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Foreword

It is with great pleasure that we present the Proceedings of the 26th Congress of Differential Equations and Applications / 16th Congress of Applied Mathematics (XXVI CEDYA / XVI CMA), the biennial congress of the Spanish Society of Applied Mathematics S$\vec{e}$MA, which is held in Gijón, Spain from June 14 to June 18, 2021.

In this volume we gather the short papers sent by some of the almost three hundred and twenty communications presented in the conference. Abstracts of all those communications can be found in the abstract book of the congress. Moreover, full papers by invited lecturers will shortly appear in a special issue of the S$\vec{e}$MA Journal.

The first CEDYA was celebrated in 1978 in Madrid, and the first joint CEDYA / CMA took place in Málaga in 1989. Our congress focuses on different fields of applied mathematics: Dynamical Systems and Ordinary Differential Equations, Partial Differential Equations, Numerical Analysis and Simulation, Numerical Linear Algebra, Optimal Control and Inverse Problems and Applications of Mathematics to Industry, Social Sciences, and Biology. Communications in other related topics such as Scientific Computation, Approximation Theory, Discrete Mathematics and Mathematical Education are also common.

For the last few editions, the congress has been structured in mini-symposia. In Gijón, we will have eighteen minis-symposia, proposed by different researchers and groups, and also five thematic sessions organized by the local organizing committee to distribute the individual contributions. We will also have a poster session and ten invited lectures. Among all the mini-symposia, we want to highlight the one dedicated to the memory of our colleague Francisco Javier "Pancho" Sayas, which gathers two plenary lectures, thirty-six talks, and more than forty invited people that have expressed their wish to pay tribute to his figure and work.

This edition has been deeply marked by the COVID-19 pandemic. First scheduled for June 2020, we had to postpone it one year, and move to a hybrid format. Roughly half of the participants attended the conference online, while the other half came to Gijón. Taking a normal conference and moving to a hybrid format in one year has meant a lot of efforts from all the parties involved. Not only did we, as organizing committee, see how much of the work already done had to be undone and redone in a different way, but also the administration staff, the scientific committee, the mini-symposia organizers, and many of the contributors had to work overtime for the change.

Just to name a few of the problems that all of us faced: some of the already accepted mini-symposia and contributed talks had to be withdrawn for different reasons (mainly because of the lack of flexibility of the funding agencies); it became quite clear since the very first moment that, no matter how well things evolved, it would be nearly impossible for most international participants to come to Gijón; reservations with the hotels and contracts with the suppliers had to be cancelled; and there was a lot of uncertainty, and even anxiety could be said, until we were able to confirm that the face-to-face part of the congress could take place as planned.

On the other hand, in the new open call for scientific proposals, we had a nice surprise: many people that would have not been able to participate in the original congress were sending new ideas for mini-symposia, individual contributions and posters. This meant that the total number of communications was about twenty percent greater than the original one, with most of the new contributions sent by students.

There were almost one hundred and twenty students registered for this CEDYA / CMA. The hybrid format allows students to participate at very low expense for their funding agencies, and this gives them the opportunity to attend different conferences and get more merits. But this, which can be seen as an advantage, makes it harder for them to obtain a full conference experience. Alfréd Rényi said: "a mathematician is a device for turning coffee into theorems". Experience has taught us that a congress is the best place for a mathematician to have a lot of coffee. And coffee cannot be served online.

In Gijón, June 4, 2021

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Flux-corrected methods for chemotaxis equations

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Abstract

The aim of this work is to review flux correction methods for chemotaxis equations with special emphasis in two directions. Firstly, to study a possible extension to the Keller–Segel equations of some recent research available on literature about well-posedness and error order of flux correction schemes. And secondly, to test the validity of the low order scheme in some practical numerical examples.

1. Introduction

The importance of mathematics to understand biological processes and the number of mathematicians studying biological and medical phenomena has been continuously increasing in recent years. In particular, for chemotaxis phenomena, which model the property of living organisms to migrate in response to chemical gradients. The celebrated classical chemotaxis model was introduced in [8, 9] and, together with all its numerous variants, has attracted significant interest from the theoretical point of view (see e.g. the compilations [4, 7]).

On the other hand, whereas there are very few numerical results in the literature, mathematical modeling of chemotaxis is a challenging task and it has developed into a relatively large and diverse discipline. In fact, the solutions exhibit interesting mathematical properties which are not easily adapted to a classical discrete methods for solving partial differential equations (EDP) like finite elements or other Galerkin methods. For instance, solutions to the Keller–Segel equations satisfy lower bounds (positivity) and enjoy an energy law, which is obtained by testing the equations against non linear functions. Generally speaking, cross-diffusion mechanisms governing the chemotactic phenomena makes them difficult to analyze not only theoretically but also numerically.

2. Setting of the Problem

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:

$$\begin{cases} u_t = \alpha_0 \Delta u - \alpha_1 \nabla \cdot (u \nabla v), & x \in \Omega,\ t > 0, \\ v_t = \alpha_2 \Delta v - \alpha_3 v + \alpha_4 u, & x \in \Omega,\ t > 0, \\ \nabla u \cdot \mathbf{n} = \nabla v \cdot \mathbf{n} = 0, & x \in \partial\Omega,\ t > 0, \\ u(x,0) = u_0(x),\ v(x,0) = v_0(x), & x \in \Omega. \end{cases} \tag{2.1}$$

Here u and v are non-negative functions in $\Omega \times [0,T]$ representing the density of cells and chemical-signal, respectively, $T > 0$ is a fixed time, and Ω is a bounded domain in $\mathbb{R}^d$, $d = 2$ or $d = 3$, where the boundary $\partial\Omega$ is Lipschitz and $\mathbf{n}$ is the unit outward normal vector.

A lot of research on this topic has been recently made from an analytical point of view (see e.g. [4, 7] 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 (2.1) occurs in many other interesting cases.

The following well-known properties can be higlighted: positivity,

$$u(x,t) > 0, \quad (x,t) \in \Omega \times [0,T], \tag{2.2}$$

and conservtion of the total mass,

$$\int_\Omega u(x,t)\,dx = \int_\Omega u_0(x)\,dx. \tag{2.3}$$

Developing numerical schemes which satisfy the discrete versions of these properties has been the object of many authors, most of whom have focused on finite volume schemes, that in principle fit well with the chemotactic cross difusion term present in (2.1). Among them we can stand out the works of Saad and coworkers [1, 12] and also of Kurganov [5] and coworkers. Some works also use Galerkin discrete schemes, for instance discontinuous Galerkin methods (Kurganov and Epshtyn [6]) and standard finite elements (Saito [13]). In all cases, the strategy is to introduce some linearization of the chemotaxis term in (2.1) and then to use some upwind technique to preserve property (2.2).

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In this work we focus in the flux correction technique for the following time-stepping numerical scheme that uncouple cells equation from chemical-signal equation: guive 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:

$$\begin{cases} (1/k)v^{m+1} - \Delta v^{m+1} + v^{m+1} = (1/k)v^m + u^m \\ (1/k)u^{m+1} - \Delta u^{m+1} + \nabla \cdot (u^{m+1}\nabla v^{m+1}) = (1/k)u^m. \end{cases} \tag{2.4}$$

Note that, for the sake of simplicty, we have taken $\alpha_0 = \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1$ and also a semi-implicit Euler scheme is introduced, altough some results will generalized to Crank-Nicolson.

Flux correction (see e.g. [11] and references therein) has been investigated for decades for transport equations with the name of FCT (flux-corrected transport). These schemes have applied in many other context like the discretization of time-dependent convection–diffusion or turbulent flows. Also they have been applied specifically to chemotaxis equations [14–16]. But, the difficulty for practical implementation on standard finitite elements libraries and and specifically the lack of solid analytical results for existence of solution and a priori error estimates have made this methods little used excepting a small circle of computer scientists. This situation may have changed because a theory has started to be developed in recent years in a serie of papers of Barrenechea et al [2,3]. Although this theory covers only the steady time-independent case for divergence-free convection-diffusion equations, the purpose of this work has been its exploration and testing the low order solutions in the framework of chemotaxis equations.

3. Algebraic Flux Correction in Chemotaxis

At each time iteration, the system of algebraic equations (2.4) consists of two decoupled subproblems for the unknowns v^{m+1} and u^{m+1}:

$$\left[\boldsymbol{M} + k\boldsymbol{L} + k\boldsymbol{M}\right]v^{m+1} = \boldsymbol{M}v^m + k\boldsymbol{M}u^m, \tag{3.1}$$

$$\left[\boldsymbol{M} + k\boldsymbol{L} + k\boldsymbol{K}(\boldsymbol{\beta}^{m+1})\right]u^{m+1} = \boldsymbol{M}u^m, \tag{3.2}$$

where $\boldsymbol{M}$, $\boldsymbol{L}$ and $\boldsymbol{K}(\boldsymbol{\beta}^{m+1})$ are respectively the mass, diffusion and convection matrices with elements defined as

$$m_{ij} = \int_\Omega \varphi_i\varphi_j\,dx, \quad l_{ij} = \int_\Omega \nabla\varphi_i\nabla\varphi_j\,dx, \quad k_{ij}(\boldsymbol{\beta}^{m+1}) = -\int_\Omega \varphi_j\boldsymbol{\beta}^{m+1}\nabla\varphi_i\,dx.$$

We denote $\boldsymbol{\beta}^{m+1} = \nabla v^{m+1}$ and φ_i is a P_1 piecewise-polynomial basis. The algebraic flux correction technique consists of a conservative manipulation of the matrices $\boldsymbol{M}$ and $\boldsymbol{K}(\boldsymbol{\beta}^{m+1})$ in order to enforce at the discrete level the positivity of the system (3.1)–(3.2). Specifically, the *consistent* mass matrix $\boldsymbol{M}$ is approximated by the diagonal matrix $\boldsymbol{M}_L$ using the well-know mass lumping technique:

$$\boldsymbol{M}_L = \mathrm{diag}(m_i), \quad m_i := \sum_j m_{ij}.$$

On the other hand, negative off-diagonal elements of $\boldsymbol{K}(\boldsymbol{\beta}^{m+1})$ are eliminated by adding an artificial diffusion operator $\boldsymbol{D}$, defined as the symmetric matrix with elements

$$d_{ij} = \max\{-k_{ij}, 0, -k_{ji}\}, \;\; j \neq i, \qquad d_{ii} = -\sum_{j\neq i} k_{ij}.$$

The result is a low order positivity-preserving discretization which, in the 1D case, transforms the linear finite element convection system (3.2) into a first-order upwind difference [10]. The 2D case is much more complicated although error estimates have been recently derived for the steady case [2]. If we denote $\boldsymbol{A}_v = \boldsymbol{M} + k\boldsymbol{L} + k\boldsymbol{M}$ and $\boldsymbol{A}_u = \boldsymbol{M} + k\boldsymbol{L} + k\boldsymbol{K}(\boldsymbol{\beta}^{m+1})$, this low-order system corresponds to

$$\left[\boldsymbol{A}_v + \boldsymbol{D}_v\right] v^{m+1} = \boldsymbol{M}v^m + k\boldsymbol{M}u^m \tag{3.3}$$

$$\left[\boldsymbol{A}_u + \boldsymbol{D}_u\right] u^{m+1} = \boldsymbol{M}u^m \tag{3.4}$$

with $\boldsymbol{D}_v = \boldsymbol{M}_L - \boldsymbol{M}$, $\boldsymbol{D}_u = \boldsymbol{M}_L - \boldsymbol{M} + k\boldsymbol{D}$. And, since the row sums of the matrix $\boldsymbol{D}$ vanish, the error with respect to the original consistent system (3.1)–(3.2) can be written in terms of two vectors

$$f_i^v = \sum_{j\neq i} f_{ij}^v \qquad f_i^u = \sum_{j\neq i} f_{ij}^u$$

where the anti-diffusive fluxes f_{ij}^v and f_{ij}^u are computed from the mass lumping and the artificial diffusion received by each node i:

$$\left((\boldsymbol{M} - \boldsymbol{M}_L)u^{m+1}\right)_i = \sum_{j\neq i} m_{ij}(u_j - u_i), \qquad \left(\boldsymbol{D}u^{m+1}\right)_i = \sum_{j\neq i} d_{ij}(u_j - u_i). \tag{3.5}$$

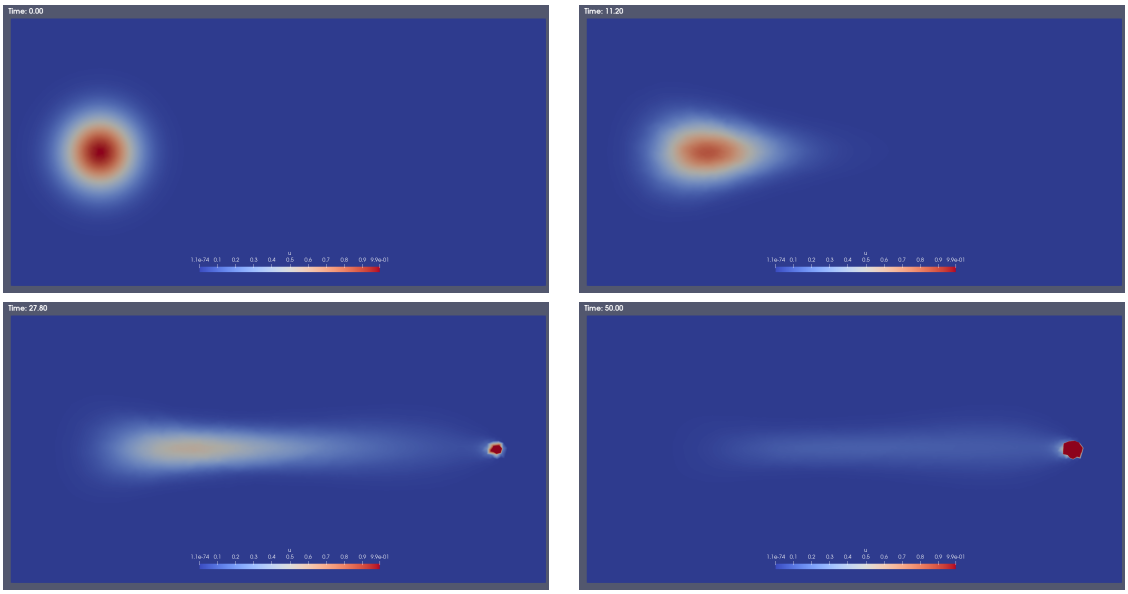

Fig. 1 Chemotatic migration towards fixed chemical concentration. Low order scheme.

Now, instead of adding this fluxes to the right hand side of (3.3), (3.4) and thus obtain the original consistent system, the idea of algebraic flux correction schemes is to limit those anti-diffusive fluxes f_{ij} that would otherwise get back to the original high order solution and cause spurious oscillations. Each flux is multiplied by a solution-dependent correction factor $\alpha_{ij} \in [0, 1]$. The original Galerkin discretization correspond to selecting $\alpha_{ij} = 1$ and may be applied where the solution is smooth, while $\alpha_{ij} = 0$ may be set in the neighborhood of steep fronts, where adding diffusion is appropriate. We impose $\alpha_{ij} = \alpha_{ji}$ to guarantee that the scheme is conservative.

Thus the final form of the algebraic flux correction scheme corresponds to the following system of nonlinear equations:

$$\boldsymbol{A}_v v_i^{m+1} + \sum_{j=1}^{N} (1 - \alpha_{ij}^v) d_{ij}^v (v_j^{m+1} - v_i^{m+1}) = \boldsymbol{M} v_i^m + k \boldsymbol{M} u_i^m, \quad i = 1, \ldots, N, \tag{3.6}$$

$$\boldsymbol{A}_u u_i^{m+1} + \sum_{j=1}^{N} (1 - \alpha_{ij}^u) d_{ij}^u (u_j^{m+1} - u_i^{m+1}) = \boldsymbol{M} u_i^m, \quad i = 1, \ldots, N, \tag{3.7}$$

where d_{ij}^v and d_{ij}^u are respectively the entries of $\boldsymbol{D}^u$ and $\boldsymbol{D}^v$ while $\alpha_{ij}^v = \alpha_{ij}^v(v^{m+1})$ and $\alpha_{ij}^u = \alpha_{ij}^u(u^{m+1})$ are in $[0, 1]$, being $\alpha_{ij}^v = \alpha_{ji}^v$ and $\alpha_{ij}^u = \alpha_{ji}^u$.

For the choice of the flux limiters α_{ij}^u and α_{ij}^v, we are going to us consider the widely used Zalesak limiters (see e.g. [2, 10, 11, 17]). Other appropriate limiters can be set, see e.g. [3]. At the present time, the authors of this work claim that, under some restrictions in the time and space discretization, the following result can be shown:

Theorem 3.1 *Assuming $u_0 \geq 0$ and $v_0 \geq 0$:*

1. *The low order discrete solution (u^{m+1}, v^{m+1}) (obtained from $\alpha_{ij}^u = \alpha_{ij}^v = 0$) is positive for all $m \geq 0$.*
2. *If $\alpha_{ij}^u, \alpha_{ij}^v$ are the Zalesak limiters*
   (a) *There exists a solution of the nonlinear problem* (3.6)–(3.7).
   (b) *The high order solution (u^{m+1}, v^{m+1}) is positive for all $m \geq 0$.*
3. *The approximate solutions (u^{m+1}, v^{m+1}) converge to the exact solution (u, v) with at least suboptimal error order.*

4. Numerical Tests

4.1. Chemotactic transport

In our first numerical test we take a static (non time-dependent) chemical source v and study the migration of the biological organisms u toward high gradients of v. Specifically, the domain Ω is taken as the rectangle

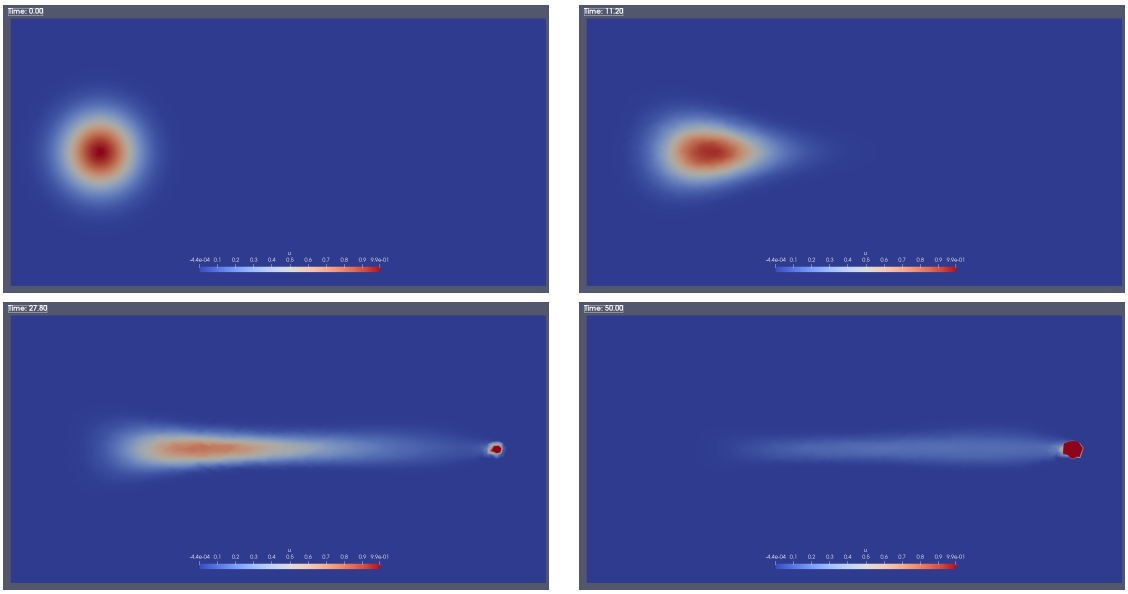

Fig. 2 Chemotatic migration towards fixed chemical concentration. High order scheme.

$[0,5]\times[-1,1]$. we introduce an unstructured mesh with size $h \simeq 0.01$. The time interval $[0,50]$ is discretized so that the CFL condition $k/h < 1$ is verified. On the other hand, v is set as the gaussian function

$$v(x,t) = v(x) = e^{-C((x-4)^2+y^2)},$$

with $C = 50$, which approximately verifies $\nabla v \cdot \mathbf{n} = 0$ on $\partial\Omega$, and u is the solution of $(2.1)_a$ with the less favorable no diffusion condition $\alpha_0 = 0$, $\alpha_1 = 1$. On the other hand, $\nabla u \cdot \mathbf{n} = 0$ on $\partial\Omega$ and the following initial state is chosen:

$$u_0(x) = e^{-C((x-1)^2+y^2)}.$$

Figure 1 shows the result obtained at times $t = 0$, $t = 11.20$, $t = 27.80$ and $t = 50$ with the low order scheme ($\alpha^u_{ij} = \alpha^v_{ij} = 0$). This initial state is transported toward maximum concentration of v. Positivity of solution is maintained strictly and no spurious ripples appear. Figure 2 shows the same test but the high-order scheme (Zalesak limiters) is introduced. In this case, fixed point iterations are introduced to avoid nonlinearity of the scheme. The results are similar although lesser diffusion can be appreciated at intermediate time steps.

4.2. Neuroblast Migration in the Brain

Secondly, we show a numerical test dealing with the migration of neuroblasts (precursor cells of neurons) in the adult brain. This test is part of a project we are working in, together with researchers of Universidad de Sevilla and Universidad de Cádiz. In recent decades, it has been known that neuroblasts are born in a specific part of the adult brain (the Subventricular Zone, SVZ) migrate to other zones: to the Olfactory Bulb (OB) and eventually to lesions in the brain). Some specific parts of the brain (the Corpus Callosum) influences the migration, obstructing it. This process can be modeled by a chemotaxis-like process.

A low order flux correction scheme has been applied in this context (together with other numerical schemes, all of which will be published in a forthcoming work). The results for different time steps are presented in Figure 3, where a source of neuroblasts starts from the SVZ and, bording the Corpus Callosum (represented as a light spot) goes to the OB, located at the left side of the brain.

4.3. Blow up for Keller–Segel System

One of the more challenging characteristics of Keller–Segel equations (2.1) is the fact that finite-time blow-up occurs in many interesting cases, for 2D and 3D, if initial data is not small enough [4]. It has been deeply investigated and many authors have worked in obtaining numerical schemes that maintain positivity and are free of spurious oscillations in blow-up regime. In particular, flux correction and chemotaxis have been studied in [14–16].

Here we just show a validation focused on the low order scheme, which can be programmed in standard finite element libraries without too much additional difficulty. In particular, the low order scheme avoids the necessity of solving nonlinear scheme and its much less computing demanding, Making feasible the use of finer meshes.

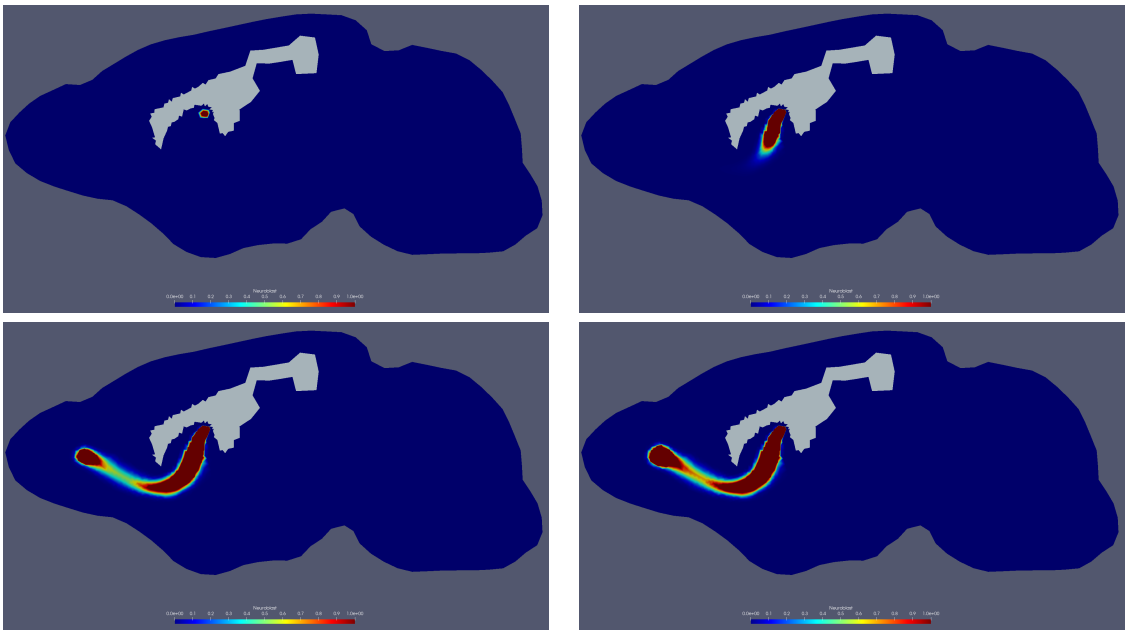

Fig. 3 Chemotatic migration towards fixed chemical concentration. Different time steps (from top left to bottom right). Low order scheme.

Specifically, we consider the numerical test studied in [5], where the domain $\Omega = (-1/2, 1/2)^2$ is meshed with $h \approx 1/100$, $h \approx 1/200$ and $h \approx 1/400$. System (2.1) is solved with $\alpha_0 = \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1$ and

$$v_0 = 0, \quad u_0 = 1000e^{-100(x^2+y^2)}.$$

The blow up which, according to the theoretical results, is expected for this initial data, is conjectured to occur at some $t^* \in (4.4 \times 10^{-5}, 10^{-4})$, where maximum values of u are around 10^4 or 10^5.

Our numerical test with the low-order scheme, maintain the positivity of u and v and reaches the following values:

- At $t = 4.4 \times 10^{-5}$: $\max(u) = 2.58586e+04$, $\min(u) = 1.41495e-18$, $\max(v) = 4.95975e+02$, $\min(v) = 1.41495e-18$.
- At $t = 10 \times 10^{-4}$: $\max(u) = 1.27965e+05$, $\min(u) = 6.35863e-18$, $\max(v) = 4.92729e+02$, $\min(v) = 6.35863e-18$.

It is interesting no observe that mass is conserved, with a constant value of $3.14159e+01$ for u in Ω.

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