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Numerische Methoden der Physik

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Exercise sheet 5

To be discussed on 01, 04 June and 08, 11 June

Exercise 1 [*The Poisson equation*]

Consider a non moving electrically charged particle with negative charge $Q = -q$ in d-dimensional space, which is positioned in the centre of a grounded sphere of radius R. The electrostatic potential ϕ produced by the particle can be calculated solving the Poisson equation

$$\Delta\,\phi(\mathbf{r}) = \frac{q}{\varepsilon_0}\,\delta(\mathbf{r})$$

with the boundary condition $\phi(\mathbf{r}) = 0$ for $|\mathbf{r}| \geqslant R$ (here ε_0 is the vacuum permittivity).

First part

(i) Rewrite the Poisson equation in d dimensions in a way such that only dimensionless quantities are used.

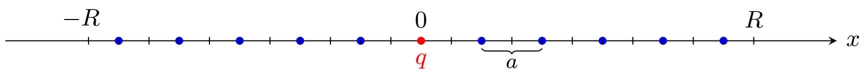
(ii) Calculate the potential $\phi(\mathbf{r})$ analytically for $d = 1$ (a 1-dimensional sphere is a set of two points at positions $x = \pm R$) and for $d = 2$.

(iii) Consider the problem in one dimension. A possibility to solve it numerically is to discretize the domain of the solution (in our case the interval $I \equiv [-R, R]$) introducing a (uniform) lattice and to approximate the derivatives with finite differences. In this way, the differential equation is mapped onto a system of linear equations, which can be solved using standard numerical techniques as discussed in the lecture.

Let us introduce a lattice

$$x \to x_j = j\,a \qquad \text{with} \qquad j \in [-n, n] \subset \mathbb{Z} \qquad \text{and} \qquad a = \frac{2R}{2n+1} \quad ,$$

which consists of $2n+1$ lattice points. At the boundary of the lattice, the conditions $\phi(x_{\pm(n+1)}) = 0$ must be imposed.



Notice that

$$\lim_{n\to\infty} x_n = R \qquad \text{and} \qquad \lim_{n\to\infty} x_{-n} = -R \quad .$$

Rewrite the Poisson equation in the form $A_{ij}\phi_j = b_i$, where $\phi_j \equiv \phi(x_j)$ is the unknown potential of the problem discretized on the lattice (now a vector with $2n+1$ components), while A and $\mathbf{b}$ are a matrix and a vector, respectively, which have to be specified before you can start the numerical implementation. Make use of the approximation

$$\frac{\partial^2\,\phi_j}{\partial\,x^2} \approx \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{a^2}$$

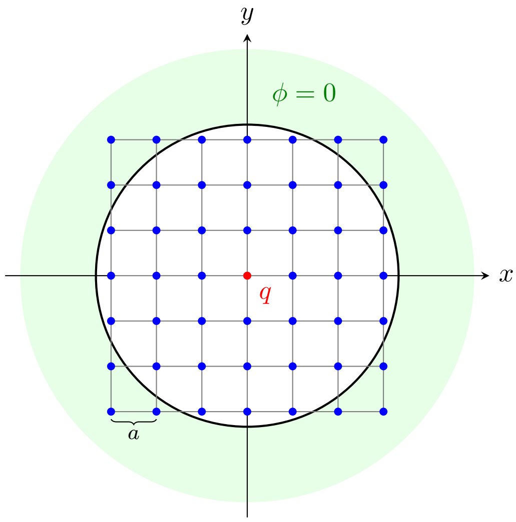
and think of how to properly treat the δ-function.

(iv) Solve the obtained linear system of equations with one of the numerical techniques which you learnt in the lecture (e.g. LU-decomposition), obtaining in this way the electrostatic potential $\phi(x)$. Study the dependence of your result on the parameter n, directly connected to the number of lattice points and compare your solution with the analytical one.

(v) Still in one dimension, put the particle inside the sphere at $x = R/2$. Solve again the Poisson equation analytically and numerically.

Second part

(vi) Consider now the above problem in two dimensions with the particle in the centre of the sphere. Repeat tasks (iii) and (iv) introducing now a $2d$-lattice.



(vii) In analogy to task (v), place the particle at position $(x, y) = (R/2, 0)$ and solve again the Poisson equation (this time only numerically).

Exercise 2 [*Lower Upper decomposition*]

Implement the LU decomposition method discussed in the lecture, to solve a system of linear equations in the form

$$A \cdot \mathbf{x} = \mathbf{b} \ ,$$

where A is a $N \times N$ matrix with real entries and $\mathbf{x}$, $\mathbf{b}$ are N-components vectors. After having added partial pivoting method to your code[1], study the advantage of using this technique when the entries of the matrix A and the components of $\mathbf{b}$ are

(i) random numbers uniformly distributed in the interval $[-1, 1]$

or

(ii) are of the form e^x with x being a random number uniformly distributed in the interval $[-5, 5]$.

In order to exhaustively understand what happens, solve the same linear system with and without partial pivoting for $10 \leqslant N \leqslant 400$ and plot the error $|A \cdot \mathbf{x} - \mathbf{b}|$ as function of N.

[1] Test your code to be sure it correctly works before using it!