Math*6020 Scientific Computing
Instructor: Prof. H.J.Eberl

Project
Due: April 15

The overall objective of the project is to implement and test solvers for 2D diffusion-reaction equations. This is broken down into three steps: P1 a linear elliptic (stationary) problem, P2 a semi-linear elliptic (stationary) problem, and P3 a semi-linear parabolic (non-stationary) problem. P1 and P2 can be considered special cases of P3. Therefore, you might directly jump to P3 and then present the results of P1, P2 as applications of P3. However, it might be helpful for the code and project development to cary them out in the given order.

Semi-linear diffusion-reaction problems of the form

$$u_t = D\Delta u - F(u)$$

for scalar or vector valued unknown functions u appear in many application areas, such as chemistry, biology, environmental (and other types of) engineering. For example, they model transport and decay/uptake of drugs and other chemicals in tissues. We treat the scalar case where the nonlinearity F is an uptake function, i.e. $F(u) \geq 0$. We consider first order uptake and uptake described by saturation kinetics (this specific form is called Holling Type-2 kinetics in ecology, Michaelis-Menten kinetics in biochemistry, Monod kinetics in microbiology and microbial engineering).

Document your programming project, both in-code in form of comments, and in a written report.

Deliverables:

- for each of the three sub-projects a compileable, documented Fortran code, along with compilation instructions,
- a written report that describes the numerical methods that are used, the testing that was done, and the results.

Key is reproducibility! The information you provide must allow me to reproduce your results.

Your project will be assessed based on the following criteria

- appropriateness and suitability of selected numerical methods [explain/justify your choice] (weight: 10)
- structure of the code (modularity!) (weight: 10)
- tidyness of the code and clarity of the in-code documentation, i.e. code readability (weight: 5)

- correctness of implementation and results (weight 25)
- thoroughness of testing [the test that you ran should be described and documented] (weight 25)
- clarity and quality of the written project report (weight: 25)

Marking scheme: A perfect P1 will give you 65%, i.e. the passing mark for a grad course. Perfect P1+P2 will give you 79%, i.e a B+. Perfect P1+P2+P3 will give 95%. The remaining 5% are reserved for **creative** work that goes beyond the minimum requirements. This could be (a) for extensive and well documented code checking, e.g. by application to problems with known exact solutions, (b) extension of the code to other (meaningful in applications) reaction kinetics, (c) application of the code/model to problems in the published literature, (d) comparison of different numerical methods, etc.

The written presentation of the project should adhere to the usual publication standards. This holds for quality and detail level of tables, figures, and text.

P1 Linear elliptic solver. Write, test, and document a solver for the non-dimensional linear elliptic boundary value problem on the rectangular domain $\Omega = [0,1] \times [0,1]$

$$\Delta u = ku.$$

The boundary conditions are

$$\frac{\partial u}{\partial x} = 0 \quad \text{at} \quad x = 0,$$

See L6A2
in part 1.

$$\frac{\partial u}{\partial y} = 0 \quad \text{at} \quad y = 0,$$

$$u = 1 \quad \text{at} \quad x = 1,$$

$$u = 1 \quad \text{at} \quad y = 1.$$

In your report make sure to include

a) a visualisation of the solution for different parameters k on grids of suitable size.

b) a convergence test of your results. This should include normed differences and/or quantities of interest, such as minimum concentration value in the domain, total substrate uptake in the domain, flux of substrate into the domain.

P2 Semilinear elliptic solver. Write, test, and document a solver for the linear elliptic boundary value problem on the rectangular domain $\Omega = [0,1] \times [0,1]$

$$\Delta u = \frac{k_1 u}{k_2 + u}.$$

The boundary conditions are

$$\frac{\partial u}{\partial x} = 0 \quad \text{at} \quad x = 0,$$

$$\frac{\partial u}{\partial y} = 0 \quad \text{at} \quad y = 0,$$

$$u = 1 \quad \text{at} \quad x = 1,$$

$$u = 1 \quad \text{at} \quad y = 1.$$

In your report make sure to include

a) a visualisation of the solution for different parameters $k_{1,2}$ on grids of suitable size (use the results of P1 to guide your experimentation).

b) a convergence test of your results. This should include normed differences and/or quantities of interest, such as minimum cpncentration value in the domain, total substrate uptake in the domain, flux of substrate into the domain.

P3 Semilinear parabolic solver. Write, test, and document a solver for the non-dimensional semilinear parabolic boundary value problem on the rectangular domain $\Omega = [0, 1] \times [0, 1]$

$$\frac{\partial u}{\partial t} = \Delta u - \frac{k_1 u}{k_2 + u}.$$

The boundary conditions are

$$\frac{\partial u}{\partial x} = 0 \quad \text{at} \quad x = 0,$$

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$$\frac{\partial u}{\partial y} = 0 \quad \text{at} \quad y = 0,$$

$$u = 1 \quad \text{at} \quad x = 1,$$

$$u = 1 \quad \text{at} \quad y = 1.$$

The initial conditions $u(0, x, y) = u_0(x, y)$ could be $u_0 \equiv 1$ or $u_0 \equiv 0$.

In your report make sure to include

a) a visualisation of the solution for different parameters $k_{1,2}$ on grids of suitable size (use the results of P1, P2 to guide your experimentation).

b) a convergence test of your results. This should include normed differences and/or quantities of interest, such as minimum cpncentration value in the domain, total substrate uptake in the domain, flux of substrate into the domain. Keep in mind that depending on your time-integration strategy, a convergence result also includes a refinement of the time-step.