

Recent Developments in the Numerical Methods for the Chemotaxis Models

YEKATERINA EPSHTEYN

In this talk we will discuss recent progress in the development of the numerical methods for the chemotaxis models and closely related problems in physics and biology. We consider the most common formulation of the classical Patlak-Keller-Segel system [7] with the 'parabolic-parabolic' coupling, which can be written in the dimensionless form as

$$(0.1) \quad \begin{cases} \rho_t + \nabla \cdot (\chi \rho \nabla c) = \Delta \rho, \\ c_t = \Delta c - c + \rho, \end{cases} \quad (x, y) \in \Omega, t > 0,$$

subject to the Neumann boundary conditions:

$$(0.2) \quad \nabla \rho \cdot \mathbf{n} = \nabla c \cdot \mathbf{n} = 0, \quad (x, y) \in \partial\Omega.$$

Here, $\rho(x, y, t)$ is the cell density, $c(x, y, t)$ is the chemoattractant concentration, χ is a chemotactic sensitivity constant, Ω is a bounded domain in \mathbb{R}^2 , $\partial\Omega$ is its boundary, and \mathbf{n} is a unit normal vector.

Chemotaxis refers to mechanisms by which cellular motion occurs in response to an external stimulus, usually a chemical one. Chemotaxis is an important process in many medical and biological applications, including bacteria/cell aggregation and pattern formation mechanisms, as well as tumor growth. There exists an extensive literature about chemotaxis models and their mathematical analysis a first place to start is [23], as well as [15, 16], and for a deeper background [2, 8, 21, 1, 7, 3, 4, 24]. The first descriptions of the mechanism owe to Keller and Segel, [17, 18, 19] and Patlak [22]. In this description, the organism or migrating enzyme chooses a direction upwards of a chemical signal which leads to aggregation.

Although there is an extensive literature on this subject, only a few numerical methods have been proposed for these models. Chemotaxis models are usually highly nonlinear due to the density dependent cross diffusion term (attracting force) that models chemotactic behavior, and hence, any realistic chemotaxis model is too difficult to solve analytically. Therefore, development of accurate and efficient numerical methods is crucial for the modeling and analysis of chemotaxis systems. Furthermore, a common property of all existing chemotaxis systems is their ability to model a concentration phenomenon that mathematically results in rapid growth of solutions in small neighborhoods of concentration points/curves. The solutions may blow up or may exhibit a very singular, spiky behavior. This blow-up represents a mathematical description of a cell concentration phenomenon that occurs in real biological systems, see, e.g., [1, 2, 3, 4, 8, 24]. In either case, capturing such solutions numerically is a very challenging problem.

Let us briefly review the numerical methods that have been proposed in the literature. A finite-volume, [13], and finite-element, [20, 26], methods have been proposed for a simplified version of the Patlak-Keller-Segel model with 'parabolic-elliptic' coupling: the equation for concentration of chemical signals c has been

replaced by an elliptic equation using an assumption that c changes over much smaller time scales than the density of the cells ρ . A fractional step numerical method for a fully time-dependent chemotaxis system from [28] has been proposed in [29]. However, the operator splitting approach may not be applicable when a convective part of the chemotaxis system is not hyperbolic, which is a generic situation for the original Patlak-Keller-Segel model with 'parabolic-parabolic' coupling. In [6], a finite-volume central-upwind scheme was derived for the original Patlak-Keller-Segel model and extended to some other chemotaxis models. Recently, in [27], an implicit flux-corrected finite element method has been developed for the original Patlak-Keller-Segel model as well. In our recent work [12, 11, 10] we developed a family of high-order Finite Element Methods (Discontinuous Galerkin Methods) for the original Patlak-Keller-Segel chemotaxis model. However, among the methods that have been proposed, only [20, 26, 27] were designed to treat complex geometry by the use of unstructured meshes. Finally, a different approach has been proposed in [14]. The authors considered the measure-valued global in time solutions of the simplified Patlak-Keller-Segel system in \mathbb{R}^2 and proposed a stochastic particle approximation. The advantage of their method is that it captures the solution even after the (possible) blow-up. However, the method was only designed for the simplified Patlak-Keller-Segel model with 'parabolic-elliptic' coupling. Moreover, at least in the 2D case, methods based on particle simulation are usually less efficient than 'conventional' finite element or finite volume methods for solving convection-diffusion equations.

Often, modeling of real biomedical problems has to deal with the complex structure of the computational domains. Therefore there is a need for accurate, fast, and computationally efficient numerical methods for different chemotaxis models that can handle arbitrary geometries. In our recent paper [9] we develop novel and efficient upwind-difference potentials method which can handle complex geometry without the use of unstructured meshes and it can be combined with fast Poisson solvers. Our method combines the simplicity of the positivity-preserving upwind scheme on Cartesian meshes [5] with the flexibility of the Difference Potentials method [25].

Therefore, in this talk we will discuss and compare recently developed high-order Discontinuous Galerkin Methods [12, 11, 10] and Upwind-Difference Potentials method [9] for the original Patlak-Keller-Segel chemotaxis model.

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