Technische Universität München
Institut für Informatik
Dr. Miriam Mehl
Dr. Sergey Pankratov

WT 2002/2003

Introduction to Scientific Computing

Mid-Term Exam, December 19th 2002

Name: ________________________________

- The exam consists of four problems and is divided into two parts:
  - The first part (problems 1 and 2) is without materials like notes, books etc. at all. You will have 50 minutes for this part.
  - For the second part (problems 3 and 4), you may use books, lecture notes etc., but no electrical devices like for example calculators, mobile phones, ... You will have 40 minutes for this part.

  You have to hand in your answers for part one before you receive the second part of the questions and may start using media.
- Part one consists of pages 2-7, part two is on pages 8 and 9. Please check your copy for completeness!
- Please, insert your answers for the first part (problems 1 and 2) in the gaps on the worksheet – the space provided should be sufficient for the expected answers.
- The level of difficulty of the questions is quite different, and we did not sort them according to difficulty. Therefor, if you have problems with some question, just proceed to the next part before loosing too much time.

1 General questions

a) Which are the two main steps of modelling?

b) Imagine you want to modell a chemical reactor. Name four basic questions you have to answer to derive an appropriate model (thinking about simulation in general, not only about your reactor)!

c) Name three general questions you have to answer if you analyse a model!

d) Name four possible ways to solve/simulate a model!

2 Continuous Models: ODE and PDE

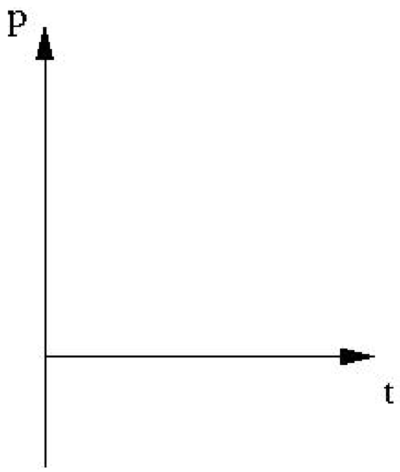
$$
\begin{aligned}
\dot{p}(t) &= a \cdot p(t), \quad p(0) = p_0, &(1)\\
\dot{q}(t) &= b \cdot q(t), \quad q(0) = q_0, &(2)
\end{aligned}
$$

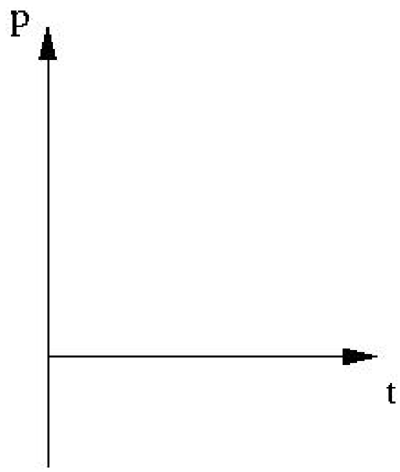
$$a, b > 0.$$

Consider the above ODEs for the growth of the population p and q of two species P and Q.

a) Describe the behaviour of p for t tending to infinity. Is this behaviour realistic?

b) Give two possible variations of equation (1) with a more realistic behaviour for t tending to infinity (but still without interactions of the two species). For both possiblities, draw the qualitative behaviour of the resulting population p in the diagrams below.





c) Why are linear ODEs not sufficient to model the s-shape form of the population curve, which can be observed for real world populations?

d) To include interactions of the two species in the above model, add suitable terms that model the following assumtion:

The decrease of population p per time unit is proportional to the number q of individuals of species Q (and vice versa for q).

e) Is there an equilibrium $\bar{p}, \bar{q} > 0$ for the system of ODEs from d)?

f) Consider the original ODE (1) for p. We now assume that the population p depends on time t *and* the position x ($x \in [0;1]$) on an east-west axis. Enhance the above model for p according to the following assumptions:

1) The growth per time unit and individual is proportional to x.

2) The movement of people to neighbouring locations is proportional to the negative steepness of p in the respective directions (thus, people move to regions with a less dense poulation).

   Hint: Imagine a small interval on the x-axis and compute the change of population within this interval from the movement of people over both borders of the interval. Compute the limit for the interval length tending to zero.

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3 Numerical Methods for ODE

Consider the first-order ODE

$$\dot{y} = f(y, t), \quad y(0) = y_0.$$

Derive a pth-order discretization on an equidistant grid

$$\{t_i = i * h; i = 1, 2, 3, \ldots \& h > 0\}$$

a) for $p = 2$ using Taylor-expansion of $y(t_{k+1})$ with respect to $y(t_k)$,

b) for $p = 3$ according to the Adams-Bashforth-approach.

4) Numerical Methods for PDE

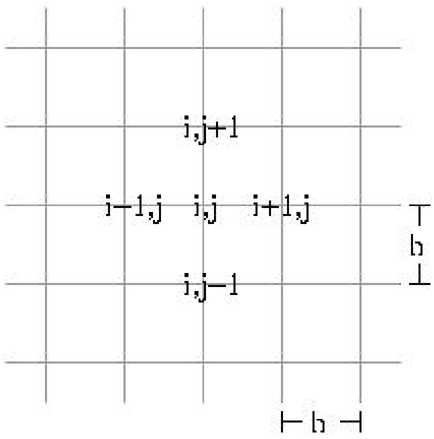
Consider the Laplace equation

$$\Delta u = f \quad \text{in} \quad]0; 1[^2$$

with Neumann boundary conditions

$$\frac{\partial p}{\partial \vec{n}} = 0 \quad \text{at} \quad \{0\} \times [0; 1] \cup \{1\} \times [0; 1] \cup [0; 1] \times \{0\} \cup [0; 1] \times \{1\}$$

and the following finite-difference discretization on a square grid:



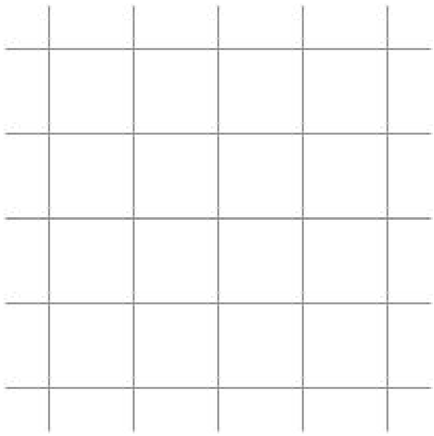
$$\Delta u(x_{i,j}) \approx \frac{u_{i-1,j-1} + u_{i-1,j+1} - 4u_{i,j} + u_{i+1,j-1} + u_{i+1,j+1}}{2h^2}$$

at all inner grid points $x_{i,j}$.

Is this discretization

a) consistent,

b) stable (hint: try to find an oscillating pattern in the following cutaway of the grid with boundary zero that is annihilated by the discrete operator),



(remark: the solution of the continuous problem is unique only up to a constant function, but oszillations cannot occur in the exact solution)

c) convergent?

Give short reasons for your answers.