



Scientific computing exam 2021

Scientific Computing (Technische Universität München)

Esolution

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Note:

- During the attendance check a sticker containing a unique code will be put on this exam.
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Scientific Computing 1

Exam: IN2005 / Endterm

Date: Friday 26th February, 2021

Examiner: Michael Bader

Time: 08:00 – 09:30

Working instructions

- This exam consists of **18 pages** with a total of **5 problems**.
Please make sure now that you received a complete copy of the exam.
- The total amount of achievable credits in this exam is 50 credits.
- Detaching pages from the exam is prohibited.
- Allowed resources:
 - all printed or electronic scripts, textbooks or lecture material
 - your own handwritten notes
- The working time for the exam is 90 minutes plus 30 minutes submission time.
- Subproblems marked by * can be solved without results of previous subproblems.
- The small scale of boxes printed next to each subproblem indicates the maximum number of credits awarded for this subproblem. **Do not write into these boxes!**
- 18 credits will be sufficient to pass the exam.
- **Answers are only accepted if the solution approach is documented.** Give a reason for each answer unless explicitly stated otherwise in the respective subproblem.
- Do not write with red or green colors nor use pencils.
- During the exam, no questions concerning the content of the exam questions will be answered.
- If you think that a question or exercise text contains an error or ambiguity, then choose a correction or variant that allows you to complete the solution – state how you have corrected or interpreted the exercise.

General Disclaimer for all solution examples: the given solution text is not intended as a “perfect answer” to the exercise; it only outlines the main aspect of the solution in compact form. It is assumed that you look up further details in the lecture material where necessary.

Left room from _____ to _____ / Early submission at _____

Problem 1 Hatching of Pigeons (8 credits)

A pair of pigeons decided to settle on a balcony and lay their eggs there. On the next day, the pigeons discovered that the balcony is visited by people and got stressed about it.

We model the pigeons' behavior by Markov chains. Suppose there are three states in our model:

1. The pigeons abandon their nest and do not return.
2. The pigeons are worried about the people and consider to abandon the nest.
3. The pigeons are not afraid of people and do not consider to abandon their nest.

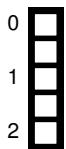
The transition matrix of the corresponding Markov chain is given by:

$$P = \begin{pmatrix} 1 & 5/16 & 0 \\ 0 & 1/2 & 1/4 \\ 0 & 3/16 & 3/4 \end{pmatrix}. \quad (1)$$

The transition matrix allows us to find the probabilities of the states f_{n+1} after $n + 1$ days when we know the probabilities after n days:

$$f_{n+1} = Pf_n = \begin{pmatrix} 1 & 5/16 & 0 \\ 0 & 1/2 & 1/4 \\ 0 & 3/16 & 3/4 \end{pmatrix} \begin{pmatrix} f_1(n) \\ f_2(n) \\ f_3(n) \end{pmatrix},$$

where $f_1(n)$, $f_2(n)$, $f_3(n)$ are the probabilities of the corresponding three states after n days.



a) * Sketch the diagram of the described Markov chain corresponding to transition matrix (1). Use Figure 1.1 to make your sketch.

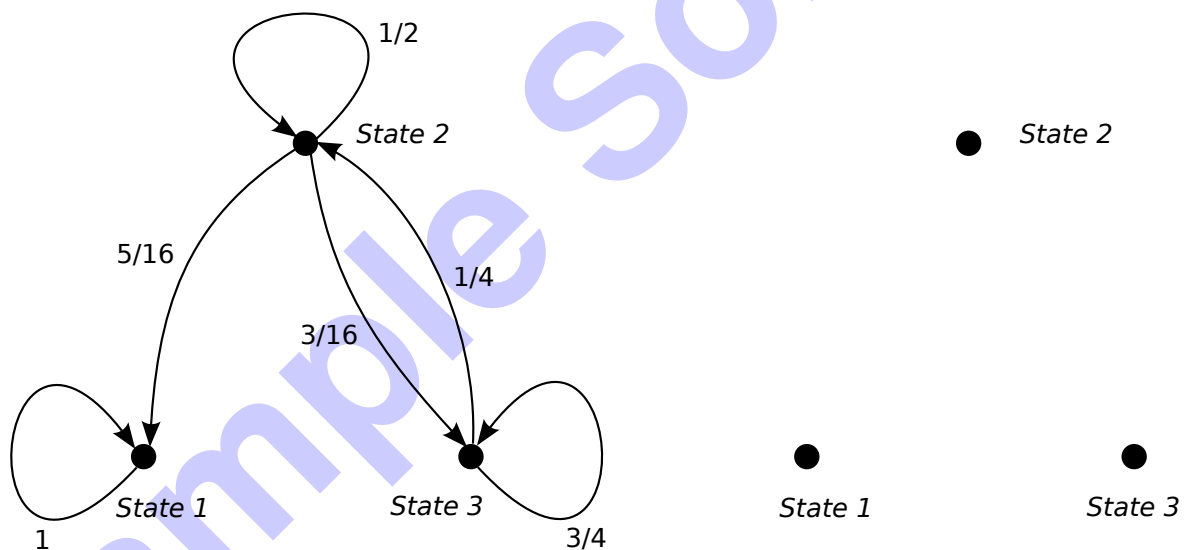


Figure 1.1: Sketch the diagram of the described Markov chain. Two empty figures are provided in case you are not satisfied with your first attempt and want to produce a second. In case you do, use the second empty figure and make sure you cross out your worse attempt.

See Figure 1.1 left.

b) * Compute the probability distribution f_n in the long term limit $n \rightarrow \infty$. Does it depend on the initial distribution? Explain your answer with reasons/arguments.



Suggested variants of answers:

1. The first state is absorbing. As soon as the system appears at this states, it stays in it forever. In the long term limit, the system eventually will get to the first state independent on the initial state. Therefore, we conclude that $f(n \rightarrow \infty) = (1 \ 0 \ 0)^T$, and it does not depend on the initial distribution.
2. We assume that in the long term limit the probability distribution converges to a certain stationary solution. Therefore, we solve the following equation to find the stationary solution

$$\begin{pmatrix} 1 & 5/16 & 0 \\ 0 & 1/2 & 1/4 \\ 0 & 3/16 & 3/4 \end{pmatrix} f_s = f_s.$$

Furthermore, the sum of f_s components must be equal one. Then the stationary solution is $f_s = (1 \ 0 \ 0)^T$. This solution corresponds to $\lambda_1 = 1$ eigenvalue, all other eigenvalues as shown in c) are smaller than one. Therefore, we conclude that contributions of other eigenvectors decays in time and the long term solution does not depend on initial condition.

3. Matrix P is column-stochastic, therefore, it has at least one eigenvalue $\lambda_1 = 1$ and the absolute values of all other eigenvalues are less than one. Indeed, from $\det(P - \lambda I) = 0$, we find that $\lambda_1 = 1$, $\lambda_2 = 7/8$, and $\lambda_3 = 3/8$, where $|\lambda_2| < 1$ and $|\lambda_3| < 1$. As a result, the long term limit solution does not depend on the initial state and will converge to the eigenvector corresponding to $\lambda_1 = 1$. Therefore, the corresponding eigenvector $f_1 = (1 \ 0 \ 0)^T$ is exactly the long term limit we are looking for.

- 0 ☐
- 1 ☐
- 2 ☐
- 3 ☐
- 4 ☐
- c) * On average, the squabs (baby pigeons) appear after 18 days. Find the probability that parent pigeons will not abandon the nest during this period, if at the first day they are at state 3.
Hint: the eigenvalues and eigenvectors of the transition matrix are:
- $$\begin{aligned}\lambda_1 &= 1 & f_{e1} &= (1 \ 0 \ 0)^\top \\ \lambda_2 &= 7/8 & f_{e2} &= (-5 \ 2 \ 3)^\top \\ \lambda_3 &= 3/8 & f_{e3} &= (-1 \ 2 \ -1)^\top\end{aligned}\quad (2)$$

Furthermore, you can use the approximations $\lambda_2^{18} = 0.1$ and $\lambda_3^{18} = 2 \cdot 10^{-8}$.

We can write down the initial probabilities vector as a linear combination of eigenvectors f_j :

$$f_0 = \sum_{j=1}^3 a_j f_{ej}.$$

Then after 18 iterations $f_{n+1} = P f_n$ we obtain:

$$f_{18} = \sum_{j=1}^3 a_j \lambda_j^{18} f_{ej}.$$

We find the coefficients a_1 , a_2 , and a_3 from the linear system

$$a_1 f_{e1} + a_2 f_{e2} + a_3 f_{e3} = f_0.$$

For our initial distribution vector $f_0 = (0 \ 0 \ 1)^\top$ we find that $a_1 = 1$, $a_2 = 1/4$, and $a_3 = -1/4$.
Now, we find the probability that in 18 days the nest is abandoned:

$$\begin{aligned}f_{18}(1) &= a_1 \lambda_1^{18} f_{e1}(1) + a_2 \lambda_2^{18} f_{e2}(2) + a_3 \lambda_3^{18} f_{e3} \\ &= 1 \cdot 1^{18} \cdot 1 - \frac{1}{4} \cdot \left(\frac{7}{8}\right)^{18} \cdot 5 + \frac{1}{4} \cdot \left(\frac{3}{8}\right)^{18} \cdot 1 \approx 0.88.\end{aligned}$$

We conclude that the squab will appear with probability $1 - f_{18}(1) \approx 0.12$.

Problem 2 ODEs: Analysis and Numerical Methods (13 credits)

Consider an electrical circuit containing a resistor, an inductor, and a capacitor, as in Figure 2.1. Such circuits are called RLC series circuits. They can be modelled by a second-order, constant-coefficient ODE:

$$L \frac{d^2 q(t)}{dt^2} + R \frac{dq(t)}{dt} + \frac{1}{C} q(t) = E(t), \quad (3)$$

where L is the inductance, R is the resistance, C is the capacitance, $E(t)$ is the variable electric potential of the electric source, and $q(t)$ is the unknown charge on the capacitor. As a reminder, the electric current passing through such a circuit is given by $I(t) = \frac{dq(t)}{dt}$.

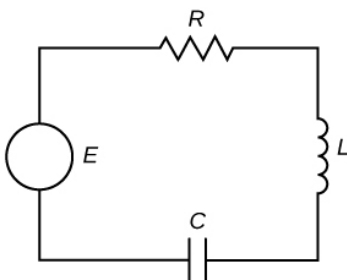


Figure 2.1: RLC serial circuit

a) * Transform equation (3) in an equivalent system of first-order ODEs, under the assumption that $L \neq 0$. Write the system of ODEs in matrix-vector form.

$$\frac{d\mathbf{q}(t)}{dt} = \begin{pmatrix} 0 & 1 \\ -\frac{1}{LC} & -\frac{R}{L} \end{pmatrix} \mathbf{q}(t) + \begin{pmatrix} 0 \\ \frac{E(t)}{L} \end{pmatrix}$$
$$\mathbf{q}(t) = \begin{pmatrix} q(t) \\ I(t) \end{pmatrix}$$

0
1
2

- 0 ☐ 1 ☐ 2 ☐ 3 ☐
- b) Physical constraints on real-life RLC series circuits are, of course, that $R > 0$, $L > 0$, and $C > 0$. Show that this is already a sufficient condition for the given ODE to have a stable critical point in the homogeneous case, i.e. $E(t) = 0$.

Method 1: Using principal minors

$$\lambda_1 + \lambda_2 = \text{tr}(A) = -\frac{R}{L} < 0$$

$$\lambda_1 \cdot \lambda_2 = \det(A) = \frac{1}{LC} > 0$$

$$\Rightarrow \Re(\lambda_{1,2}) < 0 \quad (\forall \lambda_{1,2} \in \mathbb{C})$$

Method 2: Computing the generic eigenvalues

$$\det(\lambda I - A) \stackrel{!}{=} 0 \Rightarrow \left| \begin{pmatrix} \lambda & -1 \\ \frac{1}{LC} & \lambda + \frac{R}{L} \end{pmatrix} \right| = \lambda^2 + \frac{R}{L}\lambda + \frac{1}{LC} \stackrel{!}{=} 0$$

$$\lambda_{1,2} = -\frac{R}{2L} \pm \sqrt{\left(\frac{R}{2L}\right)^2 - \frac{1}{LC}}$$

$$\Rightarrow \Re(\lambda_{1,2}) < 0 \quad (\text{checking both cases: } \lambda_{1,2} \in \mathbb{R} \wedge \lambda_{1,2} \in \mathbb{C} \setminus \mathbb{R})$$

Moving forward, we will consider a particular case of our RLC series circuit, in the form of the initial value problem

$$\dot{\mathbf{q}}(t) = A\mathbf{q}(t) + \mathbf{b}, \quad A = \begin{pmatrix} 0 & 1 \\ -18 & -6 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 180 \end{pmatrix}, \quad \mathbf{q}(0) = \begin{pmatrix} 0 \\ 9 \end{pmatrix}. \quad (4)$$

- 0 ☐ 1 ☐ 2 ☐
- c) * Find all critical points of the ODE in (4).

$$0 \stackrel{!}{=} A\hat{\mathbf{q}} + \mathbf{b} \Rightarrow \hat{\mathbf{q}} = -A^{-1}\mathbf{b}$$

$$A^{-1} = \frac{1}{18} \begin{pmatrix} -6 & -1 \\ 18 & 0 \end{pmatrix} = \begin{pmatrix} -\frac{1}{3} & -\frac{1}{18} \\ 1 & 0 \end{pmatrix}$$

$$\hat{\mathbf{q}} = \begin{pmatrix} 10 \\ 0 \end{pmatrix}$$

d) Apply the method of Heun (second order Runge-Kutta) to the ODE in (4) using a time step τ . Express the result in the form

$$\mathbf{q}^{(n+1)} = M(\tau) \mathbf{q}^{(n)} + \mathbf{d}(\tau).$$

Method of Heun:

$$\mathbf{q}_I^{(n)} = \mathbf{q}^{(n)}$$

$$\mathbf{q}_{II}^{(n)} = \mathbf{q}^{(n)} + \tau f(t^{(n)}, \mathbf{q}^{(n)})$$

$$\mathbf{q}^{(n+1)} = \mathbf{q}^{(n)} + \frac{\tau}{2} \left(f(t^{(n)}, \mathbf{q}_I^{(n)}) + f(t^{(n+1)}, \mathbf{q}_{II}^{(n)}) \right)$$

For our ODE:

$$\mathbf{q}^{(n+1)} = \mathbf{q}^{(n)} + \frac{\tau}{2} (\mathbf{A}\mathbf{q}^{(n)} + \mathbf{b} + \mathbf{A}(\mathbf{q}^{(n)} + \tau(\mathbf{A}\mathbf{q}^{(n)} + \mathbf{b})) + \mathbf{b})$$

$$\mathbf{q}^{(n+1)} = \left(\frac{\tau^2}{2} \mathbf{A}^2 + \tau \mathbf{A} + \mathbf{I} \right) \mathbf{q}^{(n)} + \left(\frac{\tau^2}{2} \mathbf{A}\mathbf{b} + \tau \mathbf{b} \right)$$

$$\mathbf{A}^2 = \begin{pmatrix} -18 & -6 \\ 108 & 18 \end{pmatrix}, \mathbf{A}\mathbf{b} = \begin{pmatrix} 180 \\ -1080 \end{pmatrix} \Rightarrow$$

$$\mathbf{q}^{(n+1)} = \begin{pmatrix} -9\tau^2 + 1 & -3\tau^2 + \tau \\ 54\tau^2 - 18\tau & 9\tau^2 - 6\tau + 1 \end{pmatrix} \mathbf{q}^{(n)} + \begin{pmatrix} 90\tau^2 \\ -540\tau^2 + 180\tau \end{pmatrix}$$

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Problem 3 Numerical Methods for ODEs (8 credits)

Consider the direction fields representing different numerical schemes for a 1D differential equation $dp/dt = f(t, p)$, as given on page 9.

The different numerical schemes are demonstrated in Figure 3.1. These schemes are used to approximate the solution at times $t_n = 0.5 \cdot n$.

Fill in the empty fields (formula, number of the figure, implicit or explicit, one- or multi-step) in the table below.

Hints:

1. The approximate values are marked by green dots.
2. The bold arrows correspond to the necessary function $f(t, p)$ evaluations to get the approximate value of p at the following time steps.
3. The green dashed lines are used to connect the bold arrows to the place where they are applied, in case they are computed at different points.
4. Multi-step methods may require several points as the initial conditions.

Nr.	Method – Formula	Figure Nr.	Implicit or Explicit	One or Multi-step
1	Ralston: $p_{n+1} = p_n + \tau \left(\frac{1}{4} f(t_n, p_n) + \frac{3}{4} f \left(t_n + \frac{2}{3} \tau, p_n + \frac{2}{3} \tau f(t_n, p_n) \right) \right)$	8	explicit	one-step
2	BDF-2: $p_{n+1} = \frac{4}{3} p_n - \frac{1}{3} p_{n-1} + \frac{2}{3} \tau f(t_n, p_n)$	7	explicit	multi-step
3	Explicit Euler: $p_{n+1} = p_n + \tau f(t_n, p_n)$	6	explicit	one-step
4	Second order modified Euler: $p_{n+1} = p_n + \tau f \left(t_n + \frac{1}{2} \tau, p_n + \frac{1}{2} \tau f(t_n, p_n) \right)$	1	explicit	one-step
5	Second order Adams-Bashforth: $p_{n+1} = p_n + \frac{3}{2} \tau f(t_n, p_n) - \frac{1}{2} \tau f(t_n - \tau, p_{n-1})$	5	explicit	multi-step
6	Crank-Nicolson (Trapezoidal rule): $p_{n+1} = p_n + \frac{1}{2} \tau (f(t_n, p_n) + f(t_{n+1}, p_{n+1}))$	2	implicit	one-step
7	Heun: $p_{n+1} = p_n + \tau \left(\frac{1}{2} f(t_n, p_n) + \frac{1}{2} f \left(t_n + \tau, p_n + \tau f(t_n, p_n) \right) \right)$	4	explicit	one-step
8	Implicit Euler: $p_{n+1} = p_n + \tau f(t_n + \tau, p_{n+1})$	3	implicit	one-step

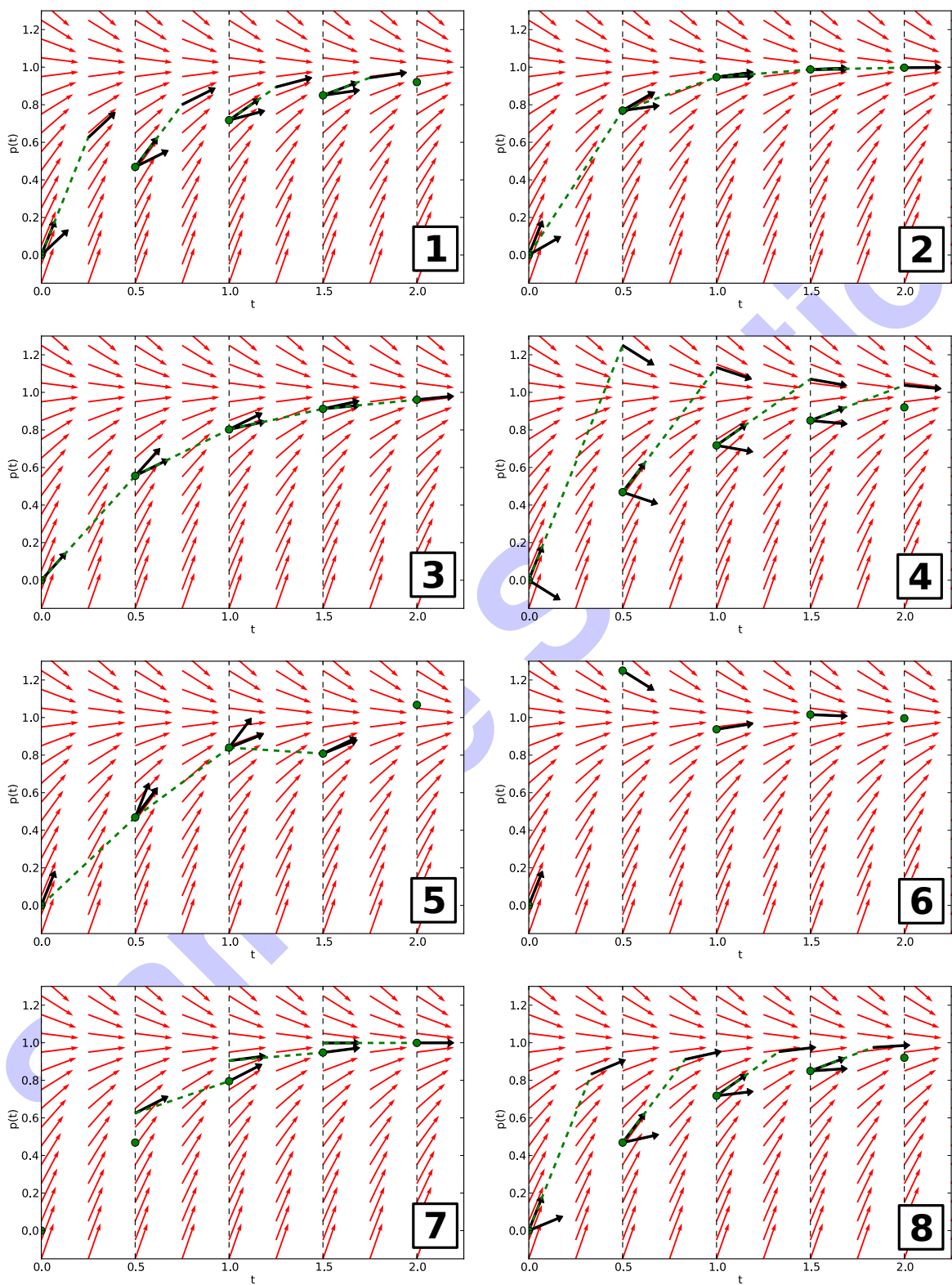


Figure 3.1: Direction field for the system of ODEs.

Problem 4 1D Flow Equation (12 credits)

For a 1D fluid that flows with very small velocity $u(x, t)$, we can derive the following 1D PDE:

$$\frac{\partial u}{\partial t} - C \frac{\partial^2 u}{\partial x^2} = g(t) \quad (5)$$

where $C \in \mathbb{R}^+$ denotes the diffusion constant of the fluid, $g(t)$ is the pressure gradient $-\partial p / \partial x$.

- 0 ☐
- 1 ☐
- 2 ☐
- a) * Develop a numerical scheme to solve equation (5): use a first-order discretisation for the temporal derivative, a time-implicit, spatial second-order finite difference discretization for the spatial second-order derivative and a time-explicit evaluation of the function $g(t)$.
You may further assume an equidistant discretization of the unit interval in space, $x \in [0, 1]$, using $N + 1$ grid points and a resulting mesh size $h := 1/N$. The time step shall be denoted by τ , the discrete velocity values for $u(t, x)$ by $u_i^n := u(n\tau, ih)$, $i = 0, \dots, N$, and the discrete representation of the function $g(t)$ by $g^n := g(n\tau)$.

The first-order time-implicit scheme is given by the implicit Euler method, the second-order spatial discretization corresponds to the default three-point stencil for the 1D Laplacian:

$$\frac{u_i^{n+1} - u_i^n}{\tau} - C \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{h^2} = g^n$$

b) Reformulate the discretised equation from a) for one particular time step $n \rightarrow n + 1$ in the form of a linear system of equations

$$\sum_{j=0}^N A_{ij} u_j^{n+1} = b_i^n, \quad i = 0, \dots, N, \quad (6)$$

with matrix $(A_{ij}) \in \mathbb{R}^{N+1 \times N+1}$. The term b_i^n should contain all contributions from the previous time step n . Assume homogeneous Dirichlet conditions at the boundaries, i.e. $u_0^{n+1} = 0, u_N^{n+1} = 0$. Make sure to give an exact definition of the matrix entries A_{ij} and right hand side entries b_i^n .



Splitting the equation from above into information from time step n and $n + 1$ results in

$$-\frac{C}{h^2} u_{i-1}^{n+1} + \left(\frac{1}{\tau} + \frac{2C}{h^2} \right) u_i^{n+1} - \frac{C}{h^2} u_{i+1}^{n+1} = g^n + \frac{1}{\tau} u_i^n$$

for all (inner and boundary) points $i = 0, \dots, N$. The matrix A can thus be defined as

$$A_{ij} := \begin{cases} -\frac{C}{h^2} & |j - i| = 1 \text{ and } i \neq 0, N \\ \frac{1}{\tau} + \frac{2C}{h^2} & \text{if } i = j \text{ and } i \neq 0, N \\ 1 & i = j \text{ and } (i = 0 \vee i = N) \\ 0 & \text{otherwise.} \end{cases}$$

The right hand side b_i^n evolves at $b_i^n := g^n + \frac{1}{\tau} u_i^n$ for $i = 1, \dots, N - 1$ and $b_0^n = 0, b_N^n = 0$.

- 0 ☐ c) Now consider the case that the pressure gradient $g(t)$ is equal to 0. The homogeneous equation is then of the
 1 form: $\frac{\partial u}{\partial t} - C \frac{\partial^2 u}{\partial x^2} = 0$.
 2 As in the von Neumann stability analysis we assume that the numerical solution is of type:

$$u_i^{(n)} = a_k^n \sin(\pi k i h) \quad (7)$$

3 Derive an explicit formula for the coefficient a_k such that $u_i^{(n)}$ solves the time-implicit scheme developed in a) and b).
 4 Hint: You may use the equality $\sin(A + B) + \sin(A - B) = 2 \sin(A) \cos(B)$.

Inserting the definition of $u_i^{(n)} = a_k^n \sin(\pi k i h)$ into the discrete update equation from b, and putting $g^n = 0$ yields:

$$-\frac{C}{h^2} a_k^{n+1} \sin(\pi k (i-1)h) + \left(\frac{1}{\tau} + \frac{2C}{h^2} \right) a_k^{n+1} \sin(\pi k (i)h) - \frac{C}{h^2} a_k^{n+1} \sin(\pi k (i+1)h) = \frac{1}{\tau} a_k^n \sin(\pi k i h)$$

Dividing by $a_k^n \sin(\pi k i h)$ results in an expression for a_k :

$$a_k = \frac{1}{1 - \frac{2C\tau}{h^2} (\cos(\pi k h) - 1)}.$$

d) Under which condition will the solution u decay? State whether and which constraints are imposed on the choice of τ and h .

0
1
2

The solution decays if it holds $|a_k| < 1$. Using the monotony of $\cos(\pi kh)$, it is enough to consider the extreme cases $\cos(\pi kh) = \pm 1$. We obtain

$$a_k \Big|_{\cos(\pi kh)=1} = 1$$

$$a_k \Big|_{\cos(\pi kh)=-1} = \frac{1}{1 + \frac{4\tau}{h^2}}$$

On the interval $\cos(\pi kh) \in (-1, 1)$, $|a_k| < 1$ is consequently fulfilled for all choices of τ and h . Our time-implicit algorithm is hence unconditionally stable.

Sample Solution

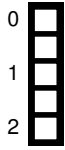
Problem 5 Cruzeix-Raviart Elements for FEM (9 credits)

The 2-dimensional heat equation is given as:

$$\frac{\partial}{\partial t} u = \Delta u, \quad (8)$$

where $\Delta u = \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial y^2} u$

a) * Derive the weak form of Equation (8) and simplify it as much as possible.



$$\begin{aligned} \frac{\partial}{\partial t} u &= \Delta u \\ \phi_i \frac{\partial}{\partial t} u &= \phi_i \Delta u && \text{multiplying with testfunction} \\ \int_{\Omega} \phi_i \frac{\partial}{\partial t} u \, d\Omega &= \int_{\Omega} \phi_i \Delta u \, d\Omega, \forall i && \text{integrating} \\ \int_{\Omega} \phi_i \frac{\partial}{\partial t} u \, d\Omega &= - \int_{\Omega} \nabla \phi_i \cdot \nabla u \, d\Omega, \forall i && \text{integration by parts; boundary=0} \end{aligned}$$

b) Using the Ritz-Galerkin approach, derive the linear system of equations. Mark the integrals corresponding to the mass and stiffness matrix and write down the matrix formulation of the equation.

with $u = \sum_j u_j \phi_j$

$$\int_{\Omega} \phi_i \frac{\partial}{\partial t} \sum_j u_j \phi_j \, d\Omega = - \int_{\Omega} \nabla \phi_i \cdot \nabla \sum_j u_j \phi_j \, d\Omega$$

sum of ansatzfunctions

$$\sum_j \frac{\partial}{\partial t} u_j \underbrace{\int_{\Omega} \phi_i \phi_j \, d\Omega}_{\text{mass matrix}} = - \sum_j u_j \underbrace{\int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j \, d\Omega}_{\text{stiffness matrix}}$$

sum outside, reordering

$$A_{\text{mass}} \dot{u} = -A_{\text{stiffness}} u$$

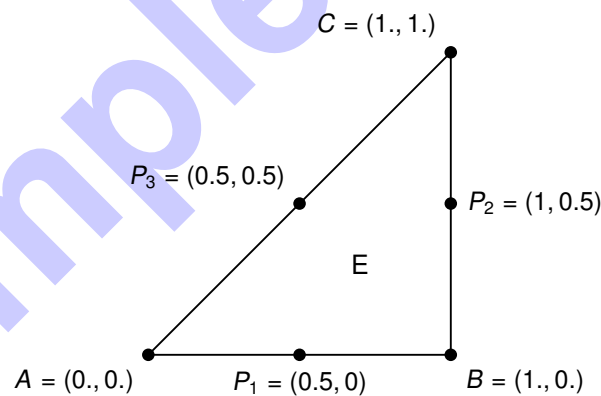


Figure 5.1: One Cruzeix-Raviart Element E defined by the points A, B and C – the basis functions are defined using the points P_1 , P_2 and P_3 that lie on the edges of the element.

c) Let us now consider the element given in Figure 5.1. The nodal basis defined through the points P_1 , P_2 and P_3 , such that $\phi_i(P_j(x, y)) = \delta_{ij}$ is given as:

$$\phi_1 = 1 - 2y$$

$$\phi_2 = -1 + 2x$$

$$\phi_3 = 1 - 2x + 2y.$$

State the general formula for the element stiffness matrix and calculate the element stiffness matrix for the particular Element E.

We calculate the stiffness matrix as follows:

$$A_{ij} = \int_E \nabla \phi_i \cdot \nabla \phi_j \, d\sigma$$

We will need the gradients of the functions ϕ_1, ϕ_2, ϕ_3 :

$$\nabla \phi_1 = (0, -2)^t$$

$$\nabla \phi_2 = (2, 0)^t$$

$$\nabla \phi_3 = (-2, 2)^t$$

The stiffness matrix is then:

$$A_{11} = A_{22} = \int_E \nabla \phi_1 \cdot \nabla \phi_1 \, d\sigma$$

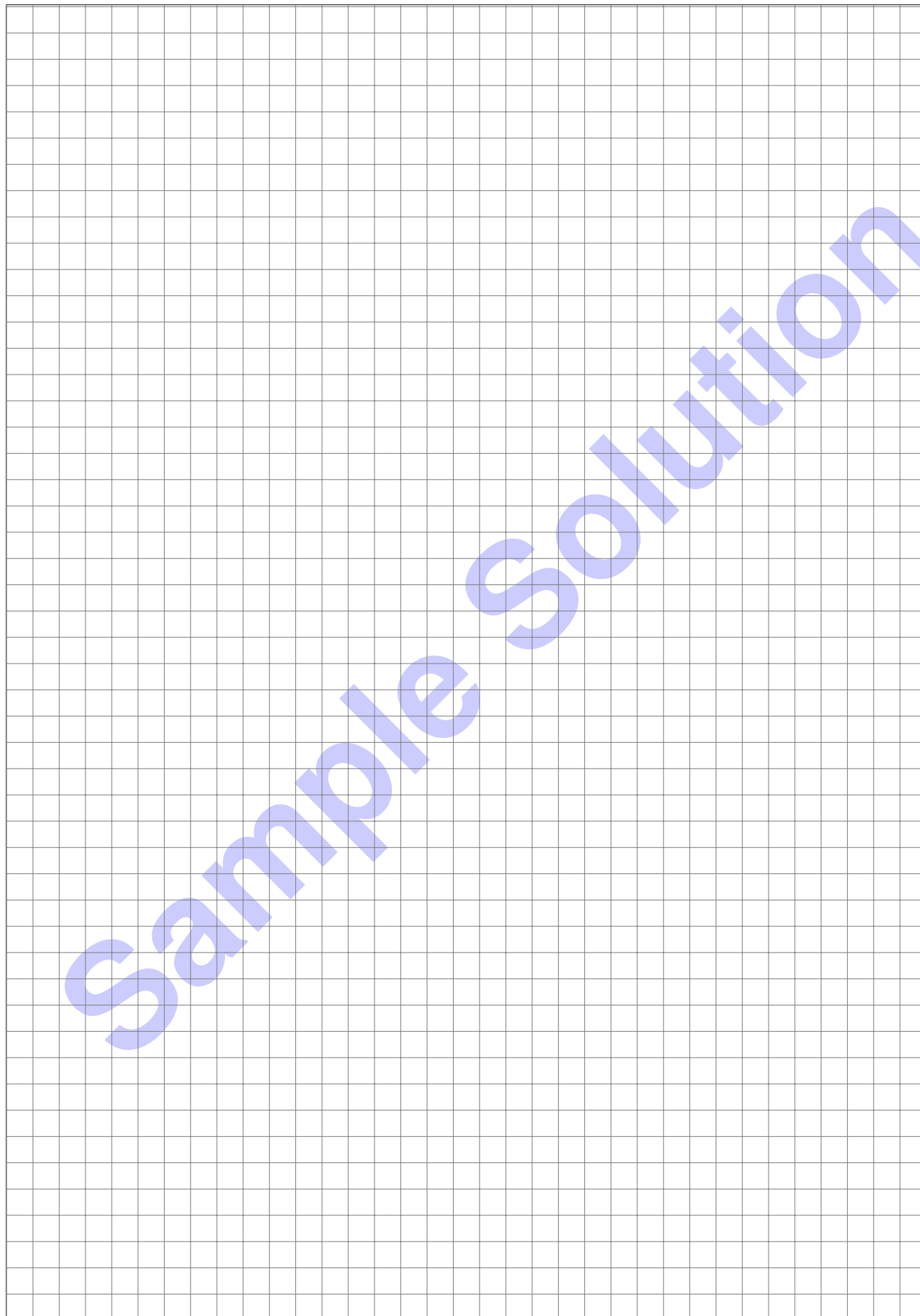
$$= 4 \cdot A_E = 4 \cdot \frac{1}{2} = 2$$

$$A_{33} = 8 \cdot A_E = 4$$

$$A_{12} = A_{21} = 0$$

$$A_{13} = A_{31} = A_{23} = A_{32} = -2$$

Additional space for solutions—clearly mark the (sub)problem your answers are related to and strike out invalid solutions.



Sample Solution