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Exercise 10

Release: 23.06.2023
Due: 27.06.2023

Question 1: Advection-Reaction-Diffusion in the QS model

In the last exercise we implemented a simplified version of the Quorum Sensing model comprising three components: (i) diffusion and exponential decay of signaling molecules outside bacteria, (ii) an ODE model for the production of molecules inside bacteria and (iii) handling of the influx and outflux of molecules across the cell membrane. This exercise we will add a fourth component: advection. We assume, however, that the bacteria are attached to the underground. The advective flow passes outside of the bacteria and hence advects the concentration field u_e while the positions of and the concentrations u_c inside the bacteria are not affected.

In the following, we will use the setup of the final test case of Exercise 8 and additionally assume the divergence-free flow field

$$\underline{v}(x, y) = \begin{bmatrix} 4\left(1 - \cos\frac{2\pi y}{50}\right) \\ 3 \end{bmatrix}.$$

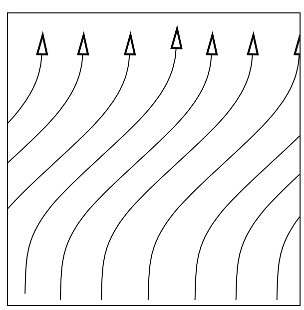

Figure 1: Flow field.

First implement the advection of the particles as

$$\begin{aligned} x_i(t + \Delta t) &= x_i(t) + \Delta t\, v_1(x_i(t), y_i(t)), \\ y_i(t + \Delta t) &= y_i(t) + \Delta t\, v_2(x_i(t), y_i(t)) \end{aligned}$$

in a function with the following input and output:

```
%%%%%%%%%%%%%%%%%%%%%%%%
% Code for Exercise 9 - move particles with advection
%%%%%%%%%%%%%%%%%%%%%%%%
% Input
% particleMat:   (numParticles x (dim+1+numStren))-Matrix of old
%                (grid-like) particle positions, cell indices and
%                particle strengths
% dt:            time step
%
% Output
% newpositions:  (numParticles x dim)-Matrix of new particle positions
%
% function newpositions = advect_particles(particleMat,dt)
```

Next, implement a remeshing function which interpolates the concentration field u_e carried by the particles at the new particle positions back to the old (grid-like) particle positions:

```
%%%%%%%%%%%%%%%%%%%%%%%%
% Code for Exercise 9 - remesh particles to grid-like positions
%%%%%%%%%%%%%%%%%%%%%%%%
% Input
% particleMat:   (numParticles x (dim+1+numStren))-Matrix of
%                (grid-like) particle positions, cell indices and old
%                particle strengths
% newpositions:  (numParticles x dim)-Matrix of new particle positions
% dt:            time step
%
% Output
% particleMat:   (numParticles x (dim+1+numStren))-Matrix of
%                (grid-like) particle positions, cell indices and new
%                particle strengths
%
% function particleMat = remesh(particleMat, index_strength, lBounds,
%                               uBounds, cutoff, newpositions)
```

To do so, use the M_4'-assignment function

$$A(s) = \begin{cases} 1 - \frac{1}{2}(5|s|^2 - 3|s|^3) & , 0 \leq |s| < 1, \\ \frac{1}{2}(2-|s|)^2(1-|s|) & , 1 \leq |s| < 2, \\ 0 & , \text{else}, \end{cases}$$

such that each particle i with position $(x,y)_i$ assigns its concentration $u_e(x_i, y_i, t)$ to the old (grid-like) positions $(x,y)_j^{\text{grid}}$:

$$u_e(x_j^{\text{grid}}, y_j^{\text{grid}}, t) = \sum_i A(x_i - x_j^{\text{grid}}) A(y_i - y_j^{\text{grid}}) u_e(x_i, y_i, t).$$

Now you can add both the advection and the remeshing function into the existing time loop of your implementation of the simplified QS model. Make sure you take care of the periodic boundaries. You can "pad" your domain in order to compensate for the loss of domain-size due to periodic boundary conditions (e.g. let your domain go from -4 to 53 and place 57 x 57 particles. Using a boundary-width of 3/h, do remeshing only for the inner domain going from -1 to 50).

Run the simulation up to time $T = 10$ for a decay rate $\gamma = 0.1$. If you use the domain properties from the example above, do you yield a total concentration of about 5488? Does the concentration field u_e look like the solution shown in figure 2? Let the simulation run until $T = 50$. How many bacteria get activated because they are located downstream of already active ones? (Starting with 7 activated bacteria, at $T = 50$ 8 should be activated.)

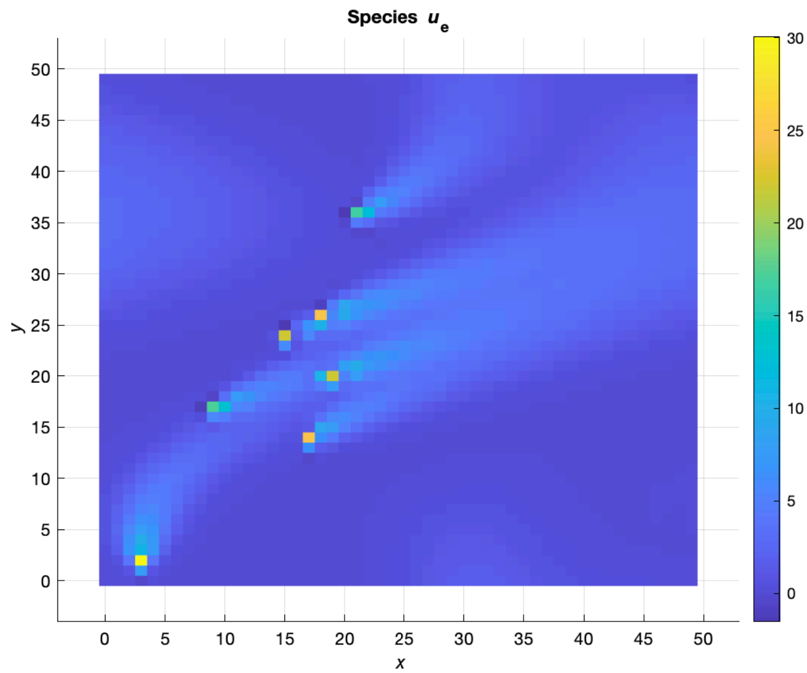

Figure 2: Concentration field u_e for $\gamma = 0.1$ at $T = 10$. (Note: negative concentration values are numerical artifacts of the remeshing procedure.)