

!APPENDIX: CODE for Simple Adsorption-Desorption Dynamic Monte Carlo
!Created by Nikolai (23 May 2001) for D.D. Johnson Lectures
!see K.A.Fichthorn, W.H.Weinberg, J. Chem. Phys. 95, 1090 (1991).
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    program dMCs
    implicit none
!glsc:
    include '../glsc-3.5/libs/src/glsc_ftn.h' !!!check_the_path!!!

    integer Lx, Ly, LT, N
    parameter( Lx=256, Ly=256, LT= 100000, N=10 )
    integer isite(Lx,Ly)
    real*8 WA, WD, rA, rD
    real*8 r !random_number
    real*8 t,dt,tl,tt !real_time
    !theta = fractional surface coverage: 0<theta<1 !
    real*8 rc,tc,theta,theta0,xc, exptt,exptl
    integer iT
    integer mx,my
    integer i,j,ic,nc
    integer Input, NoTheory
    real*8 pt !length of plot in x-direction = max real time!

! initial default parameters:
    NoTheory=0 !do not draw theoretical curve!
    Input=0 !do not read Input!
    mx=Lx
    my=Ly
    pt=LT
    rA=1.0
    rD=2.0

! Initialize time and fractional coverage
    iT=0 !integer time
    t=0 !real time
    tl=t
    dt=0.001 !realtime step
    theta=0 !fractional surface coverage, 0 <= theta <= 1 .

!here read parameters....: mx,my,pt,rA,rD:
    !.....input.....!
    Input=1
    NoTheory=1
    if(Input.ne.0) then
        read(5,*) mx,my !dimensions of simulation box
        read(5,*) pt !max real time
        read(5,*) rA,rD !parameters
    endif
    if(mx>Lx) then
        mx=Lx

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        print*, "Input Error: reducing Lx!"
    endif
    if(my>Ly) then
        my=Ly
        print*, "Input Error: reducing Ly!"
    endif

!parameters mx,my,pt,rA,rD remain unchanged after this line!
    rc=theta
    nc=mx*my
    xc=1/dfloat(nc)
    if(rA > rD) then
        WA=1.0
        WD=rD/rA
    else
        WA=rA/rD
        WD=1.0
    endif
    if(rc<0.or.rc>1) stop "Check: should be 0 < rc < 1 !!!"
    theta0=rA/(rA+rD)

!initialize lattice at random:
    ic=0
    call RANDOM_SEED
    do i=1,mx
        do j=1,my
            call RANDOM_NUMBER(r)
            if(r<rc) then
                isite(i,j)=1
                ic=ic+1
            else
                isite(i,j)=0
            endif
        enddo
    enddo

! NOTE:
!!! REMOVED THE THEORY PLOTTING CODE CALLS (SEE REAL SOURCE CODE)
!
!!!run Monte Carlo: Poisson process:
    do while(t<pt)
        !Select a random site (i,j):
        call RANDOM_NUMBER(r)
        i=int(r*mx)+1
        call RANDOM_NUMBER(r)
        j=int(r*my)+1

!Generate a random number 0<r<1:
        call RANDOM_NUMBER(r)

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!Occupied?
  if(isite(i,j).ne.0) then
    !YES
    if(r.le.WD) then
      !Remove species from lattice
      isite(i,j)=0
      ic=ic-1
    !TIME from Poisson Distr.
      call RANDOM_NUMBER(r)
      dt=-log(r)/(ic*rD+(nc-ic)*rA)
      t=t+dt
    endif
  else
!NOT Occupied
    if(r.le.WA) then
      !Add species to lattice
      isite(i,j)=1
      ic=ic+1
    !TIME from Poisson Distr.
      call RANDOM_NUMBER(r)
      dt=-log(r)/(ic*rD+(nc-ic)*rA)
      t=t+dt
    endif
  endif
  iT=iT+1
  rc=ic*xc
!
!glsc: !Plot_graphic: theta(t):
  call g_move (t1,theta)
  theta=rc
  t1=t
  call g_plot (t1,theta)

  !print*, t,rc

  enddo !while(t<pt)
!
!glsc:Termination:
  pause
  !call g_sleep (3.0d0)
  call g_term ()
!
  end
!end_of_file!

```