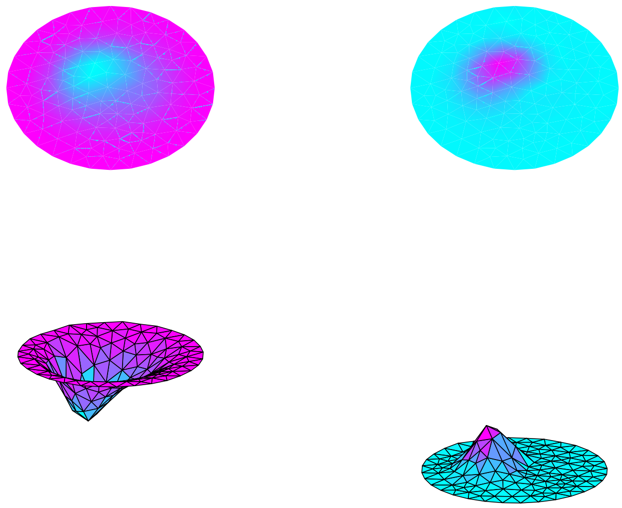
Convection–diffusion–reaction

Computer Session E5



Background

Today, we will solve a system of convection–diffusion–reaction equations,

$$
\begin{array}{rcl}
\dot{u}_1 + b \cdot \nabla u_1 - \nabla \cdot (a \nabla u_1) & = & f_1(u_1, u_2, x, t) \quad \text{in } \Omega \times (0, T], \\
\dot{u}_2 + b \cdot \nabla u_2 - \nabla \cdot (a \nabla u_2) & = & f_2(u_1, u_2, x, t) \quad \text{in } \Omega \times (0, T], \\
-\partial_n u_1 & = & 0 \quad \text{on } \Gamma \times (0, T], \\
-\partial_n u_2 & = & 0 \quad \text{on } \Gamma \times (0, T], \\
u_1(\cdot, 0) & = & u_{10} \quad \text{in } \Omega, \\
u_2(\cdot, 0) & = & u_{20} \quad \text{in } \Omega,
\end{array}
\tag{1}
$$

where we note that the right-hand side depends on the solution $u = (u_1, u_2)$ itself. This is a system of *nonlinear* equations (if f_1 or f_2 are nonlinear). Typically, f_1 and f_2 are chosen to model a chemical reaction.

The dG(0) formulation is given by

$$\begin{array}{l} \int_\Omega U_{1,n} v \, dx + k \int_\Omega (b \cdot \nabla U_{1,n} \, v + a \nabla U_{1,n} \cdot \nabla v) \, dx = \\ \quad k \int_\Omega f_1(U_{1,n}, U_{2,n}, \cdot, t) v \, dx + \int_\Omega U_{1,n-1} v \, dx \quad \forall v \in V_h, \\ \int_\Omega U_{2,n} v \, dx + k \int_\Omega (b \cdot \nabla U_{2,n} \, v + a \nabla U_{2,n} \cdot \nabla v) \, dx = \\ \quad k \int_\Omega f_2(U_{1,n}, U_{2,n}, \cdot, t) v \, dx + \int_\Omega U_{2,n-1} v \, dx \quad \forall v \in V_h, \end{array} \tag{2}$$

where $k = t_n - t_{n-1}$ denotes the size of the time step, $U_{1,n}$, $U_{2,n}$ denote the values at $t = t_n$, and $U_{1,n-1}$, $U_{2,n-1}$ denote the values at $t = t_{n-1}$.

Before today's computer session, make sure that you understand and can answer the following questions.

Question 1 Derive the variational formulation (2) from the system of equations (1).

Question 2 How does the corresponding variational formulation look for the cG(1) method? This method is also known as the Crank-Nicolson method.

Question 3 Assume that we have an (irreversible) chemical reaction of the form $A + B \rightarrow C$, let $u_1(x,t)$ be the concentration of the substance A and let $u_2(x,t)$ be the concentration of the substance B. Can you motivate that this is modeled by the system (1) if we take

$$\begin{array}{rcl} f_1(u_1, u_2, x, t) & = & -c u_1 u_2, \\ f_2(u_1, u_2, x, t) & = & -c u_1 u_2. \end{array} \tag{3}$$

The constant c determines the rate of the reaction and is called the *reaction constant*.

Preparations

Create a new directory called `e5` and the two subdirectories `problem1` and `problem2`. Then download the following files to each of the subdirectories:

- `AssembleMatrix.m`,
- `AssembleVector.m`,
- `Reaction1.m`,
- `Reaction2.m`,
- the files in the directory `mesh`.

These files are available on the web page of this session under *Programs and templates*.

Problems

Problem 1

Preparation

Go to the directory `problem1`. Create a file called `ConvDiffReacSolver.m` and write your program in this file. You also have to edit the files `Reaction1.m` and `Reaction2.m`, where you specify the variational formulation.

Problem

Solve the system of convection–diffusion–reaction equations on a circular domain (`circle.m`) with

$$\begin{aligned} f_1(u_1, u_2, x, t) &= -cu_1u_2, \\ f_2(u_1, u_2, x, t) &= -cu_1u_2 + f(x, t). \end{aligned} \tag{4}$$

Take $c = 3$, $a = 0.01$, $b = 0$ and use a time step of size $k = 0.1$ with final time $T = 1$.

As initial conditions, take $u_{10} = 1$ and $u_{20} = 0$ in the domain Ω. This corresponds to a situation where we have a beaker containing substance A (with concentration 1). There is nothing of substance B in the beaker so to get the reaction going, we need to add B to the system. We do this by taking

$$f(x,t) = \begin{cases} 2, & \text{if } |x - (0.5, 0.5)| < 0.2, \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

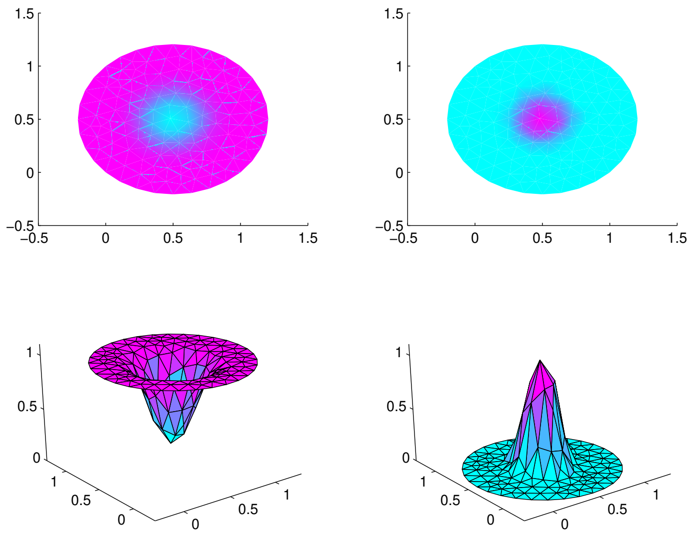
This means that we continuously pour substance B into the beaker close to $x = (0.5, 0.5)$.

To solve the problem, look at your solver for the bistable equation from computer session E4, or try yourself without looking.

Since the problem is nonlinear, we need to use fixed-point iteration. The procedure is the same as in computer session E4, but since we now have a system of two equations, we need to assemble two vectors and solve two linear systems in each fixed-point iteration.

Note also that both f_1 and f_2 depend on both u_1 and u_2, so we need to pass the values of both u_1 and u_2 (at the right-hand side of the interval) to the assembler. As before, you also need to pass the left-hand side values to the assembler (since the problem is time-dependent).

Check your answer: Compare your solution with the figure below, which shows the solution at time $t = 1$.



Problem 2

Preparation

Go to the directory **`problem2`** and copy the three files `ConvDiffReacSolver.m`, `Reaction1.m`, and `Reaction2.m` from the directory `problem1`.

Problem

Modify your program from Problem 1 so that a new drop of substance B is added at $x = (0.75, 0.5)$ every second, instead of just pouring it into the beaker. This can be accomplished by taking

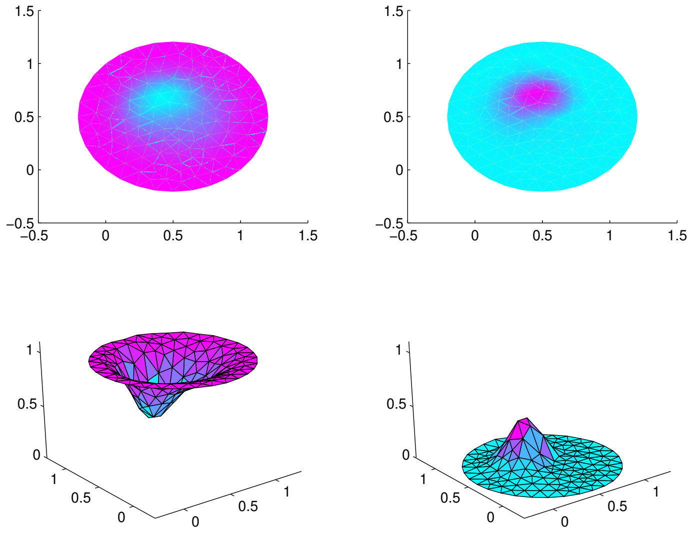
$$f(x,t) = \begin{cases} 20, & \text{if } |x - (0.75, 0.5)| < 0.1 \text{ and } |t - \text{round}(t)| < 0.1, \\ 0, & \text{otherwise,} \end{cases} \tag{6}$$

Also add a convective term corresponding to a magnetic stirrer at the bottom of the beaker, for example by taking

$$b(x,t) = 5(-(x_2 - 0.5), x_1 - 0.5). \tag{7}$$

Use a time step of size $k = 0.05$ and compute until time $T = 5$.

Check your answer: Compare your solution with the figure below, which shows the solution at time $t = 2.5$.



Hints

Problem 1

The variational formulation of the first equation that you need to specify in the file `Reaction1.m` is given by

```
u*v*dx + k*a*du'*dv*dx
```

for the left-hand side and

```
- k*c*w(2)*w(3)*v*dx + w(1)*v*dx
```

for the right-hand side.

The variational formulation of the second equation that you need to specify in the file `Reaction2.m` is given by

```
u*v*dx + k*a*du'*dv*dx
```

for the left-hand side and

```
k*(-c*w(2)*w(3) + f(x,d,t))*v*dx + w(1)*v*dx
```

for the right-hand side.

The fixed-point iteration can be implemented as follows:

```
while 1

  % Assemble vectors
  b1 = AssembleVector(p, e, t, 'Reaction1', [U10 U11 U21], time);
  b2 = AssembleVector(p, e, t, 'Reaction2', [U20 U11 U21], time);

  % Solve the linear systems
  newU1 = A1 \ b1;
  newU2 = A2 \ b2;

  % Check if the solution has converged
  if (norm(newU1 - U11) + norm(newU2 - U21))  < 0.01
    break;
  end

  % Update to the new values
  U11 = newU1;
  U21 = newU2;

end
```

Problem 2

Add the term

```
b(x,d,t)'*du*v*dx
```

to the varational formulation in both `Reaction1.m` and `Reaction2.m` where `b(x,d,t)` is a function that specifies the convection. Also modify the function `f(x,d,t)` so that it only adds a drop every second:

```
function y = f(x, d, t)

if norm(x - [0.75; 0.5]) < 0.1 & abs(t - round(t)) < 0.1
  y = 20;
else
  y = 0;
end
```

Solutions

Make sure that you really try to solve each problem before looking at the solutions. Have you really tried to solve the problem or should you try again before looking at the solution?

The solutions are available on the web page of this session under *Solutions to problems*.

About

This Computer Session is part of the Body and Soul educational program. More information can be found at

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http://www.phi.chalmers.se/bodysoul/
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This Computer session is written by Anders Logg.