

Exam Scientific Computing (T. Neckel, D. Jarema) WS 2013/14	Page 1/14
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## General Instructions

### Material:

You may only use one hand-written sheet of paper (size A4, on both pages).

Any other material including electronic devices of any kind is forbidden.

Use only the exam paper that was handed out to solve the exercises. In case the space on a page is not enough, mark that you continue with your solution and use the reverse side of the preceding page. For additional notes and sketches, you can obtain additional exam sheets.

Do not use pencil, or red or green ink.

### General hint:

Often, exercises b), c), etc. can be solved without the results from the previous exercise a); if you are stuck with exercise a), then don't immediately skip exercises b), c), etc.

### Working time:

90 minutes + 5 minutes reading time.

**Please switch off your cell phones!**

1	2	3	4	5	$\Sigma$
/12	/5	/6	/8	/12	/ $\approx$ 43

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# 1 Numerical Methods for ODE ( $\approx 4 + 4 + 2 + 2 = 12$ points)

Consider the direction field of a one-dimensional differential equation  $dp/dt = f(t, p)$ , where  $f(t, p) = (1 - p(t))/2$  (Verhust model - saturation), as given in Figure 1.

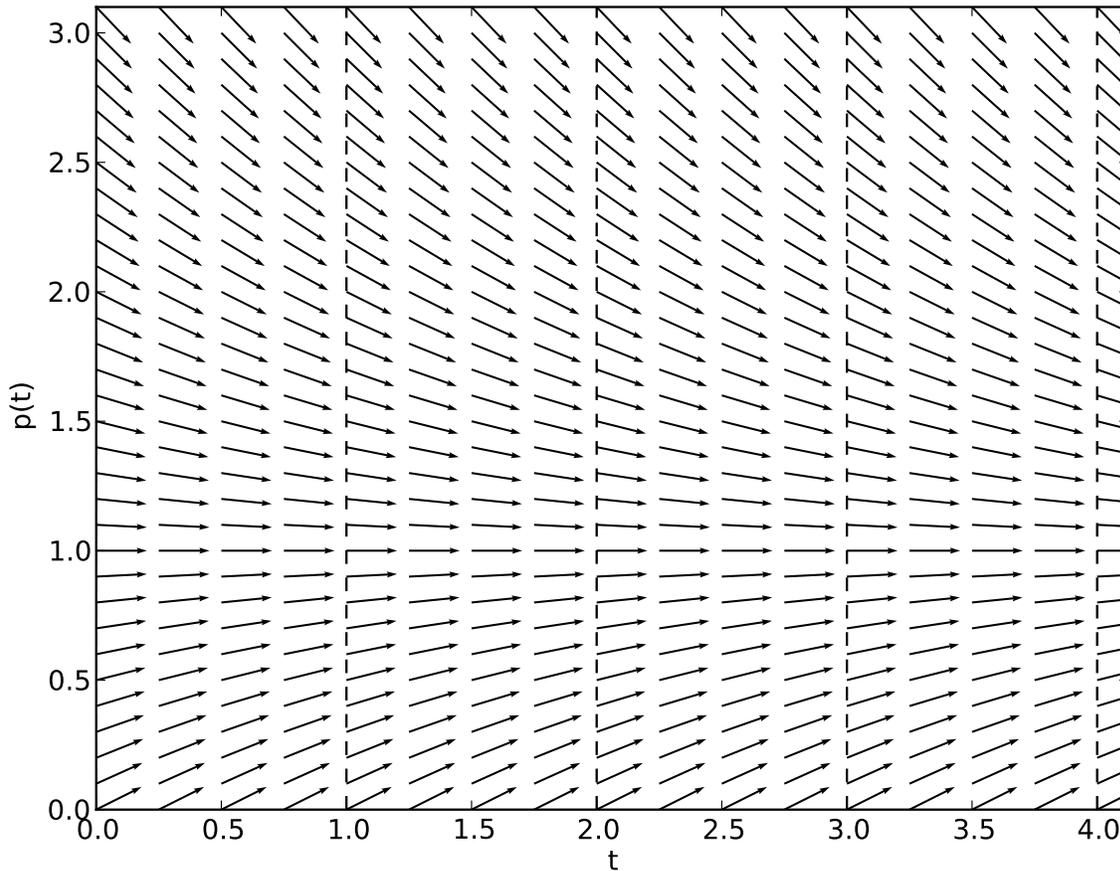


Figure 1: Direction field for  $dp/dt = (1 - p(t))/2$ .

- a) To compute approximate solutions  $p_n \approx p(t_n)$  at times  $t_n = n\tau$ , the following multistep numerical scheme is given:

$$p_0 = p(0) = 1/2 \quad (\text{initial condition}) \quad (1)$$

$$p_1 = p_0 + \tau f(t_0, p_0) \quad (2)$$

$$p_{n+1} = 5p_{n-1} - 4p_n + \tau(2f(t_{n-1}, p_{n-1}) + 4f(t_n, p_n)) \quad (3)$$

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Compute the first four steps of this scheme  $(p_1, p_2, p_3, p_4)$  with time step size  $\tau = 1$ , and draw the numerical solution (points connected by lines) on Figure 1. If a point is outside the plot domain, you do not have to visualize it.

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b) Consider a one-step Midpoint method:

$$p_0 = p(0) = 3.0 \quad (\text{initial condition}) \quad (4)$$

$$p_{n+1} = p_n + \tau f \left( t_n + \frac{1}{2}\tau, p_n + \frac{\tau}{2} f(t_n, p_n) \right). \quad (5)$$

Perform the first four steps of this scheme (to compute  $p_1, p_2, p_3, p_4$ ) by drawing the approximate solutions into the direction field in Figure 1 (graphical solution only). The step size shall be  $\tau = 1$ , as illustrated by the four intervals drawn into the direction field. Mark from which arrows you obtain the directions of the numerical steps – you are allowed to add an arrow to the direction field, if no arrow is plotted at the precise required position.

c) What can you conclude about the numerical stability of the methods from a) and b) for  $\tau = 1$ ?

d) List two advantages and two disadvantages of multistep methods in comparison to one-step methods.

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## 2 FEM – General Questions

( $\approx 1 + 1 + 3 = 5$  points)

a) Why is the nodal basis so popular and advantageous in the finite element context?

b) Why is the weak form called “weak”?

c) List three challenges in the context of implementing an FEM solver.

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### 3 FEM – The 1D Poisson Equation ( $\approx 1.5 + 0.5 + 4 = 6$ points)

Consider the one-dimensional Poisson Equation

$$-u''(x) = f(x), \quad x \text{ in } \Omega = (0, 1) \quad (6)$$

with homogeneous Dirichlet boundary conditions  $u(0) = u(1) = 0$ . We apply a finite element method with the standard linear hat functions  $\phi(x)$  on an equidistant grid with mesh size  $h = 1/N$ .

The  $k$ th element (cell) in the mesh is given by

$$\Omega^{(k)} := h \cdot [k, k + 1].$$

a) Indicate the formulas of the basis functions  $\phi_1^{(k)}(x)$  and  $\phi_2^{(k)}(x)$  on element  $\Omega^{(k)}$ .

b) What is the dimension of the element stiffness matrix  $\widehat{A}_{\mu,\nu}^{(k)}$ ?

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- c) Compute the element stiffness matrix  $\widehat{A}_{\mu,\nu}^{(k)}$  for our special setup of an equidistant grid.

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#### 4 Discrete Model: Leontief Economic Model ( $\approx 5 + 3 = 8$ points)

The Leontief economic model can be applied not only for individual companies, but also for broadly-drawn economic sectors. We will consider only the following sectors: agriculture, manufacturing, and household, where household corresponds to employees and their labor to products. The economic relations between the sectors are given in the table:

From/To	Agriculture	Manufacturing	Household
Agriculture	4	6	10
Manufacturing	8	18	4
Household	8	6	6
Total	20	30	20

Here is an example of how you should read the table: the first column shows that agriculture uses 4 units of its own production, 8 units of manufacturing, and 8 units of household production (labor) to produce 20 units of agriculture in total.

- a) Write down the production matrix  $A$  for the closed economic system described in the table.

Can the region where economy is described by the provided table survive as a closed economic system?

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- b) Alternatively, the same economy can be modeled as an open system. In this approach, the relation between the agriculture and manufacturing is described by the production matrix  $A = \begin{pmatrix} 1/5 & 1/5 \\ 2/5 & 3/5 \end{pmatrix}$ , and the household by the demand vector  $d = \begin{pmatrix} 10 \\ 4 \end{pmatrix}$ . Then, the input/output module is given by equation  $x_{in} = Ax_{out} + d$ . For which production vector  $x$  do we then obtain a stable solution?

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## 5 Continuous Model: Free Charges in Semiconductors ( $\approx 2 + 2 + 3 + 2 + 3 = 12$ points)

There are semiconductors that do not conduct electric current unless they are exposed to light. Free electrons appear in this material due to the photo-effect. They can again get trapped and localized.

- a) A thin layer of semiconductor is momentarily exposed to light. This created a homogeneous density  $n_0$  of free electrons. Write down the ODE for the free electrons density  $n(t)$  and solve it if free electrons get trapped again at a rate  $\alpha n(t)$  (number of free electrons trapped in a unit volume per unit time interval). What is  $n(t \rightarrow \infty)$ ?

- b) To improve the model, potential holes are introduced. In our model, potential holes will only keep one electron at the same time. If  $M$  is the number of potential holes,  $m(t) = n_0 - n(t)$  is the number of localized electrons, then  $\alpha(1 - m(t)/M)n(t)$  is number of trapped electrons in the potential holes per unit time interval. And the number of electrons that get free again per unit time interval is  $\beta m(t)$ . The resulting ODE is

$$\frac{dn(t)}{dt} = \beta(n_0 - n(t)) - \alpha \left(1 - \frac{n_0 - n(t)}{M}\right) n(t). \quad (7)$$

For  $n_0 = 1$ ,  $M = 1$ ,  $\alpha = 2$ ,  $\beta = 1$  find physical ( $n \geq 0$ ) stationary solution for the free electrons concentration  $n_s$  of this equation.

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c) Determine if the physical ( $n \geq 0$ ) stationary solution from b) is stable.

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- d) If the semiconductor layer is thick, the generated density of free electrons  $n$  is no longer homogeneous. More electrons are freed near the surface and less inside the layer. The simplest model for the evolution of  $n(x, t)$  considers diffusion along the layer depth  $x$  and is described by the following equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} - \gamma n, \quad (8)$$

where the coefficients  $D$  and  $\gamma$  are positive.

Provide a numerical scheme for this equation. For the time discretization use the explicit Euler scheme and for the spatial discretization a central difference second-order scheme. For a discretization grid example see Figure 2.

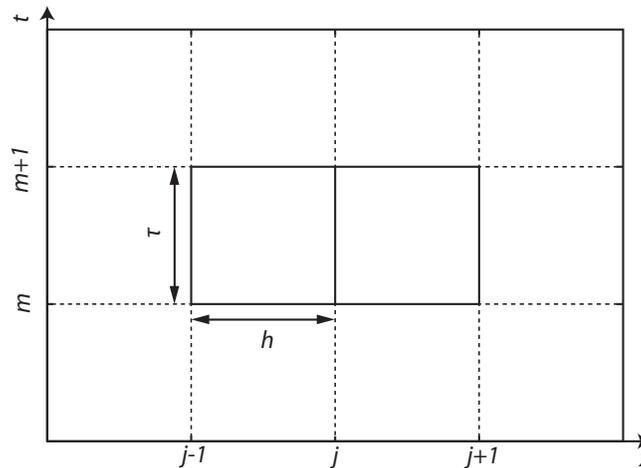


Figure 2: Discretization grid example.

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- e) Find the restriction for the time step size of the numerical scheme by using the von Neumann stability analysis.

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