Scientific Computing: Exam

General Remarks:

• You may only use one hand-written sheet of paper (size A4, on both pages). All other material including electronic devices of any kind are forbidden!
• Do not use pencil, or red or green ink.

1 Discrete Modelling: Pipe Network (6 Points)

A fluid is transported through a network of pipes, see Fig. 1. For each pipe that connects two chambers \( i \) and \( j \) \((i \neq j)\), the relative flow rate \( p_{ij} \), that is the percentage of fluid in chamber \( i \) that flows, per time unit, to chamber \( j \), is given for each pipe in the figure.

(a) Construct a model using ordinary differential equations to describe the evolution of the amount of fluid \( f_i \) in each chamber \( i \) for an arbitrary pipe network.

(b) Write down the system of ODEs for the pipe network from Fig. 1 using matrix-vector notation. Why can the respective flow rate matrix \( p_{ij} \) not be strictly diagonally dominant? Give a short explanation including the definition of strict diagonal dominance.

![Pipe network diagram](image)

Figure 1: Pipe network. Each pipe including the direction of the flow inside of the pipe is shown as arrow. The chambers are illustrated by black circles.
2 Continuous Modelling: ODEs (11 Points)

The following system of ordinary differential equations is given:

\[
\begin{align*}
\frac{dy_1(t)}{dt} &= y_1(t) + \frac{1}{2}y_2(t) \\
\frac{dy_2(t)}{dt} &= \frac{1}{2}y_2(t),
\end{align*}
\]

(1)

together with initial conditions \(y_1(0) = 1, y_2(0) = 1\).

(a) Compute the critical points of the problem and the eigenvalues and eigenvectors of the matrix \(A \in \mathbb{R}^{2 \times 2}\) of the system \(\frac{dy}{dt} = A \cdot y\). Draw the \(y_1 - y_2\)-direction field on the interval \([-1; 1] \times [-1; 1]\). Use the direction field to determine whether the critical points are stable, unstable or saddle points.

(6 points)

(b) Formulate the Crank-Nicolson (identical to second-order Adams-Moulton) method for the ODE from Eq. (1) using a time step \(\tau\). Compute the explicit form of the arising update scheme for \(y_1(t + \tau), y_2(t + \tau)\) (your computations need to be clear, and each step needs to be comprehensible).

Remark: you may use the following formula to invert \(2 \times 2\) matrices:

\[
\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}
\]

(3 points)

(c) Consider the eigenvalues of the Crank-Nicolson matrix in Eq. (?). For which time steps \(\tau\) do you expect instabilities? Explain your decision by a short computation and 1-2 sentences.

(2 points)
3 Finite Difference Methods: Chemical Transport (15 Points)

The transport equation for a chemical substance \( c(t,x,y) \) resolved in a fluid reads

\[
\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = k \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right)
\]

where \( k > 0 \) denotes the diffusivity of the substance and \( u, v \) the flow velocity in \( x \)- and \( y \)-direction, respectively. We want to solve this equation on a big two-dimensional reservoir \([0, 1000] \times [0, 1000]\).

(a) Simplify Eq. (3) by incorporating all of the following assumptions:

I The fluid properties are set to \( u = 1, \ v = 0, \ k = 1 \).

II The problem under consideration is in steady state, that is the concentration of the substance \( c \) does not change over time.

III No diffusion effects occur in \( x \)-direction.

(b) Formulate a finite difference discretisation for the simplified equation from (a) using first-order finite differences of the form

\[
\frac{\partial f}{\partial z} \approx \frac{f(z+h) - f(z)}{h}
\]

for the first-order derivatives and the usual central difference scheme for the second-order derivatives. Use an equidistant grid with \( N + 1 \) grid points which covers the square \([0, 1000] \times [0, 1000]\) and a corresponding mesh size \( h := 1000/N \) in both \( x \)- and \( y \)-direction. You may use the notation \( c_{i,j} := c(ih, jh) \). In addition, state the order of the local discretisation errors for both finite difference schemes.

(c) Sketch the arising algorithm to solve the finite difference system from (b) in pseudo-code to compute the pointwise solution \( c_{ij} \) on the whole square. How do you enforce Dirichlet boundary conditions in this algorithm?

(d) Use the von-Neumann stability analysis to investigate the stability of the discrete form from (b). Which restriction arises for the mesh size \( h \)?

Hint: the vector \( f_k(jh) = \sin(k\pi x), \ j = 0, ..., N, \) is an eigenvector of the finite difference-expression for the second-order derivative. The corresponding eigenvalue is given by

\[
\lambda_k := \frac{2}{h^2}(\cos(\pi kh) - 1).
\]
4 Finite Element Methods: Convection-Diffusion (14 Points)

The following differential equation for an unknown function $u(x,y)$ is defined on a square, $\Omega := (0, a) \times (0, b)$, with homogeneous Dirichlet conditions on all boundaries of the square:

$$\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + q(x,y)$$  \hspace{1cm} (6)

where $q(x,y)$ denotes a (known) source term.

We want to solve the problem on a Cartesian grid using the standard Galerkin procedure. For this purpose, we introduce locally bilinear basis functions which are defined on the reference element $E$ given in Fig. 2. The basis functions on the local reference element are given by

$$\begin{align*}
\varphi_0(x,y) &= (1-x)(1-y), \\
\varphi_1(x,y) &= x(1-y), \\
\varphi_2(x,y) &= (1-x)y, \\
\varphi_3(x,y) &= xy.
\end{align*}$$  \hspace{1cm} (7)

For the corners $P_0, \ldots, P_3$ of the reference element, cf. Fig. 2, this yields $\varphi_i(P_j) = \delta_{ij}$ similar to the case of using piecewise linear basis functions on triangles.

(a) Derive the weak formulation of Eq.(6) for test functions $\psi(x,y)$ which belong to some function space $V$, $\psi(x,y) \in V$. No discretisation of the function space $V$ is required. Use integration by parts to transform the second-order derivative. Give a brief explanation why this transformation is helpful.

(b) Discretise your weak formulation using the basis functions $\varphi_i(x,y)$. Re-write the system in matrix-vector form $C \cdot \vec{u} = A \cdot \vec{u} + M \cdot \vec{q}$ with matrices

- $C$ describing convection
- $A$ describing diffusion
- $M$ invoking sources terms.

Give a definition for each matrix entry $C_{ij}$, $A_{ij}$, $M_{ij}$.

(c) Compute the contributions of the matrices $A_{33}$ and $C_{33}$ on the reference element.

(4 points)