pos,L) result (f_pbc)
! use PBC, fold a coordinate from [-L,2L] in [0,L]
   real (kind = double), intent (in) :: pos,L
   real (kind = double) :: f_pbc
    if (pos < 0.0) then
        f_pbc = pos + L
    else if (pos > L) then
        f_pbc = pos - L
    else
        f_pbc = pos
    end if
end function pbc

end module periodic

module common
```

```
use periodic
private

public :: initial,allocate_arrays,Verlet,accel,force
public :: check_momentum,save_config,output

integer, public :: N
real (kind = double), public :: Lx,Ly,t,dt,dt2
real (kind = double), public, dimension (:), allocatable :: x,y,vx,vy,ax,ay
integer, dimension(2), public :: seed

contains

subroutine initial(ke,kecum,pecum,vcum,area)
   real (kind = double), intent (out) :: ke,kecum,pecum,vcum,area
   character(len = 20) :: start,file_name
   character(len = 100) :: dum
   integer :: n1,i,row,col
   real :: a_x,a_y,vmax,rnd
   dt = 0.005
   dt2 = dt*dt
!   seed(1) = 1239
!   seed(2) = 1111
!   call random_seed(put=seed)
   print *, "read data (d), read file (f), or lattice start (l) ="
   read *, start
   if (start == "D" .or. start == "d") then
      N = 16  ! for the sake of simplicity, a perfect square
      call allocate_arrays()
      Lx = 6.0
      Ly = 6.0
      x(1:8) = (/ 1.09,3.12,0.08,0.54,2.52,3.03,4.25,0.89 /)
      x(9:16) = (/ 2.76,3.14,0.23,1.91,4.77,5.10,4.97,3.90 /)
      y(1:8) = (/ 0.98,5.25,2.38,4.08,4.39,2.94,3.01,3.11 /)
      y(9:16) = (/ 0.31,1.91,5.71,2.46,0.96,4.63,5.88,0.20 /)
      vx(1:8) = (/ -0.33,0.12,-0.08,-1.94,0.75,1.70,0.84,-1.04 /)
      vx(9:16) = (/ 1.64,0.38,-1.58,-1.55,-0.23,-0.31,1.18,0.46 /)
      vy(1:8) = (/ -0.78,-1.19,-0.10,-0.56,0.34,-1.08,0.47, 0.06 /)
      vy(9:16) = (/ 1.36,-1.24,0.55,-0.16,-0.83,0.65,1.48,-0.51 /)
   else if (start == "l" .or. start == "L") then
      print *, "N (a square...)= "
      read *, N     ! assume that sqr(N) is an integer
      call allocate_arrays()
      print *, "Lx = "
      read *, Lx
      Ly = 0.5*sqrt(3.0)*Lx
```

```
   n1 = sqrt(real(N))
   a_x = Lx/n1       ! lattice spacing
   a_y = 0.5*sqrt(3.0)*a_x
   vmax = 1.0
   i = 0
   ! triangular lattice
   do row = 1,n1
      do col = 1,n1
         i = i + 1
         x(i) = (col + 0.5*modulo(row,2) - 1)*a_x
         y(i) = (row - 0.5)*a_y
         ! choose random velocities
         call random_number(rnd)
         vx(i) = (2*rnd - 1)*vmax
         call random_number(rnd)
         vy(i) = (2*rnd - 1)*vmax
      end do
   end do
   do i = 1,N
      x(i) = pbc(x(i),Lx)
      y(i) = pbc(y(i),Ly)
   end do
else if (start == "f" .or. start == "f") then
   print *, "file name = "
   read *, file_name
   open (unit=7,file=file_name,status="old",action="read")
   read (unit=7,fmt = *) N
   read (unit=7,fmt = *) Lx,Ly
   call allocate_arrays()
   read (unit=7,fmt = *) dum
   do i = 1,N
      read (unit=7,fmt = *) x(i),y(i)
   end do
   read (unit=7,fmt = *) dum
   do i = 1, N
      read (unit=7,fmt = *) vx(i),vy(i)
   end do
   close(unit=7)
end if
call check_momentum()
ke = 0.0                    ! kinetic energy
do i = 1,N
   ke = ke + vx(i)*vx(i) + vy(i)*vy(i)
end do
ke = 0.5*ke
! initialize sums
```

```
   kecum = 0.0
   pecum = 0.0
   vcum = 0.0
   area = Lx*Ly
   ! print heading for data
   write(unit=8,fmt="(t6,a,t17,a,t27,a,t37,a)")"time","E","T","P"
end subroutine initial

subroutine allocate_arrays()
   allocate(x(N))
   allocate(y(N))
   allocate(vx(N))
   allocate(vy(N))
   allocate(ax(N))
   allocate(ay(N))
end subroutine allocate_arrays

subroutine Verlet(ke,pe,virial)
   real (kind = double), intent (out) :: ke
   real (kind = double), intent (inout) :: pe,virial
   integer :: i
   real (kind = double) :: xnew,ynew

   do i = 1, N
      xnew = x(i) + vx(i)*dt + 0.5*ax(i)*dt2
      ynew = y(i) + vy(i)*dt + 0.5*ay(i)*dt2
      x(i) = pbc(xnew,Lx)
      y(i) = pbc(ynew,Ly)
      ! partially update velocity using old acceleration
      vx(i) = vx(i) + 0.5*ax(i)*dt
      vy(i) = vy(i) + 0.5*ay(i)*dt
   end do
   call accel(pe,virial)         ! new acceleration
   ke = 0.0
   do i = 1, N
      ! complete the update of the velocity using new acceleration
       vx(i) = vx(i) + 0.5*ax(i)*dt
       vy(i) = vy(i) + 0.5*ay(i)*dt
       ke = ke + vx(i)*vx(i) + vy(i)*vy(i)
   end do
   ke = 0.5*ke
   t = t + dt
end subroutine Verlet

subroutine accel(pe,virial)
  real (kind = double), intent (inout) :: pe,virial
```

```
  real (kind = double) :: dx,dy,fxij,fyij,pot
  integer :: i,j
  do i = 1, N
     ax(i) = 0.0
     ay(i) = 0.0
  end do
  pe = 0.0
  virial = 0.0
  do i = 1, N - 1            ! compute total force on particle i
     do j = i + 1,N        ! due to particles j > i
        dx = separation(x(i) - x(j),Lx)
        dy = separation(y(i) - y(j),Ly)
        ! acceleration = force because mass = 1 in reduced units
        call force(dx,dy,fxij,fyij,pot)
        ax(i) = ax(i) + fxij
        ay(i) = ay(i) + fyij
        ax(j) = ax(j) - fxij   ! Newton's third law
        ay(j) = ay(j) - fyij
        pe = pe + pot
        virial = virial + dx*ax(i) + dy*ay(i)
     end do
  end do
end subroutine accel

subroutine force(dx,dy,fx,fy,pot)
! Lennard-Jones potential
   real (kind = double), intent (in) :: dx,dy
   real (kind = double), intent (out) :: fx,fy,pot

   real (kind = double) :: r2,rm2,rm6,f_over_r

   r2 = dx*dx + dy*dy
   rm2 = 1.0/r2
   rm6 = rm2*rm2*rm2
   f_over_r = 24*rm6*(2*rm6 - 1)*rm2
   fx = f_over_r*dx
   fy = f_over_r*dy
   pot = 4.0*(rm6*rm6 - rm6)
end subroutine force

subroutine check_momentum()
   real (kind = double) :: vxsum, vysum,vxcm,vycm
   ! compute total center of mass velocity (momentum)
   vxsum = sum(vx)
   vysum = sum(vy)
   vxcm = vxsum/N
```

```
   vycm = vysum/N
   vx = vx - vxcm
   vy = vy - vycm
end subroutine check_momentum

subroutine save_config()
   character(len = 32) :: config
   integer :: i
   print *, "file name of configuration?"
   read *, config
   print *, config
   open (unit=1,file=config,status="replace",action="write")
   write (unit=1, fmt="(i4)")N
   write (unit=1, fmt="(2f13.6)")Lx,Ly
   write (unit=1,fmt="(t3,a,t20,a)")"x","y"
   do i=1,N
      write (unit=1, fmt="(2f13.6)") x(i),y(i)
   end do
   write(unit=1, fmt="(t3,a,t20,a)") "vx","vy"
   do i = 1,N
      write(unit=1,fmt="(2f13.6)")vx(i),vy(i)
   end do
   close(unit=1)
end subroutine save_config

subroutine output(ke,pe,virial,kecum,vcum,ncum,area)
   integer, intent (inout) :: ncum
   real (kind = double), intent(in) :: ke,pe,virial,area
   real (kind = double), intent(inout) :: kecum,vcum
   real (kind = double) :: E,mean_ke,P

   ncum = ncum + 1
   E = ke + pe               ! total energy
   kecum = kecum + ke
   vcum = vcum + virial
   mean_ke = kecum/ncum      ! still need to divide by N
   P = mean_ke + (0.5*vcum)/ncum  ! mean pressure * area
   P = P/area
   ! mean_ke/N    ! mean kinetic temperature
   write(unit=8,fmt="(4f10.4)") t,E,mean_ke/N,P
end subroutine output

end module common

program md
!  program adapted from Gould & Tobochnik, Chapter 8
```

```
!  simple N(N-1)/2 calculation of forces
   use periodic
   use common
   real (kind = double) :: E
   real (kind = double) :: ke,kecum,pecum,vcum,area,pe,virial
   integer :: ncum
   open(unit=8,file='energy',status='replace')
   call initial(ke,kecum,pecum,vcum,area)
   call accel(pe,virial)
   E = ke + pe                    ! total energy
   ncum = 0                       ! number of times data accumulated
   do
      if (t > 2.0) exit
      call Verlet(ke,pe,virial)
      call output(ke,pe,virial,kecum,vcum,ncum,area)
   end do
   close(8)
   call save_config()
end program md
```