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Exercise 8

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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 $u = [\mathrm{U}]$ and $v = [\mathrm{V}]$ that interact in the following way:

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

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

$$
\begin{aligned}
u_t &= a + ku^2v - (b+1)u \\
v_t &= bu - ku^2v
\end{aligned}
$$

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

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Code for Exercise 7 - Brusselator model
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
% Input
% u:          (numParticles x 1)-Vector of concentration
%             of species u
% v:          (numParticles x 1)-Vector of concentration
%             of species v
% 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:

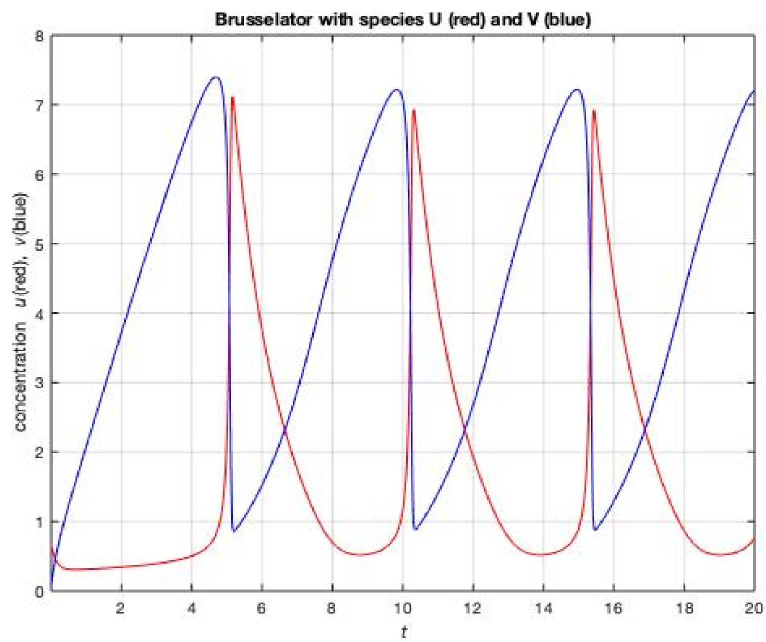

Figure 1: Solution of the Brusselator model

b) Now we couple the Brusselator reactions with diffusion. Place 51 particles per dimension on a grid in the [0,81] x [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 with an average offset of 7 compared to u_0. 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 behavior of the system and why?