CEMRACS 2018: Mathematical modeling of cell aggregation and segregation

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Introduction

1 Mathematical model

1.1 Macroscopic model

$$\begin{cases} \partial_t f^A = \nabla \cdot (f^A \nabla_x (\Phi^{AA} * f^A)) + \nabla \cdot (f^A \nabla_x \Phi^{AB} * f^B) + D_A \Delta_x f^A + \nu^A f^A \left(1 - \frac{f^A + f^B}{f^*}\right) \\ \partial_t f^B = \nabla \cdot (f^B \nabla_x (\Phi^{BB} * f^B)) + \nabla \cdot (f^B \nabla_x \Phi^{BA} * f^A) + D_A \Delta_x f^A + \nu^A f^A \left(1 - \frac{f^A + f^B}{f^*}\right) \end{cases} \tag{1}$$

1.2 Microscopic model

$$\begin{cases} dX_i^A = -\mu \nabla_{X_i^A} W^A(X^A, X^B) dt + \sqrt{2D_A} dB_i, & \forall i \in \{1, \ldots, N_A\} \\ dX_i^B = -\mu \nabla_{X_\ell^A} W^B(X^A, X^B) dt + \sqrt{2D_B} dB_\ell, & \forall \ell \in \{1, \ldots, N_B\} \end{cases} \tag{2}$$

2 From Micro to Macro model

3 Stability analysis

$$s^*_{\nu_b, \nu_d \neq 0} = \frac{(24D_A + c'^{AA}) \nu_b^B \bar{f}^B + (24D_B + c'^{BB}) \nu_b^A \bar{f}^A}{\nu_b^B \bar{f}^B \tilde{c}'^{AB} + \nu_b^A \bar{f}^A \tilde{c}'^{BA}} \tag{3}$$

with $\bar{f}^A$ and $\bar{f}^B$ constant steady states, not necessarily equal and $c'^{ST} = \frac{2\pi k^{ST} \bar{f}^A \nu_c^{ST} R^4}{\nu_d^{ST}}$, $S, T \in \{A, B\}$.

We define $c'^{AA} = k_1 \bar{f}^A, c'^{BB} = k_2 \bar{f}^B, c'^{AB} = k_3 \bar{f}^A, c'^{BA} = k_4 \bar{f}^B$. By $\bar{f}^B = f^* - \bar{f}^A$ we rewrite the following s^*:

$$s^*_{\nu_b, \nu_d \neq 0} = \frac{(24D_A + k_1 \bar{f}^A) \nu_b^B (f^* - \bar{f}^A) + (24D_B + k_2 (f^* - \bar{f}^A)) \nu_b^A \bar{f}^A}{\nu_b^B (f^* - \bar{f}^A) k_3 \bar{f}^A + \nu_b^A \bar{f}^A k_4 (f^* - \bar{f}^A)} \tag{4}$$

To simplify notation, we take into account the following function depending on $\bar{f}^A$ and its derivative :

$$F(\bar{f}^A) = \frac{\alpha\bar{f}^A + \beta(\bar{f}^A)^2 + \gamma}{\delta\bar{f}^A + \varepsilon(\bar{f}^A)^2}, \qquad \frac{\partial F(\bar{f}^A)}{\partial \bar{f}^A} = \frac{(\bar{f}^A)^2(\beta\delta - \alpha\varepsilon) - 2\varepsilon\gamma\bar{f}^A - \gamma\delta}{(\delta\bar{f}^A + \varepsilon(\bar{f}^A)^2)^2}$$

with parameters

$$\alpha = 24D_B\nu_b^A - 24D_A\nu_b^B + k_1\nu_b^B f^* + k_2\nu_b^A f^* \quad \beta = -k_1\nu_b^B - k_2\nu_b^A \quad \gamma = 24D_A\nu_b^B f^* \delta = k_3\nu_b^B f^* + k_4\nu_b^A f^* \tag{5}$$

4 Numerical scheme

4.1 Macroscopic model

A general semi-discrete finite-volume scheme can be written as follows:

$$\frac{df^A_{j,k}}{dt} = -\frac{F^x_{j+\frac{1}{2},k} - F^x_{j-\frac{1}{2},k}}{\Delta x} - \frac{F^y_{j,k+\frac{1}{2}} - F^y_{j,k-\frac{1}{2}}}{\Delta y} \tag{6}$$

$$F^x_{j+\frac{1}{2},k} = u^+_{j+\frac{1}{2},k} f^E_{j,k} - u^-_{j+\frac{1}{2},k} f^W_{j+1,k}$$

$$F^x_{j-\frac{1}{2},k} = u^+_{j-\frac{1}{2},k} f^E_{j-1,k} - u^-_{j-\frac{1}{2},k} f^W_{j,k}$$

$$F^y_{j,k+\frac{1}{2}} = u^+_{j,k+\frac{1}{2}} f^N_{j,k} - u^-_{j,k+\frac{1}{2}} f^S_{j,k+1}$$

$$F^y_{j,k-\frac{1}{2}} = u^+_{j,k-\frac{1}{2}} f^N_{j,k-1} - u^-_{j,k+\frac{1}{2}} f^S_{j,k}$$

with $u^+ = \max(u, 0)$, $u^- = \min(-u, 0)$ and with

$$u_{j+\frac{1}{2},k} = -\frac{\xi_{j+1,k} - \xi_{j,k}}{\Delta x}, \quad u_{j-\frac{1}{2},k} = -\frac{\xi_{j,k} - \xi_{j-1,k}}{\Delta x}, \quad u_{j,k+\frac{1}{2}} = -\frac{\xi_{j,k+1} - \xi_{j,k}}{\Delta y}, \quad u_{j,k-\frac{1}{2}} = -\frac{\xi_{j,k} - \xi_{j,k-1}}{\Delta y}$$

.

$$\xi_{j,k} = \Delta x \Delta y \sum_{i,\ell} \tilde{\Phi}^{AA}_{j-i,k-\ell} f^A_{i,\ell} + \tilde{\Phi}^{AB}_{j-i,k-\ell} f^B_{i,\ell}$$

with $\Phi^{AA}(x_j - x_i, x_k - x_\ell)$,

$$\xi_{j,k} = \Delta x \Delta y \sum_i \sum_\ell \tilde{\Phi}^{AA}(x_j - x_i, x_k - x_\ell) f^A_{i,\ell} + \tilde{\Phi}^{AB}(x_j - x_i, x_k - x_\ell) f^B_{i,\ell}$$

$$F_R = \nu_b^A f^A_{j,k} \left(1 - \frac{f^A_{j,k} + f^B_{j,k}}{f^*}\right).$$

$$f^{n+1}_{j,k} - F^{n+1}_D \Delta t = f^n_{j,k} + (LO)^n \Delta t + F^n_R \Delta t \tag{7}$$

$$(LO)^n = -\frac{F^{x,n}_{j+\frac{1}{2},k} - F^{x,n}_{j-\frac{1}{2},k}}{\Delta x} - \frac{F^{y,n}_{j,k+\frac{1}{2}} - F^{y,n}_{j,k-\frac{1}{2}}}{\Delta y}.$$

4.2 Microscopic model

Parameters	Values A, B	Description
L	7.5	Length half size demain
R	?	radius
μ	1	..
ν_c	.	.
ν_d	.	.
k	.	.
D		
β		
δ		

$$\beta_A = b_0^A - (b_0^A - \theta_A)\left(\frac{N_A + N_B}{N^*}\right), \qquad \delta_A = d_0^A + (\theta_A - d_0^A)\left(\frac{N_A + N_B}{N^*}\right) \quad (8)$$

5 Results

References

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