0.1 Exercise 3 - HPCSE - Leonard Wossnig

0.1.1 Task 1.

Starting with the formula

$$\frac{\rho^n_{i,j}}{\delta t} = D\left(\frac{\rho^n_{i-1,j} - 2 * \rho^n_{i,j} + \rho^n_{i+1,j}}{\delta x^2} + \frac{\rho^n_{i,j-1} - 2 * \rho^n_{i,j} + \rho^n_{i,j+1}}{\delta y^2}\right) \tag{0.1}$$

and using the 2D approach

$$u^n_{r,s} = \rho^n \mathrm{e}^{ik_x x_r} \mathrm{e}^{ik_y y_s} \tag{0.2}$$

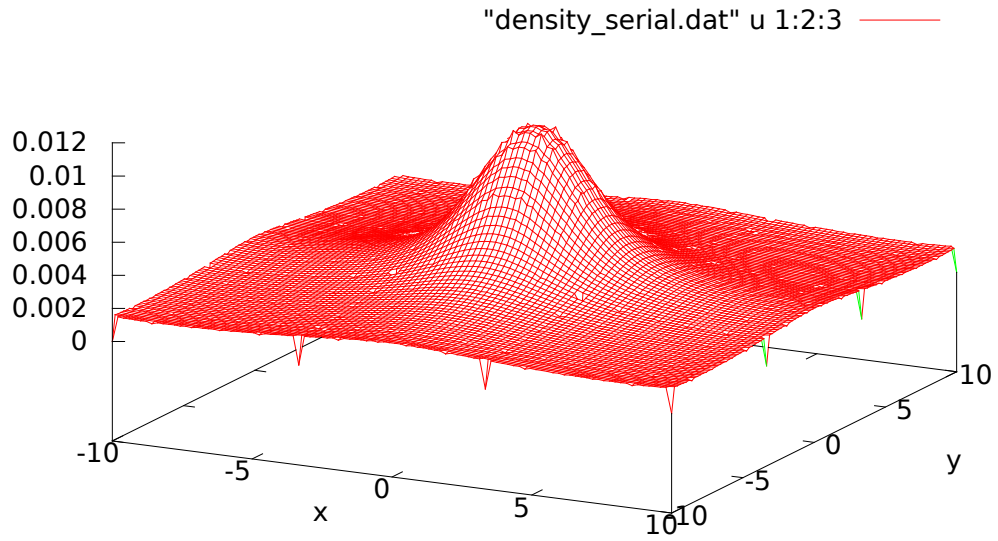
one can substitute formula (2) in (1) and find that the equation is independent (divide both sides by ρ) of ρ.

0.1.2 Task 2.

The parallelization was build using open mp with the collapsed for loop (see code below). The number of threads was individually set using

```
export OMP_NUM_THREADS=X
```

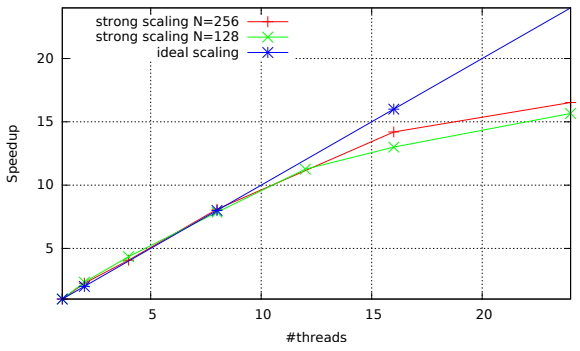
The results for a arbitrary time were approved through the sequential code (compare also graph).

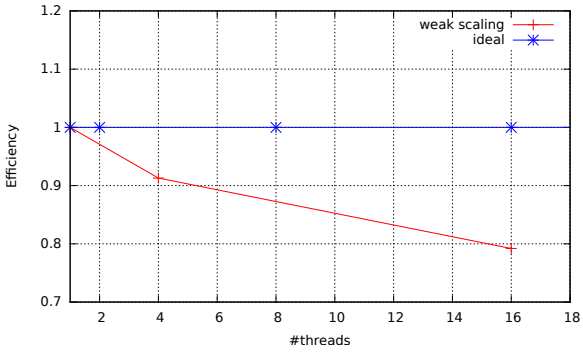


The code for the parallelization is given by:

```
52 #pragma omp parallel for collapse(2)
53         for(size_type i = 0; i < N_; ++i) {
54             for(size_type j = 0; j < N_; ++j) {
55                 rho_tmp[i*N_ + j] = rho_[i*N_ + j] +
56                 fac_
57                 *
58                 (
59                  (j == N_-1 ? 0. : rho_[i*N_ + (j+1)])
60                  +
61                  (j == 0    ? 0. : rho_[i*N_ + (j-1)])
62                  +
63                  (i == N_-1 ? 0. : rho_[(i+1)*N_ + j])
64                  +
65                  (i == 0    ? 0. : rho_[(i-1)*N_ + j])
66                  -
67                  4.*rho_[i*N_ + j]
68                  );
69             }
70         }
71         /// use swap instead of rho_=rho_tmp. this is much more efficient, because it does not have to copy
72         /// element by element.
73
74 #pragma omp barrier
75 #pragma omp master
76         using std::swap;
77         swap(rho_tmp, rho_);
```

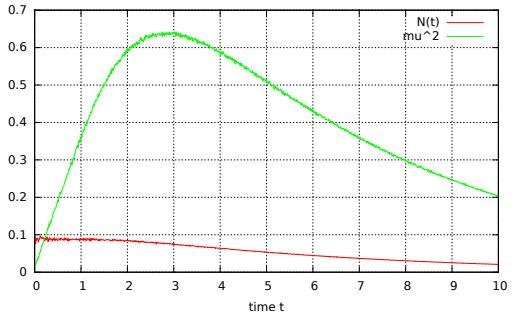
The scaling behaviour resulted in the following plots:

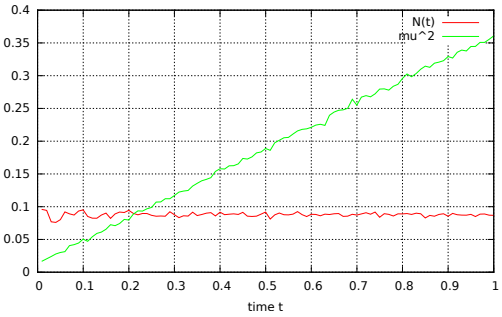




The total amount of heat and the cloud resulted in the following plots. Interestingly just a plot for a short time ($\delta t = 0.001$) with 128 steps brought a reasonable result for these quantities. For all other trials the results seemed similar to the second graph. Also changing the diffusion constant did not alter this outcome. We expect an error in the simulation. The method used was monte carlo integration (as in the code below).

```
94     value_type mc_rho()
95     {
96             size_type mc_steps2_=0;
97             value_type mc_result2_=0, mc_sum2_=0;
98
99             while(mc_steps2_ < 10000)
100            {
101                    mc_sum2_+=rho_[(rand()%N_)*N_ + (rand()%N_)];
102                    mc_steps2_++;
103            }
104            mc_result2_ = L_*mc_sum2_/10000.;
105            return (mc_result2_);
106    }
```





0.1.3 Appendix

In the following i append the source code of some of the tasks:

```
// CODE BASED ON THE LECTURE (solution) CODE FROM HPCSE-I, ETHZ
// CHANGES ARE ACCORDINGLY JUST DONE BY THE PARALLELIZATION
// OF USING OPEN MP
// Leonard Wossnig, 14.10.14
// compile and link using:
// g++ -fopenmp <codename>.cXX
// using #pragram omp parallel


#include <iostream>
#include <algorithm>
#include <string>
#include <fstream>
#include <cassert>
#include <vector>
#include <cmath>
#include <omp.h>
#include <thread>
#include <cstdlib>
#include "timer.cpp"


typedef double value_type;
typedef std::size_t size_type;

class Diffusion2D {

public:
    Diffusion2D(const value_type D, //Diffusion constant
                const value_type L, // length of interval
                const size_type N,  //steps of grid (1d)
                const value_type dt) //timestep
    : D_(D), L_(L), N_(N), Ntot(N_*N_), dt_(dt)
    {
        /// real space grid spacing
        dr_ = L_ / (N_ - 1);

        /// stencil factor
        fac_ = dt_ * D_ / (dr_ * dr_);

        rho_.resize(Ntot, 0.);
        rho_tmp.resize(Ntot, 0.);

         initialize_density();

    }

    void advance()
    {
        /// Dirichlet boundaries; central differences in space, forward Euler
        /// in time
#pragma omp parallel for collapse(2)
        for(size_type i = 0; i < N_; ++i) {
            for(size_type j = 0; j < N_; ++j) {
                rho_tmp[i*N_ + j] = rho_[i*N_ + j] +
                fac_
                *
                (
                 (j == N_-1 ? 0. : rho_[i*N_ + (j+1)])
                 +
                 (j == 0    ? 0. : rho_[i*N_ + (j-1)])
                 +
```

```
63                  (i == N_-1 ? 0. : rho_[(i+1)*N_ + j])
64                  +
65                  (i == 0    ? 0. : rho_[(i-1)*N_ + j])
66                  -
67                  4.*rho_[i*N_ + j]
68                  );
69              }
70          }
71          /// use swap instead of rho_=rho_tmp. this is much more efficient, because it does not have to copy
72          /// element by element.
73
74  #pragma omp barrier
75  #pragma omp master
76          using std::swap;
77          swap(rho_tmp, rho_);
78  //#pragma omp flush
79      }
80
81      void write_density(std::string const& filename) const
82      {
83          std::ofstream out_file(filename, std::ios::out);
84
85          for(size_type i = 0; i < N_; ++i) {
86              for(size_type j = 0; j < N_; ++j)
87                  out_file << (i*dr_ - L_/2.) << '\t' << (j*dr_ - L_/2.) << '\t' << rho_[i*N_ + j] << "\n";
88              out_file << "\n";
89          }
90          out_file.close();
91      }
92
93
94      value_type mc_rho()
95      {
96              size_type mc_steps2_=0;
97              value_type mc_result2_=0, mc_sum2_=0;
98
99              while(mc_steps2_ < 10000)
100             {
101                     mc_sum2_+=rho_[(rand()%N_)*N_ + (rand()%N_)];
102                     mc_steps2_++;
103             }
104             mc_result2_ = L_*mc_sum2_/10000.;
105             return (mc_result2_);
106     }
107
108
109     value_type mc_cloud()
110     {
111             size_type mc_steps_=0;
112             value_type mc_result_=0, mc_sum_=0;
113
114             size_type j=0;
115             size_type i=0;
116             while(mc_steps_ < 10000)
117             {
118                     j = (rand()%N_); //really bad rng but quick implementation for now
119                     i = (rand()%N_); // -"-
120                     mc_sum_ += rho_[i*N_+j]*((i*dr_ - L_/2.)*(i*dr_ - L_/2.) + (j*dr_ - L_/2.)*(j*dr_ - L_/2.)) ;
121                     mc_steps_++;
122             }
123             mc_result_ = L_*mc_sum_/10000.;
124             return (mc_result_);
125     }
126
127 private:
128
129     void initialize_density()
130     {
131         /// initialize rho(x,y,t=0)
132         value_type bound = 1/2.;
133
134         for (size_type i = 0; i < N_; ++i) {
135             for (size_type j = 0; j < N_; ++j) {
136                 if (std::abs(i*dr_ - L_/2.) < bound && std::abs(j*dr_ - L_/2.) < bound) {
137                     rho_[i*N_ + j] = 1;
138                 } else {
139                     rho_[i*N_ + j] = 0;
140                 }
141             }
142         }
143         std::cout << "Initialized density, now running programm with " << std::thread::hardware_concurrency() <<" concurrent supported thr
144 #pragma omp parallel
145 #pragma omp critical (output)
146         std::cout << "Thread " << omp_get_thread_num() << " of " << omp_get_num_threads() << " threads." << std::endl;
147
148     }
149
150     value_type D_, L_;
151     size_type N_, Ntot;
152
```

```
153     value_type dr_, dt_, fac_;
154 // MC variables
155
156     std::vector<value_type> rho_, rho_tmp;
157 };
158
159
160 int main(int argc, char* argv[])
161 {
162     std::ofstream out("rho_evolution.txt");
163     if (argc < 5) {
164         std::cerr << "Usage: " << argv[0] << " D L N dt" << std::endl;
165         return 1;
166     }
167
168     const value_type D = std::stod(argv[1]);
169     const value_type L = std::stod(argv[2]);
170     const size_type  N = std::stoul(argv[3]);
171     const value_type dt = std::stod(argv[4]);
172
173
174     Diffusion2D system(D, L, N, dt);
175     system.write_density("density.0.dat");
176
177     srand(time(NULL));
178
179     const value_type tmax = 10000 * dt;
180     value_type time = 0;
181     int w_count= 0;
182     Timer t;
183     t.start();
184
185     while(time < tmax){
186         system.advance();
187         w_count++;
188         if(w_count%100==0){
189           out << time << "    " << system.mc_rho() << "   " << system.mc_cloud() <<std::endl;
190         }
191         time += dt;
192     }
193
194     t.stop();
195
196     std::cout << "Timing : " << N << " " << t.duration() << std::endl;
197
198     system.write_density("density_serial.dat");
199
200     out.close();
201     return 0;
202 }
```