Numerische Methoden der Physik

WiSe 2023-2024 – Prof. Marc Wagner

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Exercise sheet 7

To be handed in on 29.11.2023 and discussed on 01.12.2023 and 04.12.2023.

Exercise 1 [*LU-decomposition*] (8 pts.)

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

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

where A is an $N \times N$ matrix with real entries and $\mathbf{x}$, $\mathbf{b}$ are vectors with N components. Implement the partial pivoting method to your code.[1] Next, study the advantages of this method by constructing A and b, such that their elements 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 understand what happens in detail, solve the same system of linear equations with and without partial pivoting for $N = 10, 20, \ldots 400$ and plot the error $|A \cdot \mathbf{x} - \mathbf{b}|$ as function of N.

Exercise 2 [*The Poisson equation II*] (8+2+2=12 pts.)

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 *cubic box*. In the lecture, it has been discussed that, by introducing a d-dimensional lattice, the Poisson equation

$$\hat{\Delta}\, \hat{\phi}(\hat{\mathbf{r}}) = \hat{\delta}^{(d)}(\hat{\mathbf{r}})$$

(written in terms of dimensionless quantities) can be mapped into a system of linear equations $A_{ij}\hat{\phi}_j = b_i$.

(i) Implement the conjugate gradient (CG) method and use it to solve the discretized Poisson equation in $d = 3$ dimensions. Compute the electrostatic potential $\hat{\phi}$ on a cubic lattice with $n = 50$ points in each direction, using the CG method with a precision of $|A \cdot \hat{\phi} - \mathbf{b}| \leqslant 10^{-10}$. Repeat the computation, doubling the number of lattice points in each direction. To

[1] Hint: Test your code to be sure it correctly works before using it.

illustrate your result, plot $\hat{\phi}(\hat{\mathbf{r}})$ for $\hat{r}_x \in [0.1, 1]$ and $\hat{r}_y = \hat{r}_z \equiv 0$. Compare with the analytical solution

$$\hat{\phi}(\hat{\mathbf{r}}) = -\frac{1}{4\pi}\left(\frac{1}{\hat{r}} - \frac{1}{\hat{R}}\right)$$

for a charge without a grounded box, i.e. with boundary conditions $\phi(\mathbf{r} \to \infty) = \text{const}$.

(ii) How many iterations and how much time does your algorithm take to converge to the solution? Estimate roughly how much memory your program would need and determine the maximum lattice size your computer could possibly handle, for both, direct and iterative methods.

(iii) Now, consider two particles with charges $Q_1 = -Q_2 \equiv -q$, located at $\mathbf{r}_1 = -\mathbf{r}_2 = (R/4, 0, 0)$ and solve the Poisson equation

$$\hat{\Delta}\,\hat{\phi}(\hat{\mathbf{r}}) = \hat{\delta}^{(3)}(\hat{\mathbf{r}} - \hat{\mathbf{r}}_1) - \hat{\delta}^{(3)}(\hat{\mathbf{r}} - \hat{\mathbf{r}}_2).$$

Plot your result for $\hat{r}_x \in [-1, 1]$, $\hat{r}_y \in [-1, 1]$ and $\hat{r}_z = 0.1$.