CENTRO DE CIENCIAS BÁSICAS

DEPARTAMENTO DE MATEMÁTICAS Y FÍSICA

TESIS

ON A SIMPLE FULLY DISCRETE FINITE-DIFFERENCE APPROXIMATION OF A NONLINEAR DIFFUSION-REACTION MODEL IN MICROBIAL ECOLOGY

PRESENTA

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PARA OBTENER EL GRADO DE MAESTRO EN CIENCIAS

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Aguascalientes, Ags., 5 de Julio de 2014

UNIVERSIDAD AUTONOMA DE AGUASCALIENTES

FORMATO DE CARTA DE VOTO APROBATORIO

M. en C. José de Jesús Ruiz Gallegos
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Estimado (a) alumno (a) Morales:

Por medio de este conducto me permito comunicar a Usted que habiendo recibido los votos aprobatorios de los revisores de su trabajo de tesis y/o caso práctico titulado: **"ON A SIMPLE FULLY DISCRETE FINITE-DIFFERENCE APROXIMATION OF A NONLINEAR DIFFUSIÓN-REACTION MODEL IN MICROBIOBIAL ECOLOGY",** hago de su conocimiento que puede imprimir dicho documento y continuar con los trámites para la presentación de su examen de grado.

Sin otro particular me permito saludarle muy afectuosamente.

A T E N T A M E N T E
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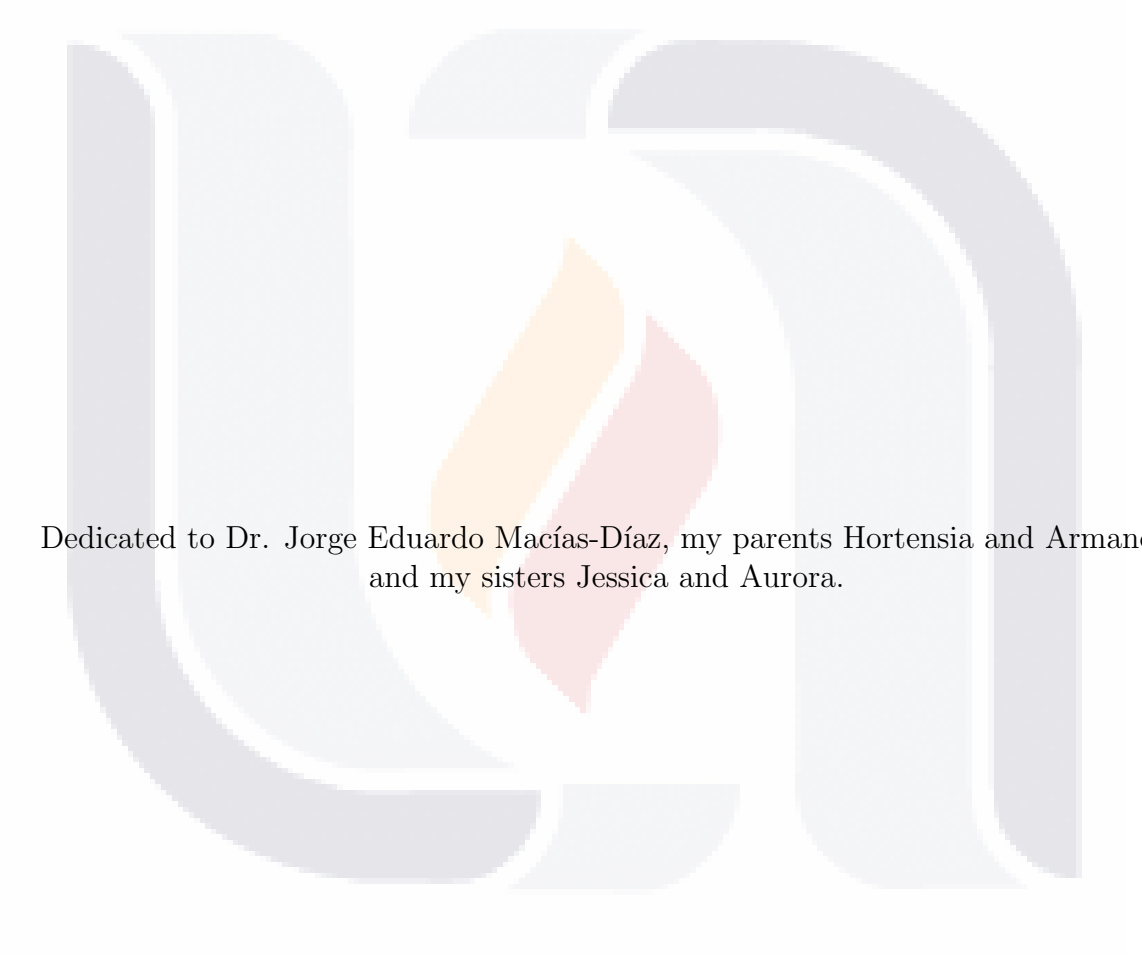

Dedicated to Dr. Jorge Eduardo Macías-Díaz, my parents Hortensia and Armando and my sisters Jessica and Aurora.

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Resumen

En este trabajo se presenta un método simple, de diferencias finitas para aproximar soluciones positivas y acotadas de una ecuación diferencial parcial parabólica con la difusión no lineal que describe la dinámica de crecimiento de colonias de bacterias. Un teorema sobre la existencia y unicidad de soluciones positivas y acotadas del modelo considerado se encuentra disponible en la literatura estándar; sin embargo, las soluciones analíticas para este modelo son difíciles de calcular en forma exacta. El enfoque lineal utilizado en este manuscrito proporciona una manera conveniente de representar el método en forma de vector a través de la multiplicación de las nuevas aproximaciones por una matriz cuadrada que, bajo condiciones adecuadas, resulta ser una M-matriz. Los hechos de que cada M-matriz es invertible y que todas las entradas de sus inversas son números positivos, se emplean para determinar las condiciones que garantizan que los perfiles iniciales positivos y acotados devienen en nuevas aproximaciones positivas y acotadas. El método es relativamente simple, el tamaño de paso temporal es variable en general, y su implementación computacional eficiente hace uso del método de gradiente de bi-conjugado estabilizado. Proporcionamos simulaciones numéricas con el fin de evidenciar que el método preserva en la práctica los aspectos positivos y acotados de las aproximaciones. Desde un punto de vista científico, nuestra técnica se puede emplear en posibles trabajos futuros relacionados con la simulación controlada del crecimiento de colonias microbianas en las ciencias de los materiales y la ingeniería biomédica.

Asbtract

In this work, we present a simple, finite-difference method to approximate positive and bounded solutions of a parabolic partial differential equation with nonlinear diffusion which describes the growth dynamics of colonies of bacteria. A theorem on the existence and uniqueness of positive and bounded solutions of the model considered is available in the standard literature; however, analytical solutions for this model are difficult to calculate in exact form. The linear approach used in this manuscript provides a convenient way to represent the method in vector form through the multiplication of the new approximations by a square matrix which, under suitable conditions, turns out to be an M-matrix. The facts that every M-matrix is invertible and that all the entries of their inverses are positive numbers, are employed to elucidate conditions which guarantee that positive and bounded initial profiles evolve into positive and bounded new approximations. The method is relatively simple, the temporal step-size is variable in general, and its efficient computational implementation makes use of the stabilized bi-conjugate gradient method. We provide numerical simulations in order to evince that the method preserves in the practice the positive and the bounded characters of the approximations. From a scientific perspective, our technique may be employed in possible future works related to the controlled simulation of the growth/decay of microbial colonies, in material science and biomedical engineering.

Introduction

Several phenomena in disciplines such as biology, chemistry, physics and economics require complex models which are described by the interaction and change of multiple variables through space and time. Those interactions can often be translated into the rigorous and well defined language of partial differential equations (PDE); differential equations that relate the partial derivatives of unknown multivariable functions. In the context of chemistry, the type of equations that we study in this manuscript describe the evolution of the concentration of chemical species in a fluid due to three factors: Advection, diffusion and reaction. Advection is the transport of a conserved property or substance by a fluid due to the fluid's bulk motion, e.g. the transport of granular material in a river by water flow. Diffusion is also a transport mechanism which causes the substances to spread out over a surface in space, e.g. when a drop of dye falls into still water and it travels from regions of high concentration to regions of low concentration. Reaction is, according to IUPAC, a process that leads to the transformation of one set of chemical substances into another, e.g. when elemental sodium is placed in water and produces hydrogen which self-ignites. PDE that involve these three phenomena are termed Advection-Diffusion-Reaction equations (ADR's). The next logical step when one has an ADR is to solve it. A naive approach would be to use the current analytical tools at our disposal to extract a solution. However simple the strategy, the truth is that solving these equations in their more general form by means of analytic techniques is fairly impossible. The way to overcome that difficulty is with the aid of numerical methods. Numerical methods for solving PDE include but are not restricted to the following: Finite differences, finite elements, finite volumes, spectral, meshfree, domain decomposition and multigrid. Among these, the one that has been most extensively studied and the one we use is the finite difference method (FDM) in which a domain is discretized and functions are represented by the calculated values at certain grid points on which the derivatives are approximated by differences. Once the equation and the numerical method have been defined, the finite difference scheme has to be designed. This last part is obviously the most complicated because at this point we are not only concerned with the approximations of the solutions, but also with their nature; since the model comes from a physical context, the solutions may only have sense under certain circumstances such as non-negativity, boundedness or monotonicity, therefore the approximations should likewise.

This manuscript is divided in 6 chapters which can be treated in an independent way so that the reader might jump to the desired section without loosing sense of content or continuity. In the first five chapters the concept and properties of M-matrices play a major role as a crucial tool to derive properties. Chapter one

presents a technique to compute bounded solutions of a Newell-Whitehead-Segel equation. In chapter two conditions to guarantee the non-negativity and boundedness of the approximations to a FitzHugh-Nagumo equation are provided. In Chapter three we propose a method that preserves the boundedness and positivity of the solutions and the skew-symmetry of the Burgers-Huxley equation from fluid dynamics. Chapter four considers a one dimensional, time-delayed, advective version of the Fisher-KPP equation from population dynamics. Chapter five develops a method to compute solutions of a non-linear ADR model in two spatial dimensions. Chapter six comes in the form of an epilogue which describes a non-linear iterative technique to approximate solutions of Burgers-Huxley equation.

Chapter 1

Preliminaries

In general, let us consider an open, connected, spatial domain $\Omega \subset \mathbb{R}^3$ which physically represents the substrate on which a biological film will grow. For every $\mathbf{x} = (x, y, z) \in \Omega$, let $u(x, y, z, t)$ represent the biomass density at the point $\mathbf{x}$ and the time $t \geq 0$, normalized with respect to the maximum biomass density. Suppose that $u : \Omega \times \mathbb{R}^+ \to \mathbb{R}$ is twice differentiable. Let α and β be real numbers with $\alpha, \beta \geq 1$, and let δ be a relatively small, positive number. Let $D : [0, 1) \to \mathbb{R}$ be the function given by

$$D(u) = \delta \frac{u^\beta}{(1-u)^\alpha}, \quad \forall u \in [0, 1). \tag{1.1}$$

Let ∇ represent the gradient operator in the three spatial dimensions. Moreover, suppose that $r : \Omega \times \mathbb{R}^+ \to \mathbb{R}$ is a continuous function which physically describes the rate at which biomass is created. Under these conventions, the equation that governs the growth dynamics of biological mass on the substrate Ω is provided by

$$\frac{\partial u}{\partial t} = \nabla \cdot (D(u)\nabla u) + ru, \quad \forall (\mathbf{x}, t) \in \Omega \times \mathbb{R}^+. \tag{1.2}$$

The function $D(u)$ is a nonlinear diffusion factor, which physically is telling us how the biomass is spreading in the domain. Its expression —as given by (1.1)— is in agreement with various experimental observations [7], one of them being that the spread of biomass is significant when u is close to the maximum biomass density, namely, when $u \approx 1$. Otherwise, the spatial rate of diffusion of the biomass should be relatively small, which is the rationale behind the choice of δ.

Evidently, suitable, initial-boundary conditions must be imposed. Throughout this work, we will assume that the initial data are given by the formula

$$u(\mathbf{x}, 0) = \varphi(\mathbf{x}), \quad \forall \mathbf{x} \in \overline{\Omega}, \tag{1.3}$$

where $\varphi : \overline{\Omega} \to \mathbb{R}$ is a function with range in $[0, 1]$, and $\overline{\Omega}$ denotes the closure of Ω in $\mathbb{R}^3$. The function u physically represents the fraction of the bacterial population together with the extracellular polymeric substances, and we may think of the spatial domain Ω as the topological interior of a glass substrate or a Petri dish.

In general, the partial differential equation (1.2) is a model for which is difficult to obtain analytical solutions given arbitrary initial-boundary data, whence the need to develop reliable numerical methods to approximate its complex dynamics is

pragmatically justified. However, some analytical results on the qualitative behavior of its solutions are available in the literature.

Let $F : [0, 1) \to \mathbb{R}$ be defined by the expression

$$F(u) = \int_0^u \frac{v^\beta}{(1-v)^\alpha} dv, \quad \forall u \in [0, 1). \tag{1.4}$$

With this nomenclature at hand, the following proposition justifies the numerical investigation reported in this work.

Proposition 1. *Let r be a nonnegative function, and suppose that φ is a nonnegative function such that $\varphi \in L^\infty(\Omega)$, $F(\varphi) \in H_0^1(\Omega)$, and $\|\varphi\|_{L^\infty(\Omega)} < 1$. Then there exists a unique solution u to (1.2) subject to the initial condition (1.3), satisfying the following properties:*

1. $u \in L^\infty(\Omega \times \mathbb{R}^+) \cap C(L^2(\Omega), [0, \infty))$,
2. $F(u) \in L^\infty(H^1(\Omega), \mathbb{R}^+) \cap C(L^2(\Omega), [0, \infty))$,
3. $0 \leq u(\mathbf{x}, t) \leq 1$ *for every* $(\mathbf{x}, t) \in \Omega \times \mathbb{R}^+$ *and* $\|u\|_{L^\infty(\Omega \times \mathbb{R}^+)} < 1$, *and*
4. $u(\mathbf{x}, t) = 0$ *for every* $(\mathbf{x}, t) \in \partial\Omega \times \mathbb{R}^+$.

Proof. See Theorem 2.1 in [8]. □

Where, $L^2(\Omega)$ is the space of square integrable functions, H^1 is a Sobolev space also denoted as $W^{1,2}(\Omega)$ consisting of the functions $f : \Omega \to \mathbb{R}$ sucht that $||F||_{H^1} < \infty$ and $C(L^2(\Omega), [0, \infty))$ consists of the square continuous integrable functions on $[0, \infty)$.

As a consequence, the existence of positive and bounded solutions of (1.2) is guaranteed under the premises of Proposition 1. Qualitatively, numerical simulations performed in [6] have shown that the solution reaches the maximum density in finite time when a nonzero initial profile and homogeneous Neumann boundary conditions are imposed. If homogeneous Dirichlet data are used on a portion or on all the boundary of Ω, then the solution is less than 1 almost everywhere, for every $t \in \mathbb{R}^+$.

Remark 2. It is important to remark that Equation (1.2) is a simplification of a more general biofilm model derived in [7] under suitable physical assumptions, such as

(a) the presence of a sharp front of biomass at the fluid/solid transition,

(b) the existence of a threshold of biomass density,

(c) the fact that the biomass spreading is significant only when the biomass is close to the threshold,

(d) the application of reaction kinetics mechanisms in the production of biomass,

(e) the compatibility of the biomass spreading mechanism with hydrodynamics and with nutrient transfer/consumption models,

among other physically motivated hypotheses. One readily notices that the expression of the diffusion factor D, as given by (1.1), satisfies conditions (b) and (c) above. On the other hand, the mathematical assumptions provided in Proposition 1 yield sufficient conditions for the existence and uniqueness of solutions of (1.2) which satisfy the physical constraints. It is worthwhile to mention that the authors do not have knowledge of more general analytical results related to the existence of positive and bounded solutions of the model (1.2).

Chapter 2

Discretization

The present discussion will focus on the design of a numerical method for Equation (1.2) in two spatial dimensions. Afterwards, we believe that its extension to the three-dimensional case and its particular treatment in the one-dimensional scenario should be straightforward. Throughout this work, we convey that $\overline{\mathbb{Z}}^+ = \mathbb{Z}^+ \cup \{0\}$. Also, for every $p \in \mathbb{Z}^+$ with $p > 1$, we let $\mathbb{Z}_p = \{1, \ldots, p-1\}$ and $\overline{\mathbb{Z}}_p = \mathbb{Z}_p \cup \{0, p\}$.

Let a, b, c and d be real numbers such that $a < b$ and $c < d$, and let M and N be positive integers greater than 1. From a physical perspective, consider a relatively thin, rectangular glass substrate whose perimeter of the base is represented by the boundary of the open rectangle $\Omega = (a, b) \times (c, d)$ in $\mathbb{R}^2$. Following a finite-difference methodology, we fix uniform partitions

$$a = x_0 < x_1 < \ldots < x_M = b, \tag{2.1}$$

and

$$c = y_0 < y_1 < \ldots < y_N = d, \tag{2.2}$$

of the intervals $[a, b]$ and $[c, d]$, respectively, with step sizes given respectively by $\Delta x = (b-a)/M$ and $\Delta y = (d-c)/N$. Likewise, fix provisionally a uniform temporal step $\Delta t > 0$, and a uniform partition

$$0 = t_0 < t_1 < \ldots < t_k < \ldots, \quad \forall k \in \overline{\mathbb{Z}}^+ \tag{2.3}$$

of the interval $[0, \infty)$.

For every $(m, n, k) \in \overline{\mathbb{Z}}_M \times \overline{\mathbb{Z}}_N \times \overline{\mathbb{Z}}^+$, we employ the notations $u_{m,n}^k$ and $r_{m,n}^k$ to represent a numerical approximation to the exact value of the solution u and the exact value of the function r, respectively, at the point (x_m, y_n, t_k). We introduce the standard, forward-difference operators

$$\delta_x^+ u_{m,n}^k = \frac{u_{m+1,n}^k - u_{m,n}^k}{\Delta x}, \quad \forall m \in \mathbb{Z}_M, \forall n \in \mathbb{Z}_N, \forall k \in \overline{\mathbb{Z}}^+, \tag{2.4}$$

$$\delta_y^+ u_{m,n}^k = \frac{u_{m,n+1}^k - u_{m,n}^k}{\Delta y}, \quad \forall m \in \mathbb{Z}_M, \forall n \in \mathbb{Z}_N, \forall k \in \overline{\mathbb{Z}}^+, \tag{2.5}$$

$$\delta_t^+ u_{m,n}^k = \frac{u_{m,n}^{k+1} - u_{m,n}^k}{\Delta t}, \quad \forall m \in \mathbb{Z}_M, \forall n \in \mathbb{Z}_N, \forall k \in \overline{\mathbb{Z}}^+, \tag{2.6}$$

which are first-order consistent approximations to the corresponding partial derivatives of u with respect to x, y and t, respectively, at (x_m, y_n, t_k). For the sake of

convenience, we introduce the following linear operators, too:

$$\delta_x^- u_{m,n}^k = \frac{u_{m-1,n}^k - u_{m,n}^k}{\Delta x}, \quad \forall m \in \mathbb{Z}_M, \forall n \in \mathbb{Z}_N, \forall k \in \overline{\mathbb{Z}}^+, \tag{2.7}$$

$$\delta_y^- u_{m,n}^k = \frac{u_{m,n-1}^k - u_{m,n}^k}{\Delta y}, \quad \forall m \in \mathbb{Z}_M, \forall n \in \mathbb{Z}_N, \forall k \in \overline{\mathbb{Z}}^+. \tag{2.8}$$

For every $m \in \mathbb{Z}_M$, every $n \in \mathbb{Z}_N$ and every $k \in \overline{\mathbb{Z}}^+$, let

$$\mu_x^{\pm} u_{m,n}^k = \frac{u_{m\pm1,n}^k + u_{m,n}^k}{2}, \quad \mu_y^{\pm} u_{m,n}^k = \frac{u_{m,n\pm1}^k + u_{m,n}^k}{2}, \tag{2.9}$$

$$\epsilon_x^{\pm} u_{m,n}^k = D(\mu_x^{\pm} u_{m,n}^k)\delta_x^{\pm} u_{m,n}^{k+1}, \quad \epsilon_y^{\pm} u_{m,n}^k = D(\mu_y^{\pm} u_{m,n}^k)\delta_y^{\pm} u_{m,n}^{k+1}, \tag{2.10}$$

$$\epsilon_x u_{m,n}^k = \frac{\epsilon_x^+ u_{m,n}^k + \epsilon_x^- u_{m,n}^k}{\Delta x}, \quad \epsilon_y u_{m,n}^k = \frac{\epsilon_y^+ u_{m,n}^k + \epsilon_y^- u_{m,n}^k}{\Delta y}. \tag{2.11}$$

To approximate the reaction and the diffusion terms in (1.2), we employ a Mickens-type, non-standard approach [11, 18]. More precisely, for every $m \in \mathbb{Z}_M$, $n \in \mathbb{Z}_N$ and $k \in \overline{\mathbb{Z}}^+$, we approximate the exact value of $r(x_m, y_n, t_{k+1})u(x_m, y_n, t_{k+1})$ by $r_{m,n}^{k+1} u_{m,n}^k$, and the diffusion term at the point (x_m, y_n, t_{k+1}) is approximated through $\nabla \cdot (D(u)\nabla u) \approx (\epsilon_x + \epsilon_y)u_{m,n}^k$. Meanwhile, the partial derivative of u with respect to t at the same point will be approximated by means of (2.6). Therefore, the finite-difference method employed in this work to approximate the solutions of (1.2) is given by the system of equations

$$\delta_t^+ u_{m,n}^k = (\epsilon_x + \epsilon_y)u_{m,n}^k + r_{m,n}^{k+1} u_{m,n}^k, \tag{2.12}$$

which is valid for every $m \in \mathbb{Z}_M$, $n \in \mathbb{Z}_N$ and $k \in \overline{\mathbb{Z}}^+$. At the initial time, we use the discrete constraint $u_{m,n}^0 = \varphi_{m,n}$, where $\varphi_{m,n} = \varphi(x_m, y_n)$ for every $m \in \overline{\mathbb{Z}}_M$ and $n \in \overline{\mathbb{Z}}_N$. It is easy to check that this method provides a consistent approximation of order $\mathcal{O}((\Delta x)^2 + (\Delta y)^2 + \Delta t)$, to the exact solutions of model (1.2).

Computationally, it is necessary to impose appropriate, discrete constraints on the edges of the rectangle Ω. In our investigation, these constraints may be homogeneous, Neumann or Dirichlet conditions; in any case, these conditions may be expressed through the identities

$$u_{m,0}^k - \lambda u_{m,1}^k = 0, \quad \forall m \in \mathbb{Z}_M, \tag{2.13}$$

$$u_{m,N}^k - \mu u_{m,N-1}^k = 0, \quad \forall m \in \mathbb{Z}_M, \tag{2.14}$$

$$u_{0,n}^k - \nu u_{1,n}^k = 0, \quad \forall n \in \overline{\mathbb{Z}}_N, \tag{2.15}$$

$$u_{M,n}^k - \xi u_{M-1,n}^k = 0, \quad \forall n \in \overline{\mathbb{Z}}_N. \tag{2.16}$$

Here, each of the constants λ, μ, ν and ξ refers to the boundary points (x_m, a), (x_m, b), (c, y_n) and (d, y_n), respectively, and each of them is equal to 0 if there is a homogeneous Dirichlet boundary condition at the point of reference, and is equal to 1 in the case of homogeneous Neumann boundary data.

Remark 3. Before we close this stage of our work, notice that each of the equations in (1.2) may be approximated by

$$\begin{aligned} \psi_{m-1,n,x}^k u_{m-1,n}^{k+1} + \psi_{m,n-1,y}^k u_{m,n-1}^{k+1} + \phi_{m,n}^k u_{m,n}^{k+1} + \\ \psi_{m,n+1,y}^k u_{m,n+1}^{k+1} + \psi_{m+1,n,x}^k u_{m+1,n}^{k+1} = \chi_{m,n}^k u_{m,n}^k, \end{aligned} \tag{2.17}$$

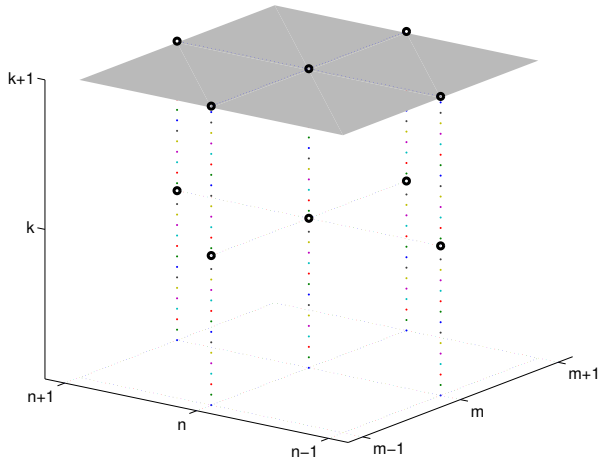


Figure 2.1: Forward-difference stencil of the numerical method (2.12) around the spatial point (x_m, y_n) at time t_k. The circles at the kth time level represent known approximations, while those at the time t_{k+1} denote the unknown estimates.

for every $m \in \mathbb{Z}_M$, $n \in \mathbb{Z}_N$ and $k \in \overline{\mathbb{Z}}^+$. Let

$$R_x = \frac{\Delta t}{(\Delta x)^2}, \qquad R_y = \frac{\Delta t}{(\Delta y)^2}. \tag{2.18}$$

Then, the coefficients in this approximation of (1.2) are provided by

$$\psi^k_{m\pm1,n,x} = -R_x D(\mu^{\pm}_x u^k_{m,n}), \qquad \psi^k_{m,n\pm1,y} = -R_y D(\mu^{\pm}_y u^k_{m,n}) \tag{2.19}$$

$$\begin{aligned} \phi^k_{m,n} &= 1 + R_x \left[D(\mu^+_x u^k_{m,n}) + D(\mu^-_x u^k_{m,n}) \right] \\ &\quad + R_y \left[D(\mu^+_y u^k_{m,n}) + D(\mu^-_y u^k_{m,n}) \right], \end{aligned} \tag{2.20}$$

$$\chi^k_{m,n} = 1 + r^{k+1}_{m,n} \Delta t. \tag{2.21}$$

In fact, Figure 2.1 presents the forward-difference stencil of the finite-difference scheme (2.12) in view of this new presentation of the method. When D assumes the form (1.1), each of the expressions in (2.19) is non-positive for example R_x is positive and $D(\mu^{\pm}_x u^k_{m,n})$, is also positive thus these terms are non-positive and each of those in (2.20) are greater than one, as we said $R_{x,y}$ are positive and D is also positive thus it is clear that these terms are greater than one.

Chapter 3

Vector representation

Beforehand, we must mention that we will use herein the nomenclature introduced in the previous sections.

It is important to notice that each iteration of the recursive method (2.12) may be rewritten conveniently in vector form. Indeed, for every $k \in \overline{\mathbb{Z}}^+$, let $\mathbf{u}^k$ be the lexicographically ordered vector of the approximate solution at the time t_k. In other words, let

$$\mathbf{u}^k = (u^k_{0,0}, u^k_{0,1}, \ldots, u^k_{0,N}, u^k_{1,0}, u^k_{1,1}, \ldots, u^k_{1,N}, \ldots, u^k_{M,0}, u^k_{M,1}, \ldots, u^k_{M,N}). \tag{3.1}$$

Let $\mathbf{u}_0$ be the vector with the information on the initial approximation, that is,

$$\mathbf{u}_0 = (\varphi_{0,0}, \varphi_{0,1}, \ldots, \varphi_{0,N}, \varphi_{1,0}, \varphi_{1,1}, \ldots, \varphi_{1,N}, \ldots, \varphi_{M,0}, \varphi_{M,1}, \ldots, \varphi_{M,N}), \tag{3.2}$$

and let I be the identity matrix of size $(N+1) \times (N+1)$. For every $m \in \mathbb{Z}_M$ and every $k \in \overline{\mathbb{Z}}^+$, let B^k_m be the matrix of the same size as I given by

$$B^k_m = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \chi^k_{m,1} & 0 & \cdots & 0 & 0 \\ 0 & 0 & \chi^k_{m,2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \chi^k_{m,N-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}, \tag{3.3}$$

and let B^k be the matrix defined by blocks through

$$B^k = \left(\begin{array}{c|ccccc|c} 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ \hline 0 & \boxed{B^k_1} & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \boxed{B^k_2} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \boxed{B^k_{M-2}} & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \boxed{B^k_{M-1}} & 0 \\ \hline 0 & 0 & 0 & \cdots & 0 & 0 & 0 \end{array}\right). \tag{3.4}$$

Evidently, B^k is a square matrix with $(M+1)(N+1)$ rows and a similar amount of columns, needless to mention that the symbol 0 in the definition of B^k represents

the zero matrix of size $(N+1)\times(N+1)$. In addition, for every $m \in \mathbb{Z}_M$ and $k \in \overline{\mathbb{Z}}^+$ we define the matrices A_m^k and C_m^k of sizes $(N+1)\times(N+1)$ by

$$A_m^k = \begin{pmatrix} 1 & -\lambda & 0 & \cdots & 0 & 0 \\ \psi_{m,0,y}^k & \phi_{m,1}^k & \psi_{m,1,y}^k & \cdots & 0 & 0 \\ 0 & \psi_{m,1,y}^k & \phi_{m,2}^k & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \phi_{m,N-1}^k & \psi_{m,N-1,y}^k \\ 0 & 0 & 0 & \cdots & -\mu & 1 \end{pmatrix}, \tag{3.5}$$

and

$$C_m^k = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \psi_{m,1,x}^k & 0 & \cdots & 0 & 0 \\ 0 & 0 & \psi_{m,2,x}^k & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \psi_{m,N-1,x}^k & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}. \tag{3.6}$$

For every $k \in \overline{\mathbb{Z}}^+$, define the block matrix

$$A^{k+1} = \left(\begin{array}{c|c|ccc|ccc} I & -\nu I & 0 & 0 & \cdots & 0 & 0 & 0 \\ \hline C_0^k & A_1^{k+1} & C_2^k & 0 & \cdots & 0 & 0 & 0 \\ \hline 0 & C_1^k & A_2^{k+1} & C_3^k & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & C_{M-2}^k & A_{M-1}^{k+1} & C_M^k \\ \hline 0 & 0 & 0 & 0 & \cdots & 0 & -\xi I & I \end{array}\right), \tag{3.7}$$

which has size $(M+1)(N+1)\times(M+1)(N+1)$. With this nomenclature, the iterative method (2.12) may be conveniently represented in vector form as the recursive system of vector equations with initial condition

$$\begin{cases} A^{k+1}\mathbf{u}^{k+1} = B^k\mathbf{u}^k, \quad \forall k \in \overline{\mathbb{Z}}^+, \\ \mathbf{u}^0 = \mathbf{u}_0. \end{cases} \tag{3.8}$$

Remark 4. Clearly, the method (2.12) is implicit. At each iteration, the matrix A^{k+1} is a function of the vector $\mathbf{u}^k$, while B^k is a function of the time value t_{k+1} and the mesh grid $\{(x_m, y_n) : m \in \overline{\mathbb{Z}}_M, n \in \overline{\mathbb{Z}}_N\}$. In our computational code of the recursive, vector system (3.8), we use an implementation of the stabilized biconjugate gradient method.

Chapter 4

Properties

In this section, we establish the fact that our method conditionally preserves the properties of positivity and boundedness. The cornerstone in the proofs is the concept of M-matrices. By an *M-matrix* we mean a square, real matrix A which satisfies all of the following properties:

1. The off-diagonal elements of A are non-positive numbers.
2. The diagonal entries of A are positive numbers.
3. A is strictly diagonally dominant, meaning that $|a_{ii}| > \sum_{j \neq i} |a_{ij}|$ where a_{ij} denotes the entry in the i-th row and j-th column.

In our study, the importance of the M-matrices lies in the facts that they are nonsingular, and that all the entries of their inverses are positive numbers [9]. Evidently, this notion will help us establish conditions which guarantee the positivity of the numerical approximations and, ultimately, their boundedness, too.

Let $\mathbf{x}$ be a real vector, and let $\mathbf{e}$ be the vector of the same dimension as $\mathbf{x}$, all of whose components are equal to 1. We say that $\mathbf{x}$ is *positive* if all its entries are positive numbers; this fact is represented by the notation $\mathbf{x} > 0$. Clearly, $\mathbf{x}$ is *non-negative* if all its components are nonnegative numbers, in which case we use the nomenclature $\mathbf{x} \geq 0$.

We use the notation $\mathbf{x} < 1$ to mean that each of the components of this vector are less than 1 and, in this case, we say that $\mathbf{x}$ is *bounded from above* by 1; evidently, the inequality $\mathbf{x} < 1$ is satisfied if and only if $\mathbf{e} - \mathbf{x}$ is positive. The inequalities $0 \leq \mathbf{x} < 1$ represent the facts that $\mathbf{x}$ is a nonnegative vector which is bounded from above by 1.

Lemma 5. *Let $k \in \overline{\mathbb{Z}}^+$, and suppose that $0 \leq \mathbf{u}^k < 1$. Then A^{k+1} is an M-matrix.*

Proof. The proof is straightforward after the closing remarks of Section 2. □

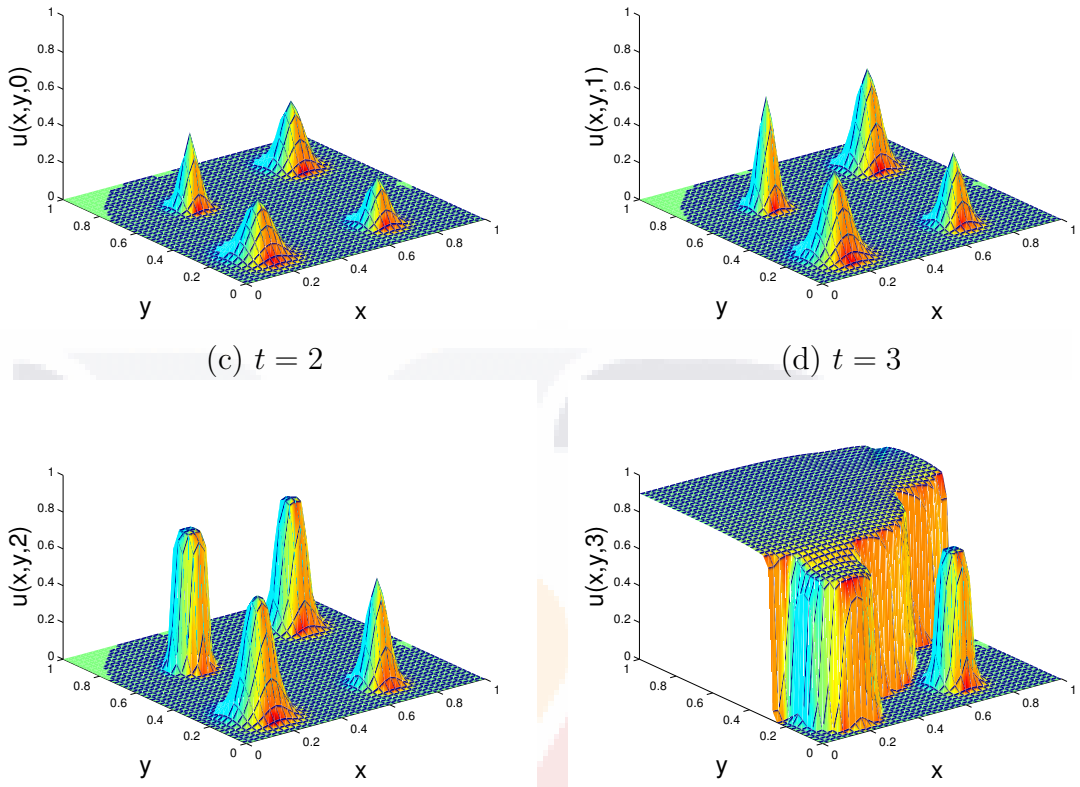
We prove next that our method is positivity- and boundedness-preserving when we consider suitable, non-constant time-steps.

Proposition 6. *Let φ and r be nonnegative functions such that $\varphi < 1$. For each $k \in \overline{\mathbb{Z}}^+$, let $(\Delta t)_k$ be the temporal step-size in the kth iteration. If the inequality*

$$r^k_{m,n} u^k_{m,n} (\Delta t)_k < 1 - u^k_{m,n} \tag{4.1}$$

is satisfied for every $m \in \mathbb{Z}_M$, $n \in \mathbb{Z}_N$ and $k \in \overline{\mathbb{Z}}^+$, then $0 \leq \mathbf{u}^k \leq 1$.

(a) $t = 0$ (b) $t = 1$



(c) $t = 2$ (d) $t = 3$

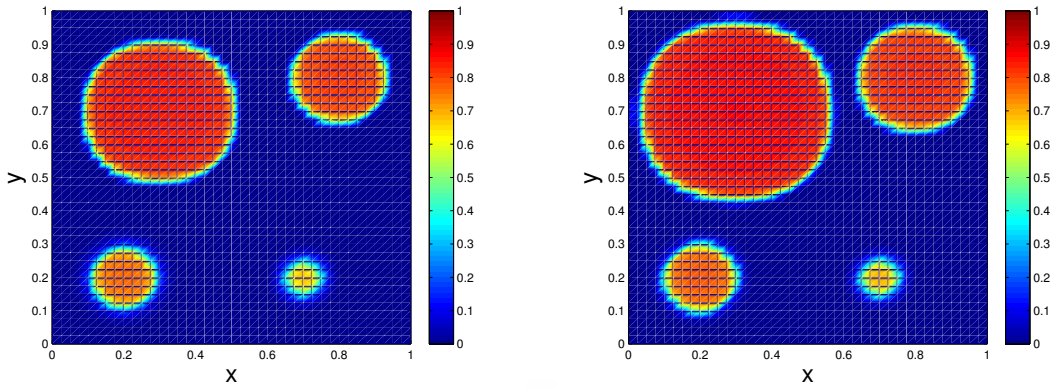
Figure 4.1: Graphs of the approximate solution of (1.2) on $\Omega = (0,1) \times (0,1)$ at four different times, namely, $t = 0, 1, 2, 3$, obtained using the finite-difference method (2.12). The following parameters were employed: $\alpha = \beta = 4$, $\delta = 1 \times 10^{-4}$, $r \equiv 0.42$; $\Delta x = \Delta y = 0.025$, and the initial temporal step-size is equal to 0.001. Discrete homogeneous Neumann conditions were imposed on the boundary of Ω, and the initial profile is given by (5.5).

Proof. The conclusion is obviously true when $k = 0$. Let us suppose that $0 < \mathbf{u}^k < 1$, for some $k \in \overline{\mathbb{Z}}^+$. Lemma 5 guarantees that A^{k+1} is an M-matrix; by hypothesis, $\chi^k_{m,n}$ is positive for every $m \in \overline{\mathbb{Z}}_M$ and $n \in \overline{\mathbb{Z}}_N$. Consequently, $B^k\mathbf{u}^k$ is a positive vector, whence $\mathbf{u}^{k+1} = (A^{k+1})^{-1}B^k\mathbf{u}^k$ is likewise positive. To establish boundedness, let $\mathbf{w}^{k+1} = \mathbf{e} - \mathbf{u}^{k+1}$. A substitution in Equation (3.8) yields $A^{k+1}\mathbf{w}^{k+1} = \mathbf{b}^{k+1}$, where

$$\mathbf{b}^{k+1} = A^{k+1}\mathbf{e} - B^k\mathbf{u}^k. \tag{4.2}$$

The first and the last $N + 1$ rows of the vector $\mathbf{b}^{k+1}$, as well as those labeled $m(N+1)+1$ and $(m+1)(N+1)$ are nonnegative for every $m \in \mathbb{Z}_M$; the components of the remaining rows are of the form $1 - (1 + (\Delta t)_k r^k_{m,n})u^k_{m,n}$, for suitable $m \in \mathbb{Z}_M$ and $n \in \mathbb{Z}_N$, and the positivity of these components follows from (4.1). The fact that $\mathbf{w}^{k+1}$ is positive follows as a result from the fact the A^{k+1} is an M-matrix, whence $\mathbf{u}^{k+1} < 1$. The result is readily established by induction. □

(a) $t = 2.7$ (b) $t = 2.8$



(c) $t = 2.9$ (d) $t = 3$

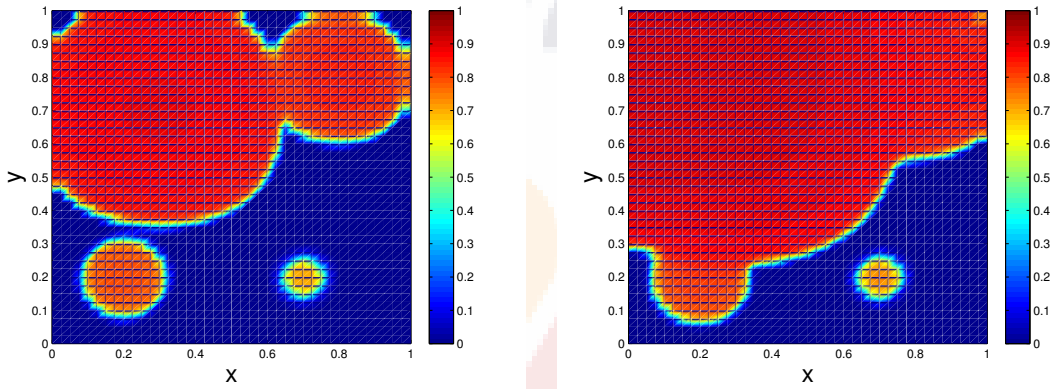


Figure 4.2: Interpolated checkerboard plots of the approximate solution of (1.2) on $\Omega = (0, 1) \times (0, 1)$ at four different times, namely, $t = 2.7, 2.8, 2.9, 3$, obtained using the finite-difference method (2.12). The following parameters were employed: $\alpha = \beta = 4$, $\delta = 1 \times 10^{-4}$, $r \equiv 0.42$; $\Delta x = \Delta y = 0.025$, and the initial temporal step-size is equal to 0.001. Discrete homogeneous Neumann conditions were imposed on the boundary of Ω, and the initial profile is given by (5.5).

Remark 7. It is worthwhile to notice that the results in this section are valid for every function D which is nonnegative in $[0, 1]$, and not only the function given by Equation (1.1).

Chapter 5

Simulations

In the present section, we will show that the method introduced in this manuscript preserves the properties of positivity and boundedness of solutions when the constraints of Proposition 6 are observed. Evidently, such results will be in qualitative agreement with Proposition 1.

In the following simulations, an initial, temporal step-size is employed; however, if the inequality (4.1) is not satisfied, then the value of $(\Delta t)_k$ is reduced by half, and this process is repeated as many times as it be necessary in order for (4.1) to hold, for every $m \in \mathbb{Z}_M$ and every $n \in \mathbb{Z}_N$. The open spatial domain is $\Omega = (0,1) \times (0,1)$, and we use the parameter values $\alpha = \beta = 4$ and $\delta = 1 \times 10^{-4}$ in the expression of the function D.

Example 8. Let r be the constant function equal to 0.42 in $\Omega \times \mathbb{R}^+$. Computationally, let $\Delta x = \Delta y = 0.025$, and choose an initial, temporal step-size equal to 0.001. Fix homogeneous Neumann conditions on the boundary of Ω, and let

$$\mathbf{x}_1 = (0.2, 0.2), \tag{5.1}$$
$$\mathbf{x}_2 = (0.8, 0.8), \tag{5.2}$$
$$\mathbf{x}_3 = (0.3, 0.7), \tag{5.3}$$
$$\mathbf{x}_4 = (0.7, 0.2). \tag{5.4}$$

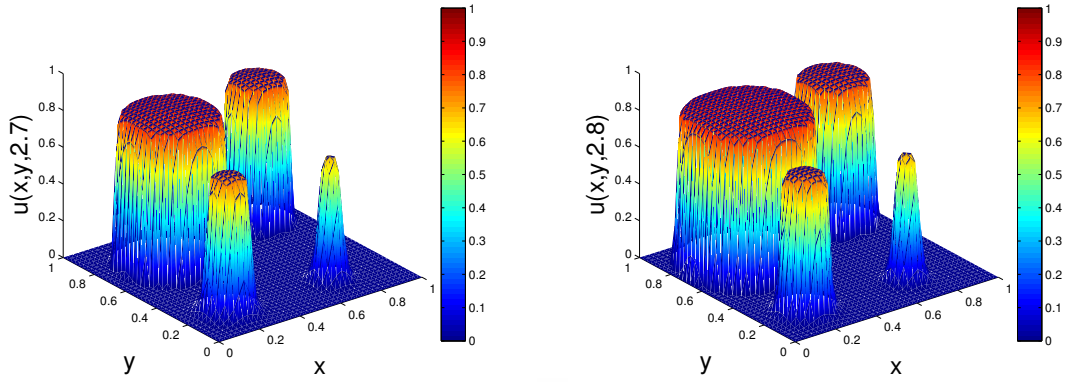
Let $\mathbf{x} = (x, y)$, and consider an initial profile of the form

$$\begin{aligned} \varphi(\mathbf{x}) = \; & 0.3e^{-200\|\mathbf{x}-\mathbf{x}_1\|^2} + 0.35e^{-300\|\mathbf{x}-\mathbf{x}_2\|^2} \\ & +0.4e^{-600\|\mathbf{x}-\mathbf{x}_3\|^2} + 0.25e^{-400\|\mathbf{x}-\mathbf{x}_4\|^2}, \quad \forall \mathbf{x} \in \overline{\Omega}, \end{aligned} \tag{5.5}$$

which is positive and bounded from above by 1, because it is a sum of functions of the form $f(x) = exp^{(-rx^2)}$ which are bounded between 0 and k and a sum of bounded terms is bounded. Under these conditions, Figure 4.1 presents the development of the solution at 4 different times, namely, 0, 1, 2 and 3. The simulations show that the solution remains bounded within $(0, 1)$ throughout time, as predicted by Proposition 6. This behavior is also observed in Figure 4.2, which presents interpolated checkerboard plots of of the solutions at the times 2.7, 2.8, 2.9 and 3, when the colonies begin to merge.

In the next example, we consider Dirichlet boundary data, instead.

(a) $t = 2.7$ (b) $t = 2.8$



(c) $t = 2.9$ (d) $t = 3$

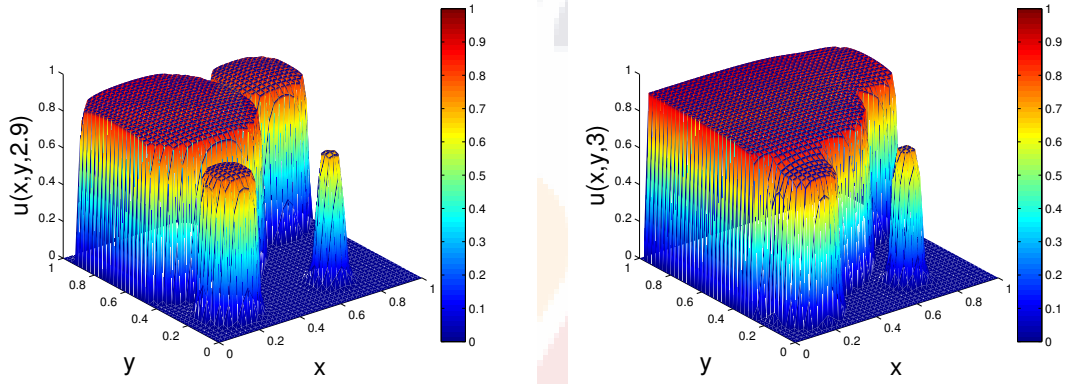


Figure 5.1: Graphs of the approximate solution of (1.2) on $\Omega = (0,1) \times (0,1)$ at four different times, namely, $t = 2.7, 2.8, 2.9, 3$, obtained using the finite-difference method (2.12). The following parameters were employed: $\alpha = \beta = 4$, $\delta = 1 \times 10^{-4}$, $r \equiv 0.42$; $\Delta x = \Delta y = 0.025$, and the initial temporal step-size is equal to 0.001. Discrete homogeneous Dirichlet conditions were imposed on the boundary of Ω, and the initial profile is given by (5.5).

Example 9. We reproduce Example 8, now with homogeneous Dirichlet data on the boundary of Ω. Figure 5.1 shows the approximate solution at the times 2.7, 2.8, 2.9 and 3. Once more, notice that positivity and boundedness are preserved in our simulations, even when different colonies of bacteria begin to merge.

Remark 10.

- It is worthwhile to remark once more that the method presented in this manuscript is capable of preserving the positivity and the boundedness of the numerical approximations, for any real numbers $\alpha, \beta \geq 1$, and any discrete reaction factor which satisfies the properties of Proposition 6.
- We have performed more simulations in order to assess the validity of this claim. The results (not shown here) suggest the fact that the method preserves the properties of interest, as postulated by Proposition 6.
- The results were obtained using ©Matlab 7.12.0.635 (R2011a) on a ©Sony Vaio PCG-5L1P laptop computer, with Kubuntu 12.04 as operating system.

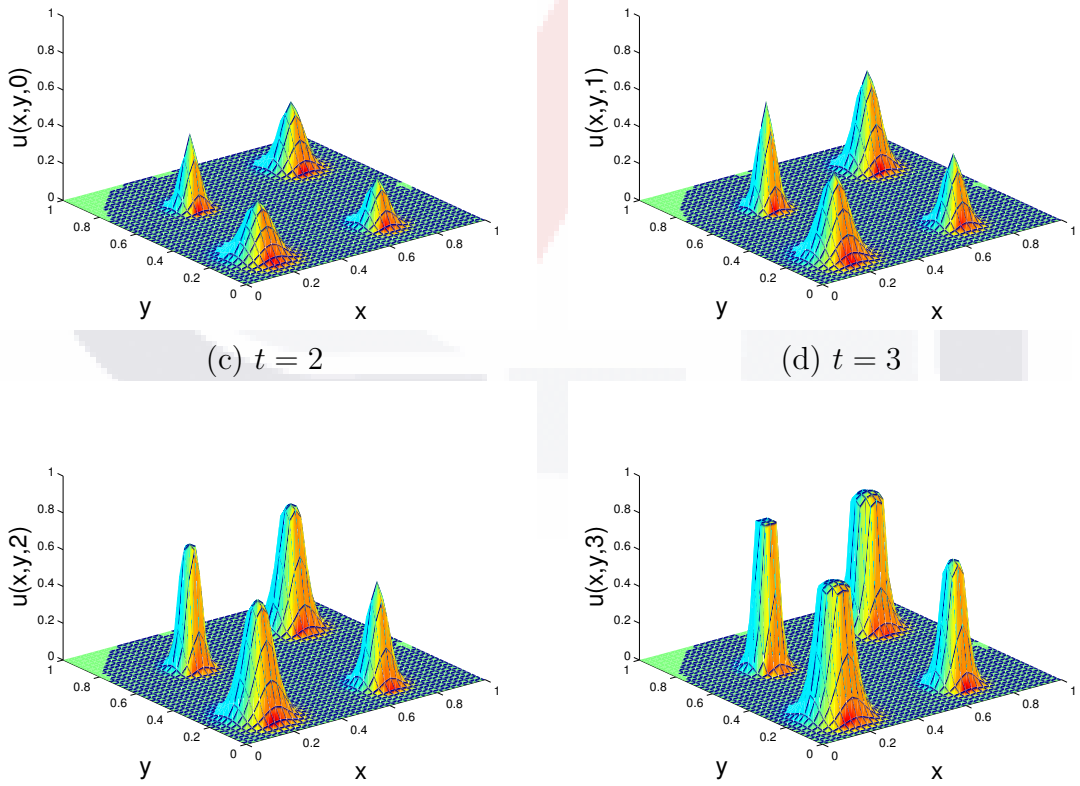
Under the computational and model parameter values employed in Examples 8 and 9, the computer time needed to simulate a time period of length 1 was equal to 3.289769 seconds, as recorded by the average of 20 such simulations.

Chapter 6

Discusion of results

This appendix reports on some incorrect simulations obtained via an implementation of the method introduced in [Int. J. Comput. Meth. 9 (2012) 1250050]. In the present note, we show the correct numerical results of Example 6.1 in that work. A new computer experiment is added in order to observe the process of merging colonies in biological films.

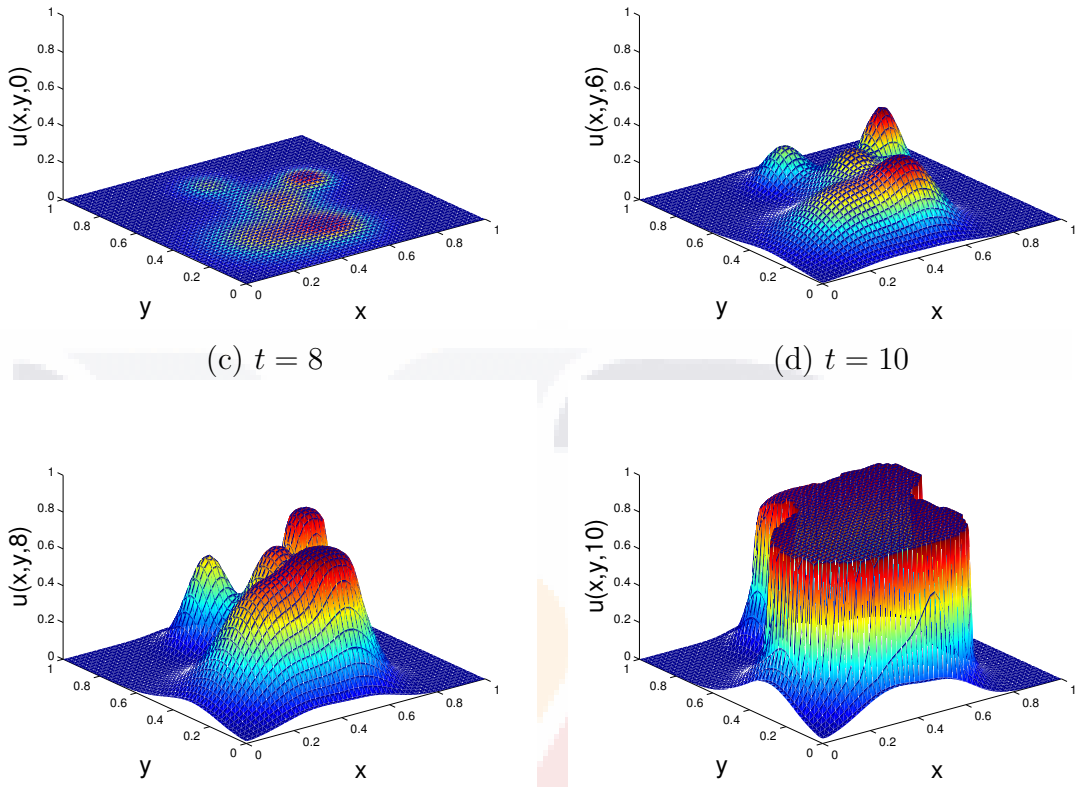
(a) $t = 0$ (b) $t = 1$



(c) $t = 2$ (d) $t = 3$

Figure 6.1: Graphs of Figure 2 in [Morales-Hernández *et al.* (2012)], obtained through a faithful implementation of the method reported in that manuscript.

(a) $t = 0$ (b) $t = 6$



(c) $t = 8$ (d) $t = 10$

Figure 6.2: Graphs of the approximate solution of (2) in [Morales-Hernández *et al.* (2012)] on $\Omega = (0,1) \times (0,1)$ at four times. We used the parameters $\alpha = \beta = 4$, $\delta = 1 \times 10^{-4}$, $r \equiv 0.4$; $\Delta x = \Delta y = 0.02$, $\Delta t = 0.01$, and the initial profile of Example 11.

Examples

Using our Matlab® code, we obtained the graphs of Figure 6.1 in the present manuscript, which are the correct versions of the corresponding graphs in Figure 2 of [17]. In this experiment, however, the process of merging of colonies is not observed. To observe it, we propose the following example.

Example 11. *let* $\Omega = (0,1) \times (0,1)$, *and consider the initial condition*

$$u_0(\mathbf{x}) = \sum_{l=1}^{5} C_l e^{-r_l \|\mathbf{x}-\mathbf{x}_l\|^2}, \quad \forall \mathbf{x} \in \Omega, \tag{6.1}$$

where $C_1 = 0.025$, $C_2 = 0.03$, $C_3 = 0.035$, $C_4 = 0.02$, $C_5 = 0.025$; $r_1 = 25$, $r_2 = 50$, $r_3 = 125$, $r_4 = 100$, $r_5 = 50$; $\mathbf{x}_1 = (0.25, .3)$, $\mathbf{x}_2 = (0.5, .25)$, $\mathbf{x}_3 = (0.7, 0.65)$, $\mathbf{x}_4 = (0.4, 0.8)$, *and* $\mathbf{x}_5 = (0.5, 0.55)$. *Let* $\alpha = \beta = 4$, $\delta = 1 \times 10^{-4}$, $r \equiv 0.4$, $\Delta x = \Delta y = 0.02$, *and* $\Delta t = 0.01$. *Consider homogeneous Neumann conditions on the boundary of* Ω. *Figure 6.2 presents the approximate solution using the method in* [17], *at the times* $t = 0$, 6, 8, 10.

Conclusions

In this work, we introduced a non-constant time-step, finite-difference scheme to approximate the solutions of a parabolic partial differential equation which governs the growth of some biological films. The linear discretization proposed is a two-step method, and each iteration of the technique may be presented in vector form through the multiplication of a real, square matrix which, under suitable conditions, is an M-matrix. As a consequence, the matrix representing each iteration of the method is nonsingular, and each of the entries of the inverse is a positive, real number. This fact guarantees the preservation of the positivity of initial profiles which are also positive. Moreover, once positivity is established, it is easy to find conditions under which the numerical technique is also capable of preserving the boundedness of the solutions at every point.

It is important to mention that the biological model investigated in this manuscript has solutions which are positive and essentially bounded; however, such solutions are not reported in the literature in an analytical form [8], whence the design of positivity- and boundedness-preserving computational technique to approximate such solutions of the model under consideration is pragmatically justified. The numerical simulations obtained through a computational implementation of our technique confirm that the mathematical properties of interest of solutions are preserved throughout time. Some of such simulations are recorded in this manuscript to support numerically these assertions.

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Appendix

Appendix: Article

From: jemaciasdiaz@hotmail.com
To: jemaciasdiaz@hotmail.com
Subject: FW: IJCM 1250050
Date: Tue, 3 Jun 2014 10:00:07 -0500

Dear Dr. Macias-Diaz,

Enclosed are the page proofs of your article, scheduled to be published in _International Journal of Computational Methods_ (IJCM) Vol. 9, issue 4, for your review and go-ahead. If you wish to make any corrections, you can list them in point form with the corresponding page & line numbers and send to me as a doc. attachment, or simply mark the corrections directly on the proofs and email them back to me. I would appreciate it if you (or one of the other contributors) could return the proof by 29 NOV 2012. Please also provide answers for the queries listed below. ------Queries-------- 1. Kindly provide us with the date of submission of your paper as well as the date it was accepted. ---------- The article will be published online first once you have proofread it. As the corresponding author, you are entitled to a complimentary pdf of your published article. We will send you the pdf after the journal issue is published. Thank you and with best regards.

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