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Department of Mathematical
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TMA4212 Num.diff.
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Project 1

Practical information

- *Deadline and hand-in:* Friday February 28 (before midnight). Hand in the project in ovsys.
- *Supervision:* There will be a few additional meeting hours, these will be announced at the wiki-page.
- *Report:* Submit the report as a pdf-document (L^AT_EX), with the python code in a separate file. Write the report as a scientific report, not as a solution to an exercise. Meaning: Describe the problem you want to solve, describe the method you are using, write mathematical results as mathematical statements, and make sure there is a consistency between theoretical and numerical results etc. Use plots whenever appropriate, make sure they are readable, and explain clearly what you observe, and if it is as expected.

Include the name of all the group members on the title page.

The tex-report should not exceed 10 pages, all included.

If you are using any kind of AI or other tools or references, it should be clearly stated how it is used, and what it is used for.

- *Grading:* Out of 20 points, the report counts for 5 points, Problem 1 for 8 and Problem 2 for 7. Roughly.
- *Learning objectives:* When completed this project you should demonstrate that you are able to:
 - perform an error and stability analysis for a time dependent problem,
 - to justify the theoretical results by numerical experiments,
 - to apply a scheme to a realistic problem,
 - communicate the results in a scientific manner.

In addition, we hope that working with the application is a bit motivating.

- Both references can be downloaded from Springer.

Some advice:

- *Implementation:* Make a plan. Do not implement everything at once, split the work in small pieces, and make sure each of them works before you continue. If possible, use nontrivial test problems of which the numerical solution is exact to check that the implementation is correct, but please do not include such results in the report.
- *Writing:* Imagine you are writing to a fellow student, who do not know about this project. How you make him/her understand and be interested in what you have done and learned during the project?

Do not include huge amounts of trivial calculations, this is a report, not an exam paper.

Writing takes a lot of time, so start early. And accept that you may want to rewrite parts, that is a part of the writing process.

- *Time organisation:* Think about how much time you are willing to use on this project. If you are completely stuck at one point, maybe it is better to skip it and concentrate on writing a good report instead.

In this project the topic is reaction-diffusion equations. Such equations are given by

$$u_t = \mu u_{xx} + f(u)$$

where μ is some positive constant. We will in the following assume the reaction term $f(u)$ to be nonstiff, in the sense that explicit methods can be used to solve the ODE $u_t = f(u)$.

As at this point should be well known, time dependent PDEs with diffusion terms should be solved by implicit methods. Using implicit methods for solving the whole system requires solutions of nonlinear equations for each step, and we would all be happy to avoid that. One option would be to use an implicit method for the diffusion term and an explicit for the reaction.

Use constant stepsizes h in the x -direction, and k in the t -direction, so that $x_{m+1} = x_m + h$ and $t_{n+1} = t_n + k$. A scheme based on forward and backward Euler, together with a central difference in space could be:

$$\frac{1}{k} \nabla_t U_m^{n+1} = \frac{\mu}{h^2} \delta_x^2 U_m^{n+1} + f(U_m^n)$$

which written out becomes

$$U_m^{n+1} = U_m^n + r(U_{m+1}^{n+1} - 2U_m^{n+1} + U_{m-1}^{n+1}) + kf(U_m^n), \quad r = \mu \frac{k}{h^2}.$$

We now propose the following modification of the Crank-Nicolson scheme:

$$\begin{aligned} U_m^* &= U_m^n + \frac{r}{2}(\delta_x^2 U_m^* + \delta_x^2 U_m^n) + kf(U_m^n), & r &= \mu \frac{k}{h^2}, \\ U_m^{n+1} &= U_m^* + \frac{k}{2}(f(U_m^*) - f(U_m^n)). \end{aligned} \tag{1}$$

For pure diffusion ($f = 0$), this is nothing but the usual Crank-Nicolson scheme, and for a pure reaction equation ($\mu = 0$), it is nothing but a second order explicit Runge-Kutta method (convince yourself about that).

1 *Theory*

Do a consistency/stability analysis of the proposed method (1) on a linear PDE, that is, let $f(u) = au$ for some constant a .

For the stability analysis, you can choose whether you do a complete matrix analysis for the PDE on a given domain (e.g. $x \in (0,1)$) with boundary conditions, or a Neumann analysis. Is the method unconditionally stable? What can be said about the global error?

Formulate your results as a mathematical statements (lemmas or theorems) with proofs.

Justify your theoretical results by numerical experiments.

2 *Application*

In this exercise, we will look at a model from epidemiology; how an infectious disease will develop in space and time.

At a given time t , a population N can be divided into

- **Susceptible S :** A person is susceptible if she/he may get the disease.
- **Infective and infectious I :** A person is infective if she/he has the disease and is able to transfer it to others.
- **Removed: R** Part of the population that for some reason will never again be infected or infect others (immune, isolated from the population or dead).

The following model (SIR) is described in [1], chapter 3, and describe the development of a disease over time:

$$\begin{aligned}\frac{dS}{dt} &= -\beta SI, \\ \frac{dI}{dt} &= \beta SI - \gamma I, \\ \frac{dR}{dt} &= \gamma I.\end{aligned}\tag{2}$$

Notice that $N(t) = S(t) + I(t) + R(t)$ is constant.

In the following, we will assume a scaled model, so S , I and R are the fraction of the population that are susceptible, infected and removed respectively. In this case, $S(t) + I(t) + R(t) = 1$.

The usual SIR model only describe how a disease may develop over time at one specific location, not how a disease is spread in space. Murray [2], chapter 13, proposes the following modification to include spatial spread:

$$\begin{aligned}S_t &= -\beta IS + \mu_S \Delta S, \\ I_t &= \beta IS - \gamma I + \mu_I \Delta I,\end{aligned}$$

where $\Delta u = u_{xx} + u_{yy}$ (see the appendix). Your exercise is now: Try to understand the model. Choose an appropriate numerical scheme for solving the PDEs, and use

this to study the spread of a disease. That is, at $t = 0$ assume a small portion of the population is infected at some particular place, and see how the disease will spread from there. You are free to choose the domain, the parameters and boundary conditions, but you should be able to get some interesting results out of it. And you should justify your choices.

As soon as you have a working model, play with it! As an example: In the present model, we assume that the population is equally distributed over the domain. You can for instance model a more dense populated area (or an event that gather a lot of people) by making β larger over there (and then dependent on x).

Some hints:

- To get a certain feeling for the dynamics of the model, solve (2) first. As a first try, you can use $\beta = 3$ and $\gamma = 1$, but then change the parameters and see what happens. Use a standard ODE solver if you prefer.
- The diffusion parameters μ_* describes how fast people are moving around. If your domain is small, you should probably use quite small diffusion parameters.
- For a full score, the 2d problem should be solved. But if this seems difficult, solve the 1d problem first.

References

- [1] N.F. Britton *Essential Mathematical Biology* Springer, 2003.
- [2] J.D. Murray *Mathematical Biology II: Spatial Models and Biomedical Applications*, 3th ed., Springer, 2003.

A Numerical solution of the two-dimensional heat equation.

This appendix gives a very brief description on how to discretize the Laplace operator in two space dimensions $\Delta u = u_{xx} + u_{yy}$ on a unit square.

Consider the heat equation in two space variables (x, y) :

$$u_t = \alpha \Delta u \quad \alpha > 0$$

on $\Omega = [0, 1] \times [0, 1]$ with Dirichlet boundary conditions and $u(x, y, t) = f(x, y)$ as initial condition.

Make a grid in space: Let $h = 1/M$, and $x_i = ih$, $y_j = jh$, $i, j = 0, \dots, M$. Replace u_{xx} u_{yy} by the corresponding central difference approximations, thus

$$\begin{aligned} u_{xx}(x_i, y_j, t) &= \frac{1}{h^2} (u(x_i - h, y_j, t) - 2u(x_i, y_j, t) + u(x_i + h, y_j, t)) + \mathcal{O}(h^2), \\ u_{yy}(x_i, y_j, t) &= \frac{1}{h^2} (u(x_i, y_j - h, t) - 2u(x_i, y_j, t) + u(x_i, y_j + h, t)) + \mathcal{O}(h^2) \end{aligned}$$

which inserted into the heat equations gives

$$\partial_t u(x_i, y_j, t) = \frac{\alpha}{h^2} \left(u(x_{i-1}, y_j, t) + u(x_{i+1}, y_j, t) + u(x_i, y_{j-1}, t) + u(x_i, y_{j+1}, t) - 4u(x_i, y_j, t) \right) + \mathcal{O}(h^2)$$

Let $U_{i,j}(t) \approx u(x_i, y_j, t)$, and the result is the following set of ordinary differential equations

$$\begin{aligned} \frac{dU_{i,j}}{dt} &= \frac{\alpha}{h^2} (U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - 4U_{i,j}), \quad i, j = 1, \dots, M-1, \\ U_{i,j}(0) &= f(x_i, y_j). \end{aligned}$$

For i and j equal to 0 or M , $U_{i,j}$ is given from the boundary conditions.

This can be solved by your favourite ODE solver. However, if you choose the forward Euler scheme, the solution is stable only for $\alpha k/h^2 \leq 1/4$, where k is the step size in time.