Name:	Matr.Nr.:	No. Sheets:

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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.

(3 points)

(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.

(3 points)

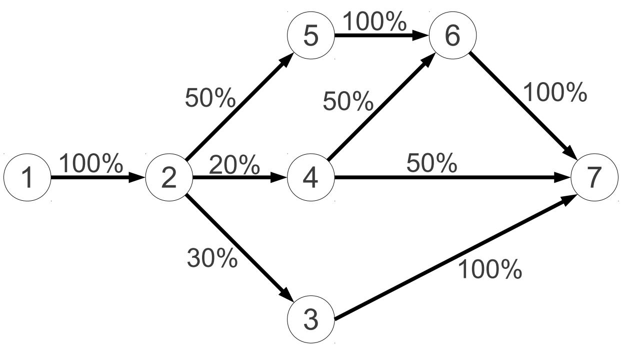

Figure 1: Pipe network. Each pipe including the direction of the flow inside of the pipe is shown as arrow. The chambers are illustrated by black circles.

2 Continuous Modelling: ODEs (11 Points)

The following system of ordinary differential equations is given:

$$\begin{aligned} \frac{dy_1(t)}{dt} &= y_1(t) + \tfrac{1}{2}y_2(t) \\ \frac{dy_2(t)}{dt} &= \tfrac{1}{2}y_2(t), \end{aligned} \tag{1}$$

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 τ. 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 2×2 matrices:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \tag{2}$$

(3 points)

(c) Consider the eigenvalues of the Crank-Nicolson matrix in Eq. (**??**). For which time steps τ 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

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = k\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) \tag{3}$$

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.

(3 points)

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

$$\frac{\partial f(..., z, ...)}{\partial z} \approx \frac{f(..., z+h, ...) - f(..., z, ...)}{h} \tag{4}$$

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.

(4 points)

(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?

(5 points)

(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

$$\lambda_k := \frac{2}{h^2}(\cos(\pi k h) - 1). \tag{5}$$

(3 points)

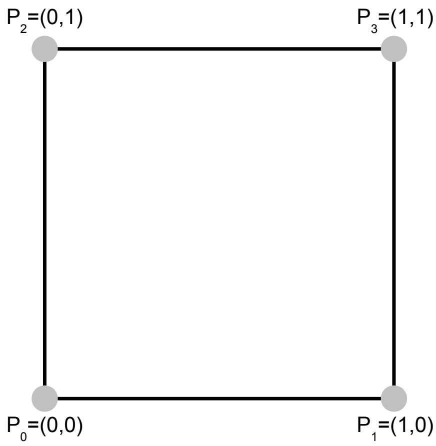

Figure 2: Cartesian grid cell for the application of bilinear ansatz functions.

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:

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

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

$$\begin{aligned} \varphi_0(x, y) &= (1 - x)(1 - y), \\ \varphi_1(x, y) &= x(1 - y), \\ \varphi_2(x, y) &= (1 - x)y, \\ \varphi_3(x, y) &= xy. \end{aligned} \tag{7}$$

For the corners P_0,..., 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.

(4 points)

(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}.

(4 points)

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

(6 points)