



# Scientific Computing II

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## Sheet 4

Submission on **Thursday, 7.6.18.**

### Exercise 1. (1D heat equation)

We consider a metal rod and its temperature distribution

$$y: [0, 1] \times [0, T] \longrightarrow \mathbb{R}$$

with initial condition  $y(\cdot, 0) = y^0$ . Additionally, we assume that we are able to control the heat flux of the metal rod at the end points. More precisely, we model  $y(x, t)$  to satisfy the partial differential equation

$$\begin{aligned} y_t - y_{xx} &= f && \text{in } [0, 1] \times [0, T] \\ -y_x(0, \cdot) &= l && \text{in } [0, T] \\ y_x(1, \cdot) &= r && \text{in } [0, T] \\ y(\cdot, 0) &= y^0 && \text{in } [0, 1] \end{aligned}$$

with control parameters  $l(t)$ ,  $r(t)$  and additional environmental influence  $f(x, t)$  (material conditions, additional heat source...).

As a first step, we want to do a time discretization of the partial differential equation. We interpret  $y(x, t) = y(t)(x) = y(t) \in V$  (f likewise), where  $y$  is now a function of time mapping into a function space  $V$ , which consists of functions defined on  $[0, 1]$  (for instance  $C[0, 1]$ ). Introducing the time steps  $t_n = nT/N$  for  $n = 0, \dots, N$  we define  $y^n = y(t_n) \in V$ ,  $f^n = f(t_n) \in V$ ,  $l(t_n) = l^n \in \mathbb{R}$ ,  $r(t_n) = r^n \in \mathbb{R}$ .

- a) Use the implicit Euler scheme to derive the time-discretized formulation

$$\begin{aligned} y^n &= y^{n-1} + \frac{T}{N}(f^n + y_{xx}^n), & n = 1, \dots, N \\ -y_x^n(0) &= l^n, & n = 1, \dots, N \\ y_x^n(1) &= r^n, & n = 1, \dots, N. \end{aligned}$$

This is a system of  $N$  Poisson-like differential equations, which from now on we consider in their weak form. Next, we do a spatial discretization  $V_h \subset V$  with basis functions  $\{\phi_0, \dots, \phi_m\}$ .

- b) Using the coefficient vector  $\underline{y}^n \in \mathbb{R}^{m+1}$  with the Ansatz

$$y^n \approx \sum_{i=0}^m \underline{y}_i^n \phi_i,$$

derive the time-space discretized formulation

$$\left( M + \frac{T}{N} K \right) \underline{y}^n = \frac{T}{N} L^n + M \underline{y}^{n-1}, \quad n = 1, \dots, N. \quad (1)$$

Here,  $M \in \mathbb{R}^{(m+1) \times (m+1)}$  is the mass matrix with  $M_{ij} = \int \phi_i \phi_j$ ,  $K \in \mathbb{R}^{(m+1) \times (m+1)}$  is the stiffness matrix with  $K_{ij} = \int (\phi_i)_x (\phi_j)_x$ , and  $L^n \in \mathbb{R}^{m+1}$  is the load vector with  $L_i^n = \int f^n \phi_i + \phi_i(0) l^n + \phi_i(1) r^n$ .

**Programmieraufgabe 1.** (1D heat equation)

The goal of this programming exercise is the implementation of the routine outlined in Exercise 1. This will take several steps:

- Calculation and Assemblation of  $M$ ,  $K$  and  $L$  for a given finite element basis. For  $M$  and  $K$ , we assemble the matrices as sparse multiplication routines to gain computational speed.
- Implementation of an iterative solver for the equations (1).
- Solution plotting, variation of input parameters, ...

For the space discretization, we use piecewise linear, continuous elements.

Let  $m \in \mathbb{N}$ . We consider the spacial nodes  $x_i = i/m$ ,  $i = 0, \dots, m$ . The nodal basis to the piecewise linear, continuous finite element space is given by

$$\phi_i(x) = \begin{cases} m(x - (i - 1)/m) & x \in [(i - 1)/m, i/m] \\ 1 - m(x - i/m) & x \in [i/m, (i + 1)/m] \\ 0 & \text{else} \end{cases}$$

for  $i = 0, \dots, m$ .

- Calculate  $K_m, M_m \in \mathbb{R}^{(m+1) \times (m+1)}$  for this basis. Calculate  $L_{m,i}^n$  for the case that  $f^n$  is piecewise constant on the intervals  $[i/m, (i + 1)/m]$  for  $i = 0, \dots, m - 1$ .
- Implement a routine which takes  $m \in \mathbb{N}$ ,  $l, r \in \mathbb{R}$  and  $b \in \mathbb{R}^m$  as input and returns as output the vector

$$L = [L_i]_{i=0}^{m+1} = \left[ \int_0^1 \phi_i(x)b(x) dx + \phi_i(0)l + \phi_i(1)r \right]_{i=0}^{m+1}.$$

Here,  $b(x)$  is the piecewise constant function with  $b|_{[i/m, (i+1)/m]} \equiv b_{i+1}$  for  $i = 0, \dots, m - 1$ .

- Implement a routine which takes  $m \in \mathbb{N}$ ,  $a \in \mathbb{R}$  and a vector  $b \in \mathbb{R}^{m+1}$  as input and returns as output the vector  $(M_m + aK_m)b \in \mathbb{R}^{m+1}$ . Make sure that this routine has runtime  $\mathcal{O}(m)$  (use the sparse structure of the matrices).
- Implement an iterative solver for linear equation systems of the form

$$(M_m + aK_m)b = c$$

which uses the matrix-vector-product routine from part b). Possible choices are for instance the CG-method or the Jacobi method.

- Write the final routine which solves the system (1). The input is given as  $T \in \mathbb{R}$ ,  $m, N \in \mathbb{N}$ ,  $\underline{y}^0 = [\underline{y}_i^0]_{i=0}^m \in \mathbb{R}^{m+1}$ ,  $f = [f_i^n]_{n=1, i=0}^{N, m-1} \in \mathbb{R}^{N \times m}$ , and  $l = [l^n]_{n=1}^N, r = [r^n]_{n=1}^N \in \mathbb{R}^N$ . For  $n = 1, \dots, N$ , one obtains  $\underline{y}^n \in \mathbb{R}^{m+1}$  sequentially as stated in (1). The output is given by  $y = [y_i^n]_{n=0, i=0}^{N, m+1} \in \mathbb{R}^{(N+1) \times (m+1)}$ .
- Test your implementation with the following input data:  $T = 10$ ,  $m = 100$ ,  $N = 1000$ ,  $\underline{y}^0 \equiv 0 \in \mathbb{R}^{m+1}$ ,  $l \equiv r \equiv -0.1 \in \mathbb{R}^N$ , and  $f = [f_i^n]_{n=1, i=0}^{N, m-1} \in \mathbb{R}^{N \times m}$  defined via

$$f_i^n = \begin{cases} 1 & i = 50, \\ 0 & \text{else.} \end{cases}$$

Visualize the solution in a comprehensive manner, e.g. a GIF-animation.

g) One can easily show that the solution  $y$  to the original PDE satisfies

$$\int_0^1 y(x, 0) dx = \int_0^1 y(x, t) dx \quad \forall t \in [0, T].$$

Does the computed approximation show an analogous behaviour? Why/Why not?  
(30 points)

The programming exercise should be handed in either before/after the exercise class on 14.6.18 (bring your own laptop!) or in the HRZ-CIP-Pool, after making an appointment at 'angelina.steffens@uni-bonn.de'. All group members need to attend the presentation of your solution. Closing date for the programming exercise is the 14.6.2018. You can choose the programming language yourself.