**Metropolis – MC: 2D-particles**

function [ehist,xhist,yhist]=metro1\_surf\_esimple

global xymax epslj siglj

naccept=0; % acceptance counter

nuphill=0; % uphill counter

nstart=1; % initial step number

nfreq=100; % plotting frequency

[np,nstep,inimode,rmax,kT]=iniset('test');

while 1, % infinite loop

[np,nstep,inimode,kT]=setupinp(np,nstep,inimode,kT);

switch inimode

case 'random',

xco=rand(np,1)\*xymax; yco=rand(np,1)\*xymax;

ehist=zeros(nstep,1); xhist=zeros(nstep,np); yhist=xhist;

subplot(1,2,1); fp=get(gcf,'pos'); set(gcf,'pos',fp.\*[1 1 1.5 1]);

p0=plot(xco,yco,'sb','markerfacecolor','b','markersize',10);

axis square; set(gca,'xlim',[0 xymax],'ylim',[0 xymax]); title('initial');

case 'continue',

ehist=[ehist;zeros(nstep,1)]; xhist=[xhist;zeros(nstep,np)]; yhist=[yhist;zeros(nstep,np)];

end

subplot(1,2,2); p1=plot(xco,yco,'sb','markerfacecolor','b','markersize',10);

axis square; set(gca,'xlim',[0 xymax],'ylim',[0 xymax]); title('running');

etot=e(xco,yco,np);

%\*\*\* START of MC loop \*\*\*

for istep=nstart:nstep+nstart-1,

n=round(rand\*np+0.5); % random particle

xconew=xco; xconew(n)=xconew(n)+(rand\*2-1)\*rmax;

yconew=yco; yconew(n)=yconew(n)+(rand\*2-1)\*rmax;

if xconew(n)>xymax, xconew(n)=xconew(n)-xymax; end

if xconew(n)<0, xconew(n)=xconew(n)+xymax; end

if yconew(n)>xymax, yconew(n)=yconew(n)-xymax; end

if yconew(n)<0, yconew(n)=yconew(n)+xymax; end

etotnew=e(xconew,yconew,np);

dE=etotnew-etot;

if dE<0 || rand < exp(-dE/kT), % accept move

naccept=naccept+1; if dE>0, nuphill=nuphill+1; end

etot=etotnew; xco=xconew; yco=yconew;

end

if mod(istep,nfreq)==1,

set(p1,'xdata',xco,'ydata',yco); drawnow;

fprintf('i=%6i nacc=%6i nup=%6i dE=%15.5g E=%15.5g nmov=%3i\n', ...

istep,naccept,nuphill,dE,etot,n)

end

ehist(istep)=etot; xhist(istep,:)=xco; yhist(istep,:)=yco;

end

%\*\*\* END of MC loop \*\*\*

figure(2); title('Energy'); subplot(1,2,1); fp=get(gcf,'pos');

set(gcf,'pos',fp.\*[1 0.1 1 1]);

plot(ehist); set(gca,'xlim',[0 istep]); title('total');

subplot(1,2,2); plot(ehist); set(gca,'xlim',[istep/2+nstart/2 istep]);

ans2= questdlg('what do you want do do ?','next', ...

'quit','continue','start new','quit');

switch ans2

case 'quit', break;

case 'continue', figure(1); nstart=istep+1; inimode='continue';

case 'start new', figure(1); nstart=1; inimode='random';

end%switch

end % infinite loop

function e=e(x,y,np)

global xymax epslj siglj

xy2=xymax/2;

xm=x(:,ones(np,1)); ym=y(:,ones(np,1));

dx=xm-xm'; dy=ym-ym';

mask=dx>xy2; dx(mask)=dx(mask)-xymax; mask=dx<-xy2; dx(mask)=dx(mask)+xymax;

mask=dy>xy2; dy(mask)=dy(mask)-xymax; mask=dy<-xy2; dy(mask)=dy(mask)+xymax;

dist=sqrt(dx.^2+dy.^2); % all distances

emat=epslj\*((siglj./dist).^12-2\*(siglj./dist).^6);

e=sum(emat(~isnan(emat)))/2; % or sum(sum(tril(emat,-1));

function [np,nstep,inimode,kT]=setupinp(np,nstep,inimode,kT);

default1={num2str(np),num2str(nstep),inimode,num2str(kT)};

prompt1={'number of particles','number of steps','initial coordinates','kT'};

ans1=inputdlg(prompt1,'setup values',1,default1);

np=str2num(ans1{1}); nstep=str2num(ans1{2});

inimode=ans1{3}; kT=str2num(ans1{4});

function [np,nstep,inimode,rmax,kT]=iniset(iset)

global xymax epslj siglj

% select sets of useful initial conditions

switch iset

case 'cryst' % crystallizes after ~ 5000 steps

epslj=40; siglj=3; % interaction parameters

xymax=10; % size of system (surface)

np=30; % np particles somewhere on the surface [0 xymax]^2

nstep=10000; % steps

inimode='random'; % initial configuration

rmax=0.1; % maximal displacement

kT=100; % temperature

case 'vibcryst' % crystallizes after ~ 5000 steps and vibrates

epslj=40; siglj=3; % interaction parameters

xymax=10; % size of system (surface)

np=30; % np particles somewhere on the surface [0 xymax]^2

nstep=10000; % steps

inimode='random'; % initial configuration

rmax=0.1; % maximal displacement

kT=1000; % temperature

case 'melt' % crystallizes after ~ 5000 steps and vibrates

epslj=40; siglj=3; % interaction parameters

xymax=10; % size of system (surface)

np=30; % np particles somewhere on the surface [0 xymax]^2

nstep=10000; % steps

inimode='random'; % initial configuration

rmax=0.1; % maximal displacement

kT=1e6; % temperature

case 'gas' % crystallizes after ~ 5000 steps and vibrates

epslj=40; siglj=3; % interaction parameters

xymax=20; % size of system (surface)

np=30; % np particles somewhere on the surface [0 xymax]^2

nstep=10000; % steps

inimode='random'; % initial configuration

rmax=0.4; % maximal displacement

kT=1e2; % temperature

case 'islands' % crystallizes after ~ 5000 steps and vibrates

epslj=40; siglj=3; % interaction parameters

xymax=30; % size of system (surface)

np=30; % np particles somewhere on the surface [0 xymax]^2

nstep=10000; % steps

inimode='random'; % initial configuration

rmax=0.1; % maximal displacement

kT=1e2; % temperature

end