Exercise 7
Release: 26.05.2020
Due: 02.06.2020

Question 1: Reaction-Diffusion in 2D - The Brusselator

We couple diffusion with a complex reaction system, the Brusselator equations. These equations exhibit under certain conditions a Turing pattern. The Brusselator model assumes two species U and V with concentrations $u = [U]$ and $v = [V]$ that interact in the following way:

$$
\begin{align*}
A & \to U \\
2U + V & \to 3U \\
B + U & \to V + C \\
U & \to D
\end{align*}
$$

The two species of interest, U and V, are autocatalytic species. The differential equations given in dimensionless form for these species are:

$$
\begin{align*}
\frac{du}{dt} &= a + ku^2v - (b + 1)u \\
\frac{dv}{dt} &= bu - ku^2v
\end{align*}
$$

a) Please implement the right hand side of the ODE system for reaction terms in `applyBrusselator.m`. The function reads like this:

```matlab
%% % Code for Exercise 7 – Brusselator model % % Input % u: (numParticles x 1) – Vector of concentration % v: (numParticles x 1) – Vector of concentration % a: Scalar parameter a % b: Scalar parameter b
```
% k: Scalar reaction rate

% Output
% du: (numParticles x 1) – vector of concentration
% change of species u
% dv: (numParticles x 1) – vector of concentration
% change of species v

% function [du, dv] = applyBrusselator(u, v, a, b, k)

Test the code using $a = 2$, $b = 6$ and $k = 1$. Choose the time step $dt = 0.01$ and end time $T = 20$. Set the initial values $u_0 = 0.7$ and $v_0 = 0.04$. Plot the time evolution of $u$ and $v$. The resulting plot should look like this:

![Figure 1: Solution of the Brusselator model](image)

b) Now we couple the Brusselator reactions with diffusion. Place 51 particles per dimension on a grid in the $[0,81] \times [0,81]$ domain. Add the applyBrusselator term to the RHS of the time integrator in your code. Initialize the strengths for $u_0$ uniformly at random and $v_0$ uniformly at random. Use the settings for $a$, $b$, and $k$ as described above. Set the diffusion constant $D = 10$ and simulate the system until $T = 10$. Plot the time evolution of $u$ and $v$ in the 2D domain. What do you observe? Look at the scales of the two species $u$ and $v$. How do they change? Play with the setting of the diffusion constant $D$ and the rate constant $k$ in the reaction term! What influence do the changes of $D$ and $k$ have on the behaviour of the system and why?