08/07/2015 Francesco Pancaldi

I am trying to list here several possible directions that I thought of for the project. Some of these may be undertaken at the same time or in succession, but some are probably exclusive with respect to one another.

The model right now is a 1D model simulating RomR dynamics through a reaction-advection-diffusion PDE system.

We were able to qualitatively replicate the behaviour of RomR before and during division)not yet after division). Moreover, we observed asymmetry during division and variables starting times for the start of oscillations. Note that these are typically observed phenomena in the experiments, but they were not directly implemented in the model, and came instead from the simple PDEs that controls diffusion and attachement of RomR to receptors.

Problems with the model are mainly two:

- 1- The receptors are controlled by a MinCDE like system, but we have no concrete candidate for this role.
- 2- Diffusion is assumed to change in time (during division) and space (at the center) due to changes in shape during the division process. However, the diffusion coefficient as a physical quantity most probably does not change, but what changes is the effectiveness of the diffusion (i.e. how many particles can pass from one side to the other of the diffusion locus). I attempted to solve this problem re-deriving the equations taking into account the change in cross-sectional area during division. However, there seem to be some problems either at the theoretical or at the programming level with this approach.

This said here is a list of possible directions:

- 1. keep developing our 1D model:
 - first step producing simulations after the two daughter cells split. This is just a Matlab programming issue that can probably be solved in a week or so.
 - Calibrate the model parameters to have more quantitative adherence to the experiments. This will hugely depend on the availability of processed data (Shant told me that there was some progress, but I am not sure how much). Once I have the data I can probably produce some preliminary fitting in 1-2 weeks and some more definite one in a month.
 - Work more on the derivation of new reaction diffusion equation dependent on the cross-sectional area change. I am not sure if this is doable or how quickly. I hope to discuss this with you soon.
 - Determine candidates for the role played by the MinCDE system and/or determine alternatives for the control of RomR oscillations. I am reading some more on Myxo and RomR, but for these task we definitely need Dr. Shrout's opinion. I also have an idea about using a chemical potential term in the equations similarly to a trap potential for non linear wave equations.
 - Finally we may want to add some stochastic element to our equations. This will probably become more evident once a first fitting is done using the experimental data.
- 2. Change our model to 2D
 - This will eliminate the problem of having to re-derive the diffusion equation since the cross-sectional change and the forces leading to that will already be included. One preliminary way of determining if this is a suitable approach we could use the final element software-package Frefem++. I should be able to set up code for a changing 2D domain during division in 1 week and post-division in at most an other week. After that we will need to determine the equivalent in 2D of our equations from the 1D model.

- This should require not much more than 1 month.
- Use a stochastic agent based model in a 2D domain instead of PDE equations. I am not familiar with packages to do this so this would require more time. Moreover, I am not sure if they support domain change during the simulations, and the extra forces due to compression at the center will have to be forced into the governing laws for our chemicals.
- 3. For both approach we will eventually pass to analysis of the model simulations
 - In the courses during my summer school in Canada I have seen different techniques used to analyze PDE equations and their solutions (ansatz solution, variational approach, conserved quantities, Euler-Lagrange equations, multiple scales method, etc...). This could be done with the current model or after some more development is done depending on our intentions concerning the contents of the next myxo-RomR paper.