Highly Accurate Numerical Methods for Chemotaxis and Related Models

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Many microorganisms exhibit a special pattern formation at the presence of a chemoattractant, food, light or areas with high oxygen concentration. Collective cell movement can be described by a system of nonlinear PDEs: a convection-diffusion equation for the cell density coupled with a reaction-diffusion equation for the chemoattractant concentration. For instance, the Patlak-Keller-Segel (PKS) system reads

$$\begin{cases} \rho_t + \chi \boldsymbol{\nabla} \cdot (\rho\, \mathbf{Q}\,(\nabla c)) = \nu \Delta \rho, \quad \mathbf{Q}\,(\nabla c) = \nabla c, \\ c_t = \Delta c - \alpha c + \beta \rho. \end{cases} \tag{1}$$

Here, ρ is the cell density, c is the chemoattractant concentration, χ is a positive chemosensitivity constant, α, β and ν are positive constants.

A distinctive feature of the chemotactic behavior is a concentration phenomenon: sharp increase in the cell density at isolated points or along certain manifolds. It is well-known that solutions of the PKS system may blow up (develop δ-type singularities) in finite time. This blowup represents a mathematical description of a cell concentration phenomenon that occurs in real biological systems. More realistic scenarios include emergence of (bounded) spiky structures that may be obtained as solutions of regularized PKS systems.

Capturing such rapidly growing solutions, especially when the convection term loses its hyperbolicity is quite a challenging task. We have recently discovered that the convective part in most chemotaxis models is generically of a mixed hyperbolic-elliptic type and developed a second-order positivity preserving (and thus, nonlinearly stable) central-upwind scheme. Positivity preserving is an absolutely crucial property a good numerical method used to simulate chemotaxis should satisfy: this is the only way to guarantee a nonlinear stability of the method. Unlike many other models, in which appearance of unphysical (small) negative values is numerically tolerable, in the chemotaxis models negative, even small negative values of the cell density, generated by a numerical method, will trigger the development of negative cell density spikes, which in turn will make the computed solution completely irrelevant. It is quite easy to design first-order positivity preserving schemes, but first-order schemes are typically impractical.

In this talk, I will present new efficient, high-order and positivity preserving numerical methods that will enhance resolution of spiky solutions of the PKS system and some related models. In particular, in addition to the above PKS model, I will consider a two-species chemotaxis model, which can be viewed as direct extensions of the PKS system to the case of the chemotaxis motion of two noncompeting species that both consume and produce the same chemoattractant. I will also present a model of a fluid-chemotaxis coupling, which describes the collective behavior of a suspension of oxygen-driven bacteria in an aquatic fluid.

The new numerical approach applied to the above models is based on a hybrid finite-difference finite-volume methods, in which the ρ-equation is discretized using a high-order finite-volume scheme, while a much simpler c-equation is solved by a high-order finite-difference method. To ensure positivity of the hybrid method, we implement a high-order positivity preserving reconstruction techniques. I will also present a number of numerical examples that illustrate accuracy, stability, and robustness of the proposed method.