# Computational Physics SuSe 2023
# 4. Exercise Sheet

**Handing out:** 15.05.2023 Prof. H. Jelger Risselada
**Submission:** 19.05.2023 8 pm

## Exercise 0: Comprehension questions 0 Points

1) What methods do you know for solving a time-independent partial differential equation? What advantages do these methods offer?

2) How does the FTCS scheme differ from the Crank-Nicolson scheme? What additional considerations should be taken into account when implementing the Crank-Nicolson scheme?

## Exercise 1: Poisson's equation 12 Points

*In a suitable electrodynamics lecture, you have already become acquainted with Poisson's equation, with the help of which an electrostatic potential can be calculated from a static charge density. Since this equation cannot be solved analytically except in a few cases, in this assignment you are to implement a procedure to solve Poisson's equation numerically for arbitrary charge densities.*

Solve the two-dimensional Poisson equation ($\epsilon_0 = 1$)

$$\left(\partial_x^2 + \partial_y^2\right)\phi(x,y) = -\rho(x,y)$$

using the Gauss-Seidel method for the following system: we consider a square with dimensions $Q = [0,1]^2$ and Dirichlet boundary conditions with given potential $\phi$. Inside the square are discrete charges $q_i$ at locations $\vec{r}_i$ such that

$$\rho(\vec{r}) = \sum_i q_i \delta(\vec{r} - \vec{r}_i)$$

holds for the charge density. Use a discretization with $\Delta = 0.05$ in the whole task. Use as a termination criterion for the Gauss-Seidel integration an error bound of $\kappa = 10^{-5}$. Present your results graphically in each part of the task.

Proceed as follows for your implementation:

a) Discretize the system and implement the Gauss-Seidel method. Also write an output routine for $\phi(\vec{r})$ and the electric field $\vec{E}(\vec{r}) = -\nabla\phi(\vec{r})$.
*Note: At each iteration steps, the algorithm should update each lattice site within the square once, without changing the boundaries.*

b) Choose as initial conditions $\phi(x,y) = 1$ within the square and test the algorithm for $\rho(x,y) = 0$ with Dirichlet boundary condition $\phi = \text{const} = 0$.

c) Solve the Poisson equation for $\rho(x,y) = 0$ within the square and with boundary conditions

$$\phi(x=0,y) = \phi(x=1,y) = \phi(x,y=0) = 0,$$
$$\phi(x,y=1) = 1.$$

Compare the analytical result with your numerical result. The analytical solution for $\phi(x,y)$ is

$$\Phi(x,y) = \sum_{n=1}^{\infty} \frac{2(1-\cos(n\pi))}{n\pi \sinh(n\pi)} \sin(n\pi x)\sinh(n\pi y).$$

d) Set $\phi = \text{const} = 0$ on all edges and now place a charge $q_1 = +1$ in the center of $Q$. Calculate $\phi(\vec{r})$ and $\vec{E}(\vec{r})$ inside the square by iteration.

e) Again, set $\phi = \text{const} = 0$ on all edges and now place two positive charges with $q = +1$ on points $\vec{r}_1 = (0.25, 0.25)^\top$ and $\vec{r}_2 = (0.75, 0.75)^\top$ and two negative charges with $q = -1$ on points $\vec{r}_3 = (0.25, 0.75)^\top$ and $\vec{r}_4 = (0.75, 0.25)^\top$. Again calculate $\phi(\vec{r})$ and $\vec{E}(\vec{r})$ inside the square by iteration.

## Exercise 2: Diffusion equation — 8 Points

*While you have dealt with the discretization of a static problem in the last task, you shall now look at a problem with additional time dependence. For the numerical solution of the diffusion equation, time must be discretized in addition to the spatial degrees of freedom. In this task you are to consider one of the simplest methods for this, the so-called FTCS (forward in time, centered in space) scheme.*

For solving the diffusion equation

$$\partial_t u(x,t) = D\,\partial_x^2 u(x,t)$$

implement the explicit FTCS scheme. We consider a one-dimensional system on $L = [0,1]$ with a spatial discretization $\Delta x = 0.01$ throughout the task. Let the edges be "isolating", so that no concentration $u(x,t)$ can flow in or out from the outside. Also, set the diffusion constant to $D = 1$ throughout the task. Graph all your results, for example using an animation with *FuncAnimation* from *matplotlib.animation*.

1. Write an algorithm that on $L$ is given an arbitrary initial condition $u(x,0)$ and is propagates the system with a time discretization $\Delta t$. Also consider the boundary conditions. Check your implementation for a system with the initial condition

$$u(x,0) = \text{const} = 1.$$

2. For the FTCS scheme, the stability criterion can be written as follows

$$\frac{2D\delta t}{\delta x^2} < 1.$$

Check this for the initial condition ($\delta$-peak).

$$u(x,0) = \delta(x - 0.5),$$

by comparing results for a time discretization just above and just below the criterion.

3. Now choose a reliable step size and determine the time-dependent solution of the diffusion equation for the initial conditions ($\delta$-peak, Heaviside, Dirac ridge).

$$u_1(x,0) = \delta(x - 0.5),$$
$$u_2(x,0) = \theta(x - 0.5),$$
$$u_3(x,0) = \frac{1}{9}\sum_{n=1}^{9} \delta(x - 0.1n).$$

For which initial condition does the system approach its equilibrium state the fastest? How does the space integral of the concentration $u(x,t)$ behave over time?