

Zależność D=f(gęstość). Symulacje przeprowadzono na 50 000 cząsteczek I 80 000 kroków dla każdego punktu pomiarowego. Zauważymy nieliniowość tendencji

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główny program:
diffuse23.cpp
#include <cmath>
#include <vector>
#include <iostream>
#include <boost/random/mersenne_twister.hpp>
#include <boost/random/uniform_int_distribution.hpp>
#include <algorithm>
#include <tuple>
boost::random::mt19937 rng;
class point
public:
        point(int x,int y):p{x,y}{};
int& operator[](char i){return p[i];};
int p[2];
};
class lattice
{public:
         lattice(int size)
                 size_x=fĺoor(sqrt(size)+0.5);
                 size_y=floor(sqrt(size)+0.5);
                 stor.resize(size_x*size_y,0);
         auto& at(point p)
                 int xp=p[0]%size_x;
```

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if(xp<0)xp+=size_x;</pre>
                 int yp=p[1]%size_y;
                 if(yp<0)yp+=size_y;
                 return stor.at(xp*size_x+yp);
        auto len() {return stor.size();};
//private:
        std::vector<char> stor;
        int size_x,size_y;
};
auto create_state(auto lattice_size,auto particlecount)
{std::vector<point> particles;
        particles.reserve(particlecount);
        lattice particle_lattice(lattice_size);
        std::cout<<double(particlecount)/particle_lattice.len()<<std::endl;</pre>
        boost::random::uniform_int_distribution<> randompos(0,particle_lattice.size_x);
        while(particles.size()<particlecount)
{      point new_particle(randompos(rng),randompos(rng));</pre>
                 if(particle_lattice.at(new_particle)==0)
                         auto sl=lattice_size;
                          auto p=new_particle;
                          particle_lattice.at(new_particle)=1;
                          particles.push_back(new_particle);
        return std::make_tuple(particles,particle_lattice);
auto step(auto& particles,auto& particle_lattice)
        boost::random::uniform_int_distribution<> direction(0,3);
        for(int i=0;i<particles.size();i++)</pre>
                 auto& it=particles[i];
                 char dir=direction(rng);
                 auto new_particle=it;
                 new_particle[dir>>1]+=-1+2*(dir%2);
                 if(particle_lattice.at(new_particle)==0)
                          particle_lattice.at(new_particle)=1;
                         particle_lattice.at(it)=0;
it=new_particle;
                 }
        }
void analyze(auto origins, auto particles, int t)
        double mean_accumulator=0;
        for(int i=1;i<=particles.size();i++)</pre>
                 long xdev=(particles[i][0]-origins[i][0]);
                 xdev*=xdev;
                 long ydev=(particles[i][1]-origins[i][1]);
                 ydev*=ydev;
                 mean_accumulator+=xdev+ydev;
        double mean=mean_accumulator/4/particles.size();
std::cout<<t<<' '<<mean<<'\n';</pre>
int main(int argc, char** argv)
{          rng.seed(100);
        //check validity of arguments
        if(argc!=4)
                 std::cout<<"Usage: <Fill rate> <Number of steps> <Number of particles>"<<std::endl;
                 exit(-1);
        double fill_rate=atof(argv[1]);
        int number_of_steps=atoi(argv[2]);
        int particlecount=atoi(argv[3]);
        auto lattice_size=particlecount/fill_rate;
        auto [particles,particle_lattice]=create_state(lattice_size,particlecount);
        auto origins=particles;
                 for(int i=1;i<=number_of_steps;i++)
                          step(particles,particle_lattice);
                          if(i%256==0) analyze(origins,particles,i);
        return 0;
}
```

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Program do ostatecznej analizy wyników:
analysis.py:
from sys import argv
def get_data(filename):
       datavector=[]
       with open(filename, 'r') as data:
              while(True):
                     c=data.readline()
                     if c =='': return datavector
                     l=[float(x) for x in c.split(' ')]
                     datavector.append(l)
def mean(sample):
       return sum(sample)/len(sample);
#accepts data in form (list of X,list of Y)
def linear_slope(data):
       covariance=mean([x[0]*x[1] \text{ for } x \text{ in data}])
       variance_of_square=mean([x[0]*x[0] for x in data])
       return covariance/variance_of_square
def variance(data):
       avg_x=sum(data)/len(data)
       avg_x2=sum([x**2 for x in data])/len(data)
       ans=avg_x2-avg_x*avg_x
       return ans;
if len(argv)!=2:
       print("You need to specify a file to analyse")
       exit(-1)
with open(argv[1]) as densities_list:
       while True:
              density=densities_list.readline();
              density=density[0:-1]
if density=='':
                     break;
              data=get_data('fresults/'+str(density)+'.txt')
              slope=linear_slope(data)
              stdun=(variance([x[1]/x[0]-slope for x in data]))**(1/2)
              print(float(density),slope,stdun)
Oprócz tych dwóch, do efektywnego zrównoleglenia obliczeń użyłem dwóch dodatkowych
skryptów które zajmują się uruchamianiem I monitorowaniem głównego programu na
wszystkich rdzeniach procesora:
runone.sh:
#!/bin/bash
###
DENSITY=$1
STEPS=80000
PARTICLES=50000
./diffuse23 $DENSITY $STEPS $PARTICLES > intermresults/$DENSITY.txt
FILENAME="$(head -n 1 intermresults/$DENSITY.txt)"
sed -i 1,1d intermresults/$DENSITY.txt
cp intermresults/$DENSITY.txt fresults/$FILENAME.txt
echo $FILENAME >> fresults/truedensities.txt
doall.sh:
rm fresults/truedensities.txt
cat densities.txt | parallel --verbose ./runone.sh
python3 analysis.py fresults/truedensities.txt > fins.txt
```