Introduction to Computational Physics – Exercise 5

Simon Groß-Bölting, Lorenz Vogel, Sebastian Willenberg

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Numerical linear algebra methods: Tridiagonal matrices

We consider the following tridiagonal $N \times N$ matrix equation:

$$\underbrace{\begin{pmatrix} b_1 & c_1 & 0 & \cdots & 0 \\ a_2 & b_2 & c_2 & \ddots & \vdots \\ 0 & a_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & c_{N-1} \\ 0 & \cdots & 0 & a_N & b_N \end{pmatrix}}_{=:\, M = (m_{ij})} \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{pmatrix}}_{=:\, \vec{x} = (x_j)} = \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix}}_{=:\, \vec{y} = (y_i)} \tag{1}$$

Gauß elimination is the method of choice when one is interested in the solution $\vec{x}$ of the linear set of equations $M\vec{x} = \vec{y}$, but does not need the information about the inverse matrix M^{-1} (Gauß-Jordan method). In this case, it is sufficient to convert the matrix A into an upper (or lower) triangular matrix M'

$$M\vec{x} = \vec{y} \qquad \xrightarrow{\text{Gauß elimination}} \qquad M'\vec{x} = \vec{y}' \tag{2}$$

Then we can obtain the solution vector $\vec{x}$ by back substitution. Let us assume, we have already obtained a system $M'\vec{x} = \vec{y}'$ with M' being in upper triangular form, i.e. $m'_{ij} = 0$ for $i > j$, then we can compute $\vec{x}$ as

$$x_N = \frac{y'_N}{m'_{N,N}} \qquad x_{N-1} = \frac{1}{m'_{N-1,N-1}} \left(y'_{N-1} - m'_{N-1,N-1} x_N\right) \qquad \cdots \tag{3}$$

Thomas algorithm:

$$m_{i+1,i} = m_{i+1,i} - m_{i,i} \frac{m_{i+1,i}}{} \tag{4}$$