

## FILE: RW.F90

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1 program rw
2
3   use global_env
4   use calendar
5   use walker
6   use cell
7
8   implicit none
9
10  integer :: max_events
11  integer :: action, opt1, opt2
12
13  real(DP) :: time, time_limit, time_stat
14  real(DP) :: sigma, rho, xx
15
16  integer, dimension(:,:), allocatable :: p0
17
18  real(DP), dimension(:), allocatable :: rn
19
20  integer :: i, j, k, l, m, n
21  integer :: n_errors
22
23  character(len=10) :: arg
24
25  debug = .false.
26
27  ! The following if statement checks to see whether you supply
28     any
29  ! flags to the compiler. The possible flags are "debug" and
30  ! "newseed". The debug flag will output information about the
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30 ! running of the program and will introduce additional stop
31 ! commands. The newseed flag ensures that all the random
    numbers are
32 ! generated from a different seed. This is something that we
    would
33 ! like to turn off during testing.
34
35 if(iargc(>0) then
36     do i=1,iargc()
37         call getarg(i,arg)
38         select case (trim(arg))
39             case ('-debug')
40                 debug = .true.
41             case ('-newseed')
42                 call newseed()
43             end select
44         end do
45     end if
46
47 ! Extract the needed data from the configuration file
48
49 open(10,file='config.dat')
50 read(10,*) n_walkers
51 read(10,*) box_size
52 read(10,*) cell_size
53 read(10,*) k_3d, k_2d
54 read(10,*) k_on, k_off
55 read(10,*) time_limit
56 read(10,*) time_stat
57 close(10)
58

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59     ! open log file for output
60
61     open(fmain,file='rw.log')
62
63     write(fmain,*) '*** KMC FRAP *** '
64     write(fmain,*) 'Started at ',time_stamp()
65     write(fmain,' (/a,i5)') 'Number of Random Walkers=',n_walkers
66     write(fmain,' (3(a,i4))') 'Box size=',box_size(X),' x',
        box_size(Y),' x',box_size(Y)
67     write(fmain,' (3(a,i4))') 'Cell size=',cell_size(X),' x',
        cell_size(Y),' x',cell_size(Y)
68     write(fmain,' (2(a,f8.4),a)') 'Transition rate=',k_3d,' (3d)
        ',k_2d,' (2d)'
69     write(fmain,' (2(a,f8.4),a)') 'Transition rate=',k_on,' (on)
        ',k_off,' (off)'
70     write(fmain,' (a,e15.3)') 'Total simulation time=',time_limit
71     write(fmain,*)
72
73     ! open a data file #1
74     write(fmain,*) 'outout: onoff.dat'
75     open(fdat1,file='onoff.dat')
76
77     ! open a data file #2
78     write(fmain,*) 'output: diffusion.dat'
79     open(fdat2,file='diffusion.dat')
80
81     ! open a file for debug information, iff the debug flag is
        issued
82     if(debug) then
83         write(fmain,*) 'output: debug.dat'
84         open(fdbg,file='debug.dat')

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85     endif
86
87     ! set the maximum number of walkers.
88     !(this determines the size of array)
89     max_walkers = 2*n_walkers
90
91     ! set the maximum number of events recorded in the calendar
92     at a time.
93
94     max_events = 2*max_walkers
95
96
97     ! initialize the event calendar
98     call calendar_init(n_walkers,max_events)
99
100    ! initialize the random walkers
101    call walker_init(n_walkers)
102
103    ! initial position of walkers
104    !(for example uniformly random distribution)
105    allocate(rn(n_walkers)) ! Create a vector for the random
106    numbers
107    call random_number(rn)
108    walker_pos(1:n_walkers,X) = ceiling(rn*box_size(X))
109    call random_number(rn)
110    walker_pos(1:n_walkers,Y) = ceiling(rn*box_size(Y))
111    call random_number(rn)
112    walker_pos(1:n_walkers,Z) = ceiling(rn*box_size(Z))
113    deallocate(rn) ! Not needed anymore, so there isn't any sense
114    in
115    ! letting rn take up any memory
116
117    ! initialize the cell configuration

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113  call cell_init(n_walkers,max_walkers,walker_pos)
114  ! This is used for determining particle collisions
115
116  if(debug) call cell_test(n_walkers) ! check the consistency
      in cell assignment
117
118  ! predict the jump time for all walkers
119  do i=1,n_walkers
120      call walker_predict_event(i)
121  end do
122
123  ! save the initial position
124  allocate(p0(max_walkers,3))
125  p0 = walker_pos
126
127  ! schedule the first data output
128  call calendar_schedule_event(11,0,0,time_stat)
129  call calendar_schedule_event(12,0,0,time_stat)
130
131  n_collisions = 0
132  time_current = 0.0_DP
133
134  do while (time_current<=time_limit)
135
136      ! find the next event to happen
137      call calendar_find_event(action,opt1,opt2)
138
139      ! execute the event
140      if (action<=10) then ! simple jump event
141
142          ! walker 'opt1' jumps

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143      call walker_action(opt1,action)
144      ! predict next jump of walker 'opt1'
145      call walker_predict_event(opt1)
146
147  else if(action<=20) then    ! non-physical events
148
149      select case(action)
150      case(11)
151          ! evaluate surface density
152          sigma = count(walker_pos(:,Z)>box_size(Z))
153          rho = count(walker_pos(:,Z)==box_size(Z))
154          write(fdat1,'(f10.2,2e13.5)') time_current, rho,
              sigma
155          ! set the next evaluation time
156          call calendar_schedule_event(11,0,0,time_current+
              time_stat)
157      case(12)
158          ! evaluate mean square displacement
159          xx = real(sum((walker_pos-p0)**2),kind=DP)/real(
              n_walkers,kind=DP)
160          write(fdat2,'(f10.2,e13.5)') time_current, xx
161          ! set the next evaluation time
162          call calendar_schedule_event(12,0,0,time_current+
              time_stat)
163      case default
164          ! unknown event
165          write(fmain,'(f10.2,a)') time_current, 'unknown
              event'
166          ! emergency stop
167          stop
168  end select

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169
170     else if(action>20) then
171         ! binary event (\such as reaction
172         write(fmain,'(f10.2,a)') time_current, 'binary event'
173         ! binary events have not implimented yet.
174     end if
175
176 end do
177
178 write(fmain,'(a,i10)') 'Number of collisions =',n_collisions
179
180 if(debug) call cell_test(n_walkers)
181
182 ! close output files
183
184 close(fdat1)
185 close(fdat2)
186
187 !
188 open(fdat1,file='walkers.dat')
189 ! creation of particles has not been considered yet.
190 write(fdat1,'(3i5)') (walker_pos(i,:), i=1,n_walkers)
191 close(fdat1)
192
193 if(debug) close(fdbg)
194
195 write(fmain,*) '*** Done at ',time_stamp(), '***'
196 end program rw

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