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COURSE: CHE 5382

COURSE NAME: MOLECULAR SIMULATION

Assignment-6

**QUESTION 1**

1. ***CODE***

//CHE 5382

//Assignment-6

//Apr-26-2011

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//This code is a code to generate coordinates of atoms in a cybic simulation //box of box length 18.The number density of atoms is 0.75. The following are //the parts of the code.

//(a)Create a simulation box of length 18, plot the initial RDF

//(b)Get the Lennard Jones Potential which is shifted by 2.5

//(c)NVT ensemble of Temperature 1.

//(d)NPT ensemble of Pressure 1.011.

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#include<iostream>

#include<fstream>

#include<cmath>

#include<cstdlib>

#include<ctime>

using namespace std;

// In\_Line Definitions //

double PI=atan(1.0)\*4.0; //PI\_Value

const int N=2700; //Number of atoms

const double box\_len=15; //Box\_Length

const double half\_box\_len=7.5; //Half\_Box\_Length

const double bin\_size=0.1; //Bin\_Size

const double T=1; //Reduced Temperature

const double R\_cut=2.5; //Cut\_off Distance

const int N\_iter=10000; //MC steps

const double dist=0.05; //Time\_size

// Function Definition for Periodic Boundary Condition //

int roundoff(double d)

{

return int(floor(d + 0.5));

}

// Function Definitions for Random Number Generation //

double unifRand()

{

return rand() / double(RAND\_MAX);

}

// Function for seeding the Random Numbers //

void seed()

{

srand(time(0));

}

// Main Function //

int main()

{

// Initialization //

double R[2700][4]={0};

long double U=0;

double RxIJ,RyIJ,RzIJ,RIJ;

double U\_r=4\*(pow((1/R\_cut),12)-pow((1/R\_cut),6));

int q;

double p=0;

seed();

ofstream coord\_init;

ofstream LJ\_pot;

ofstream energy\_out;

ofstream coord\_final;

int Bin\_No[200]={0},bin=0,Out\_box=0,i;

double r,Shell\_vol,V\_box,gofr,Denom;

ofstream RDF;

ofstream Final\_pos;

ofstream energy;

// Part (a) //

coord\_init.open("init\_coord.txt");

int n=0;

for(int i=0;i<box\_len-1;i++)

for(int j=0;j<box\_len-1;j++)

for(int k=0;k<box\_len-1;k++)

{

if(n<N)

{

R[n][1]=i\*1.07;

R[n][2]=j\*1.07;

R[n][3]=k\*1.07;// Generation of coordinates in a cubic lattice

coord\_init<<R[n][1]<<"\t"<<R[n][2]<<"\t"<<R[n][3]<<"\n";

n=n+1;

}

}

coord\_init.close(); // Data file containing coordinates

// Part (b) //

LJ\_pot.open("LJ\_pot.txt");

U=0;

for( i=0;i<N-1;i++)

{

for (int j=i+1;j<N;j++)

{

RxIJ=R[i][1]-R[j][1]-box\_len\*roundoff((R[i][1]-R[j][1])/box\_len);

RyIJ=R[i][2]-R[j][2]-box\_len\*roundoff((R[i][2]-R[j][2])/box\_len);

RzIJ=R[i][3]-R[j][3]-box\_len\*roundoff((R[i][3]-R[j][3])/box\_len);

RIJ=sqrt(pow(RxIJ,2)+pow(RyIJ,2)+pow(RzIJ,2));

if (RIJ<=R\_cut)

U=U-U\_r+4\*(pow((1/RIJ),12)-pow((1/RIJ),6));

}

LJ\_pot<<U<<"\n";

}

LJ\_pot.close();

// Part(c) //

double O\_energy,N\_energy,Rand\_no,Num1,Num2,Num3,Fin[4],Temp[4],prob,a,b,c;

int M\_atom,acc;long int N\_acc=0;

O\_energy=U;

cout<<"O\_energy"<<O\_energy<<"\n";

U=0;

//cout<<O\_energy<<"\n";

energy.open("Energy.txt");

Final\_pos.open("Final\_pos.txt");

for(i=1;i<N\_iter;i++)

{

U=0;

for(int t=1;t<5;t++)

{

Rand\_no=unifRand();

M\_atom=roundoff(N\*Rand\_no);

if(M\_atom==0) M\_atom=1;

//cout<<"M\_atom"<<"\t"<<M\_atom<<"\n";

for(int h=1;h<=3;h++)

{

Num1=unifRand();

Fin[h]=R[M\_atom][h]-(2\*Num1-1)\*dist;

}

for(int j=1;j<=3;j++)

{

if(Fin[j]>=box\_len)

Fin[j]=Fin[j]-box\_len;

else if(Fin[j]<=0)

Fin[j]=Fin[j]+box\_len;

Temp[j]=R[M\_atom][j];

R[M\_atom][j]=Fin[j];

}

}

for(int k=0;k<N-1;k++)

{

for (int j=i+1;j<N;j++)

{

RxIJ=R[i][1]-R[j][1]-box\_len\*roundoff((R[i][1]-R[j][1])/box\_len);

RyIJ=R[i][2]-R[j][2]-box\_len\*roundoff((R[i][2]-R[j][2])/box\_len);

RzIJ=R[i][3]-R[j][3]-box\_len\*roundoff((R[i][3]-R[j][3])/box\_len);

RIJ=sqrt(pow(RxIJ,2)+pow(RyIJ,2)+pow(RzIJ,2));

if (RIJ<=R\_cut)

U=U-U\_r+4\*(pow((1/RIJ),12)-pow((1/RIJ),6));

}

}

//cout<<"U"<<U<<"\n";

N\_energy=U;

if (N\_energy<=O\_energy)

{

acc=1;

N\_acc=N\_acc+1;

}

else

{

prob=exp(O\_energy-N\_energy);

Num1=unifRand();

if (r<=prob)

{

acc=1;

N\_acc=N\_acc+1;

}

else

{

R[M\_atom][1]=Temp[1];

R[M\_atom][2]=Temp[2];

R[M\_atom][3]=Temp[3];

}

}

//cout<<"N\_acc"<<"\t"<<N\_acc<<"\n";

if (acc==1)

O\_energy=N\_energy;

ener[i]=O\_energy;

cout<<"O\_energy"<<O\_energy<<"ener{i}"<<ener[i]<<"N\_energy"<<N\_energy<<"\n";

energy<<i<<"\t"<<ener[i]<<"\n";

//cout<<"i"<<"\t"<<i<<"\n";

if(N\_acc>2760)break;

}

for (int t=0;t<N;t++)

{

Final\_pos<<t<<"\t"<<R[t][1]<<"\t"<<R[t][2]<<"\t"<<R[t][3]<<"\n";

}

Final\_pos.close();

energy.close();

}

1. ***PLOTS***

***Initial Cubic box of atoms with 1.07 as lattice parameter.***

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***RDF of initial configuration***

***Potential energy vs timesteps***



After 2800 steps the potential goes to zero, this is possibly because of a flaw in coding.

***RDF***

**References:**

1. <http://www02.mpikg.mpg.de/th/physik/allen_tildesley/allen_tildesley.11>