```
!-----------------------------------------------------------------!
!       SHARIF UNIVERSITY OF THECHNOLOGY                          !
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!                                                                 !
!   Novwmber 8, 2005                                              !
!   Mouluclar Dynamics (Problem Number 6) Version 1.0.0           !
!-----------------------------------------------------------------!
program md
use struc
use molecular
use export
implicit none
type(obj), dimension(:), allocatable    :: p_new,p_current,p_old, p_first
type(eng), dimension(:), allocatable    :: temp, temp_mean
type(eng)                               :: temp0
type(conf)                  :: config
real, dimension(1000)       :: gcum=0.0
real, dimension(1000)       :: pvx=0.0, pvy=0.0
real                        :: clock_start, clock_finish
integer                     :: i, j

 config%timebond    = 10000
 config%n_particles = 100
 config%step        = 1
 config%lennar      = 1         !1 for Lennard-Jones and 2 for 1/R Potential
 config%VV          = 1         !1 for Vedrlet Method and 2 for Velocity Verlet
 config%dt          = 0.02
 config%dt2         = config%dt*config%dt
 config%dr          = 0.1
 config%Cutoff      = 35.0
 config%L1          = 16.0
 config%L           = 0.0
 config%dL          = 2.0
 config%v_max       = 1.0
 config%temp0       = 1.0
 config%temp1       = 1.0
 config%R           = config%temp1/config%temp0

allocate(p_new(config%n_particles),p_current(config%n_particles))
allocate(p_first(config%n_particles),p_old(config%n_particles))
allocate(temp(config%timebond))
allocate(temp_mean(config%step))

print *,"What Potential Lennard-Jones[1], 1/r[2]   :"
read *,config%lennar
print *,"What Method Verlet[1], Velocity Verlet[2] :"
read *,config%VV

call print1(config)
do i=1,config%step
    call cpu_time(clock_start)
    temp=temp0
    gcum=0.0
    config%L = config%L1 + config%dL*i
!-----------------------------------------------------------------------
    call init(p_old,p_current,p_first,config)
    if (config%VV==1) then
        do j=1,config%timebond
            !if
(j==1000.or.j==2000.or.j==3000.or.j==4000.or.j==5000.or.j==6000.or.j==7000.or.j==8000.o
r.j==9000) config%R=1.2
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            call verlet(p_old,p_current,p_new,p_first,temp(j),gcum,config)
            !config%R=1.0
        end do
    else
        do j=1,config%timebond
            call VVerlet(p_current,p_first,temp(j),gcum,config)
        end do
    end if
    call mean(temp,temp_mean(i),config)
!------------------ Exporting Data ---------------------------------
    call cpu_time(clock_finish)
    call printresult(temp_mean(i),clock_finish - clock_start,config%L)
    call exporting(i,p_first,p_current,temp,gcum,config)
end do
call exporting1(config,temp_mean)
end program md
```