```
/* ------------------------------------------------------------------------- */

/* Metropolis algorithm, generic illustration
   [Note: One point particle in 3d cube. You will not get "good
   statistics" with one particle, of course. Illustration only!
   Use as template for Project 5.] */

/* Header files */
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
/* #include "f2c.h" */
/* #include "slatec.h" */

/* Global constants */
#define N 6
#define M 1000
#define L 50

/* Aliases*/
#define RAN (rand()/(float)RAND_MAX)

/* Prototypes */
float p(float *x, int n);  /* probability distribution function */

/* ------------------------------------------------------------------------- */
int main (void)
{
/*      declarations */
        unsigned int seed;
        const int n=N;
        int i,ii,j,k;
        float x[N],xx[N],r,acpt,eps, ekin,ekin1,ekin2,epot,epot1,epot2;

        FILE *mtout;

        seed=305;
        srand(seed);

    eps=0.2;

/*      Initial X, counters */
        x[0]=0.0;
        x[1]=0.0;
        x[2]=0.0;
        x[3]=0.5;
        x[4]=0.5;
        x[5]=0.0;
        i=0;
        j=0;
        acpt=0.0;

/*      Initialize observables, counters */
        ekin1=0.0;
        ekin2=0.0;
        epot1=0.0;
        epot2=0.0;
        k=0;
```

this code is for only one particle

I need to change it for many interacting particles.

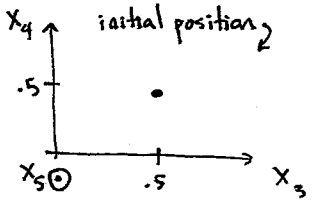
# of dimensions; 3 momenta, 3 position

reduces statistical dependence

momentum

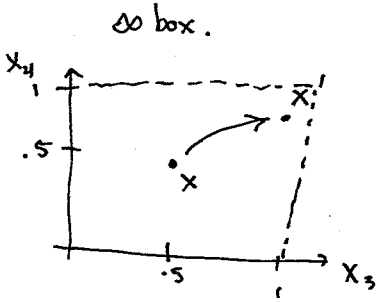
space

initial conditions.



```
59
60  /*      For the record */
61          mtout=fopen("metropolis.out","w");
62
63  /*      Initial energies */
64          ekin=(powf(x[0],2.0)+powf(x[1],2.0)+powf(x[2],2.))/2.0;
65          epot=x[5];
66          fprintf(mtout,"%6i%15.7e%15.7e\n",i,ekin,epot);
67
68  /*      Limit length of chain to M */
69
70          A:
71          if (i>=M) goto C;
72
73  /*              Trial X'   */
74  /*              momenta    */
75                  xx[0]=x[0]+(RAN-.5)*eps;
76                  xx[1]=x[1]+(RAN-.5)*eps;
77                  xx[2]=x[2]+(RAN-.5)*eps;
78  /*              positions */
79                  xx[3]=x[3]+(RAN-.5)*eps;
80                  xx[4]=x[4]+(RAN-.5)*eps;
81                  xx[5]=x[5]+(RAN-.5)*eps;
82
83  /*              Metropolis update */
84                  if ( p(xx,n) >= p(x,n) )
85  /*                      Accept */
86                          goto B;
87                  else {
88                          r=RAN;
89                          if ( p(xx,n) > r*p(x,n) )
90  /*                              Accept */
91                                  goto B;
92                          else {
93  /*                              Reject */
94                                  j++;
95                                  goto A;
96                          }
97                  }
98
99                  B:
100
101 /*              Next element of chain */
102                 i++;
103                 for (ii=0; ii<n; ii++) x[ii]=xx[ii];
104                 acpt=(float)i/(float)(i+j);
105
106 /*              Energies */
107                 ekin=(powf(x[0],2.0)+powf(x[1],2.0)+powf(x[2],2.0))/2.0;
108                 epot=x[5];
109
110 /*              For the record */
111                 fprintf(mtout,"%6i%15.7e%15.7e\n",i,ekin,epot);
112
113                 if (L*(int)(i/L)==i) {  /* mod function */
114 /*                      accumulate 1st and 2nd moments */
115                         k++;
116                         ekin1=ekin1+ekin;
```

eps = small # (set to .2)



```
117                         ekin2=ekin2+powf(ekin,2.0);
118                         epot1=epot1+epot;
119                         epot2=epot2+powf(epot,2.0);
120                         printf("%6i%7.4f%4i%14.6e\n",i,acpt,k,(ekin1+epot1)/(float)k);
121                 }
122                 goto A;
123
124                 C:
125
126 /*              Final results */
127         ekin1=ekin1/(float)k;
128         ekin2=ekin2/(float)k;
129         ekin2=sqrt(ekin2-powf(ekin1,2.0))/sqrt((float)k);
130         epot1=epot1/(float)k;
131         epot2=epot2/(float)k;
132         epot2=sqrt(epot2-powf(epot1,2.0))/sqrt((float)k);
133                 printf("%6i%7.4f%4i%14.6e%12.4e%14.6e%12.4e\n",i,acpt,k,ekin1,ekin2,epot1,epot2);
134
135         return 0;
136
137 }
138
139 /* ------------------------------------------------------------------------- */
140
141 /*      Probability distribution function, def */
142
143 float p(float *x, int n)
144 {
145                 float s, beta=4.0;
146                 int i;
147
148 /*              outside box */
149                 s=0.0;
150                 for (i=3; i<5; i++) if (x[i]<0.0 || x[i]>1.0) return s;
151                 if (x[5]<0.0) return s;
152
153 /*              Boltzmann */
154                 s=exp(-beta*(powf(x[0],2.0)+powf(x[1],2.0)+powf(x[2],2.0))/2.0+x[5]);
155
156                 return s;
157 }
158
159 /* ------------------------------------------------------------------------- */
```

line 68-124 is looking @ his outline

if they are interac[ting] then ∃ an interaction potential

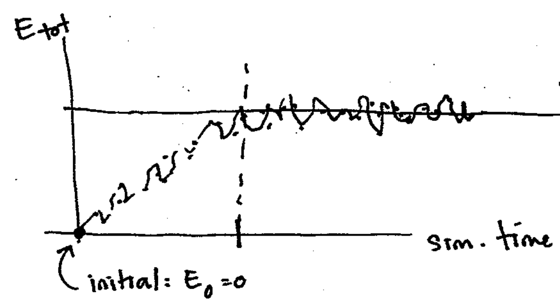
this line reads: $s = e^{-\beta[\frac{1}{2}(p_x^2 + p_y^2 + p_z^2) + z]}$ — The K.E ($\frac{1}{2}(p_x^2+p_y^2+p_z^2)$); the P.E. w/ mg=1 ($z$)

actually 1/2m w/ m=1.

so this is

$s = e^{-\beta E_{tot}}$, the Boltzmann factor.

make a plot of E_{tot} vs. simulation time



the average energy is const but ∃ fluctuations about that average.

(the kinetic energy is going to be similar in shape, but not @ same time.)

Markov Chain Process

Implementation

0 Generate initial config's X_i, $p(X_i)$, $i=0$

1 Generate a (new) trial config X', $p(X')$

2 if $p(X') \geq p(X_i)$

accept, $i = i+1$, $X_i = X'$

goto 1

else

gen $r \in [0,1)$ uniform

if $p(X')/p(X_i) > r$

accept, $i = i+1$, $X_i = X'$

goto 1

else

reject

goto 1

endif

endif