On some Numerical Schemes for the Classical Keller-Segel System

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In this work we focus on the numerical analysis and simulation of some discrete schemes for the classical Keller-Segel system on chemotaxis, which is given by the following equations:

$$\begin{cases} u_t = \Delta u - \alpha_1 \nabla \cdot (u \nabla v), & x \in \Omega,\ t > 0, \\ v_t = \alpha_2 \Delta v - \alpha_3 v + \alpha_4 u, & x \in \Omega,\ t > 0, \\ \nabla u \cdot \mathbf{n} = \nabla v \cdot \mathbf{n} = 0, & x \in \partial\Omega,\ t > 0, \\ u(x,0) = u_0(x),\ v(x,0) = v_0(x), & x \in \Omega. \end{cases} \tag{1}$$

Here u and v are non-negative functions representing the density of cells and chemical-signal, respectively. A lot of research on this topic has been recently made from an analytical point of view (see e.g. [1] and references therein). Global in time existence and boundedness of the solution has been show if the initial data is small enough, while blow-up in some solutions of (1) occurs in many other interesting cases.

Firstly, we analyze a certain family of time-stepping numerical schemes for the Keller-Segel model, focusing on those cases that uncouple cells equation from chemical-signal equation. Specifically, let us consider a partition of the time interval $[0,T]$ into subintervals of size $k > 0$. At each time step t^{m+1}, we approximate $u(t^{m+1})$ and $v(t^{m+1})$ as follows:

$$\begin{cases} (1/k)u^{m+1} - \Delta u^{m+1} + \nabla \cdot (u^{m+s_1} \nabla v^{m+s_2}) = (1/k)u^m \\ (1/k)v^{m+1} - \Delta v^{m+1} + v^{m+s_3} - u^{m+s_4} = (1/k)v^m \end{cases} \tag{2}$$

where $S = (s_1, s_2, s_3, s_4) \in \{0,1\}^4$ and, for simplicity, we take coefficients $\alpha_i = 1$, $i = 1, \ldots, 4$. We are interested in linear and uncoupled schemes which are energetically stable with respect to the well-known energy law of (1)

$$\frac{d}{dt}\mathcal{E}\big(u(\cdot,t), v(\cdot,t)\big) = -\mathcal{D}\big(u(\cdot,t), v(\cdot,t)\big),$$

with $\mathcal{E}(u,v) = \frac{1}{2}\int_\Omega |\nabla v|^2 + \int_\Omega v^2 - \int_\Omega uv + \int_\Omega u \ln u$ and $\mathcal{D}(u,v) = \int_\Omega v_t^2 + \int_\Omega \left| \frac{\nabla u}{\sqrt{u}} - \sqrt{u}\nabla v \right|^2$. We can show:

Theorem 1. *Let $\{(u^m, v^m)\}_{m=0}^N$ be a solution of scheme $S = (s_1, s_2, s_3, s_4)$. The following discrete energy law holds:*

$$\delta_t \mathcal{E}_S^{m+1} \leq -\mathcal{D}_S^{m+1} - \mathcal{N}_S^{m+1} + \mathcal{M}_S^{m+1} \quad \forall m = 0, ..., N-1,$$

where $\delta_t(w^m) = (w^{m+1} - w^m)/k$, $\mathcal{E}_S^{m+1} = \mathcal{E}(u^{m+1}, v^{m+1})$, $\mathcal{D}_S^{m+1} = \mathcal{D}(u^{m+1}, v^{m+1}) + \mathcal{R}^{m+1} \geq 0$, $N_{i,S}$, $M_{i,S} \geq 0$ (numerical dissipation and sources), $N_{i,S}, M_{i,S} \to 0$ as $k \to 0$.

Indeed, the terms $N_{i,S}$ and $M_{i,S}$ (also $\mathcal{R}^{m+1}$) are explicitly computed and we can show that the scheme $S = (1,1,1,0)$ is optimal, in the sense of minimization of numerical dissipation and sources. Other conclusions are obtained from Theorem 1, relating discrete and continuous energy laws.

Secondly, we propose two different types of space discretizations. For the first one, we use continuous $\mathbb{P}_r$ finite elements, both for cells and for chemical equations, using different polynomial families and

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high-order ($r \geq 8$) polynomials, in demanding tests where blow-up is expected in finite time. Some 3D tests are also included, where we make use of parallel computing, and numerical blow-up is detected for some sets of initial values.

For the second space discretization, we take advantage of the scheme $S = (1, 1, 1, 0)$, which allows the use of continuous $\mathbb{P}_r$ finite elements for computing v^{m+1} as a solution of the parabolic equation (2.b). Then we use an upwind discontinuous Galerkin scheme for computing u^{m+1} as solution of the diffusion-convection-reaction equation (2.a).

References

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