Linear finite-difference discretizations that preserve positivity and boundedness

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Let Ω be an open and bounded set in $\mathbb{R}^2$. The problem of interest is the following initial-boundary-value problem:

$$\begin{cases} \dfrac{\partial u}{\partial t}(\mathbf{x}, t) = f(\mathbf{x}, t, u, \nabla u), & \mathbf{x} \in \Omega, t \in \mathbb{R}^+, \\ u(\mathbf{x}, 0) = \phi(x), & \mathbf{x} \in \Omega, \\ u(\mathbf{x}, t) = \psi(\mathbf{x}, t), & \mathbf{x} \in \partial\Omega, t \in \mathbb{R}^+. \end{cases}$$

Alternative problem

After integrating with respect to t on both sides, we reach the equivalent problem

$$u(\mathbf{x}, t) = u(\mathbf{x}, 0) + \int_0^t f(\mathbf{x}, t, u, \nabla u) dt, \quad \mathbf{x} \in \Omega, t \in \mathbb{R}^+,$$
$$u(\mathbf{x}, t) = \psi(\mathbf{x}, t), \quad \mathbf{x} \in \partial\Omega, t \in \mathbb{R}^+,$$

which is a boundary-value problem.

A simple model

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Nomenclature

- $\Omega \subset \mathbb{R}^n$ is open, bounded and connected.
- $\alpha, \beta \in \mathbb{R}$ such that $\alpha, \beta \geq 1$, and $\delta \in \mathbb{R}$ satisfies $0 < \delta \ll 1$.
- $D : [0, 1) \to \mathbb{R}$ is the function

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

- $r : \Omega \times \mathbb{R}^+ \to \mathbb{R}$ is a continuous function such that $0 \leq r < 1$.

Model

$u : \overline{\Omega} \times \mathbb{R}^+ \to \mathbb{R}$ is a twice-differentiable function satisfying

$$\begin{cases} \dfrac{\partial u}{\partial t} = \nabla \cdot (D(u)\nabla u) + ru, & \forall (\mathbf{x}, t) \in \Omega \times \mathbb{R}^+, \\ u(\mathbf{x}, 0) = \varphi(\mathbf{x}), & \forall \mathbf{x} \in \Omega. \end{cases}$$

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

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

Theorem

Suppose that $\varphi \geq 0$ is a function such that $\varphi \in L^\infty(\Omega)$, $F(\varphi) \in H_0^1(\Omega)$, and

$$\|\varphi\|_{L^\infty(\Omega)} < 1.$$

There exists a unique solution u satisfying:

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

Dimensional restriction

We will restrict our attention to the $(2+1)$-dimensional case.

Nomenclature

- $\Omega = [a, b] \times [c, d] \subset \mathbb{R}^2$, for $a, b, c, d \in \mathbb{R}$ such that $a < b$ and $c < d$.
- Fix uniform partitions

$$\begin{aligned} a = x_0 < x_1 < \ldots < x_m < \ldots < x_M = b, \\ c = y_0 < y_1 < \ldots < y_n < \ldots < y_N = d. \end{aligned}$$

- Fix a uniform partition $0 = t_0 < t_1 < \ldots < t_k < \ldots$
- Let Δx, Δy and Δt be the respective step-sizes, let $u_{m,n}^k \approx u(x_m, y_n, t_k)$.
- Define the finite-difference operators

$$\delta_x u_{m,n}^k = \frac{u_{m+1,n}^k - u_{m,n}^k}{\Delta x}, \quad \delta_y u_{m,n}^k = \frac{u_{m,n+1}^k - u_{m,n}^k}{\Delta y}, \quad \delta_t u_{m,n}^k = \frac{u_{m,n}^{k+1} - u_{m,n}^k}{\Delta t}.$$

Finite-difference scheme

$$\delta_t u^k_{m,n} = \delta_x(D(u^k_{m-1,n})\delta_x u^{k+1}_{m-1,n}) + \delta_y(D(u^k_{m,n-1})\delta_y u^{k+1}_{m,n-1}) + r^{k+1}_{m,n} u^k_{m,n},$$

$$\begin{cases} u^k_{m,0} - \lambda u^k_{m,1} = 0, & \forall m \in \mathbb{Z}_M, \\ u^k_{m,N} - \mu u^k_{m,N-1} = 0, & \forall m \in \mathbb{Z}_M, \\ u^k_{0,n} - \nu u^k_{1,n} = 0, & \forall n \in \overline{\mathbb{Z}}_N, \\ u^k_{M,n} - \xi u^k_{M-1,n} = 0, & \forall n \in \overline{\mathbb{Z}}_N, \\ u^k_{m,n} = \varphi(x_m, y_n), & \forall m \in \mathbb{Z}_M, \forall n \in \overline{\mathbb{Z}}_N. \end{cases}$$

where

- $\nabla \cdot (D(u)\nabla u) \approx \delta_x(D(u^k_{m-1,n})\delta_x u^{k+1}_{m-1,n}) + \delta_y(D(u^k_{m,n-1})\delta_y u^{k+1}_{m,n-1})$.
- $r(x_m, y_n, t_{k+1})u(x_m, y_n, t_{k+1}) \approx r^{k+1}_{m,n} u^k_{m,n}$, with $r^{k+1}_{m,n} = r(x_m, y_n, t_{k+1})$.

Boundary conditions

- λ, μ, ν, ξ refer to (x_m, a), (x_m, b), (c, y_n) and (d, y_n), respectively.
- Each constant $= 0$ in case of Dirichlet conditions, and $= 1$ in case of Neumann.

Nomenclature

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

$$\begin{aligned} \psi^k_{m,n,z} &= -R_z D(u^k_{m,n}), \quad z = x, y, \\ \phi^k_{m,n} &= 1 + (R_x + R_y)\, D(u^k_{m,n}) + R_x D(u^k_{m-1,n}) + R_y D(u^k_{m,n-1}), \\ \chi^k_{m,n} &= 1 + r^{k+1}_{m,n} \Delta t, \end{aligned}$$

where

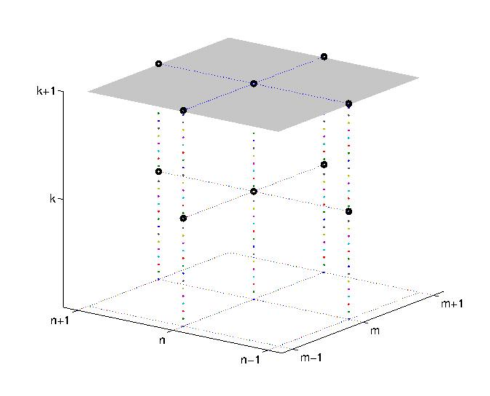
$$R_z = \frac{\Delta t}{(\Delta z)^2}.$$

Implicit representation

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

$$\begin{aligned} \psi^k_{m-1,n,x} u^{k+1}_{m-1,n} + \psi^k_{m,n-1,y} u^{k+1}_{m,n-1} + \phi^k_{m,n} u^{k+1}_{m,n} + \\ \psi^k_{m,n,y} u^{k+1}_{m,n+1} + \psi^k_{m,n,x} u^{k+1}_{m+1,n} &= \chi^k_{m,n} u^k_{m,n}. \end{aligned}$$

Stencil



Forward-difference stencil of the method around (x_m, y_n, t_k). The circles at time t_k are the known approximations, while those at time t_{k+1} are unknowns.

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Vector notation

- Let $\mathbf{u}^k$ be the vector of the approximate solution at the time t_k, namely, let

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

- 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

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

Let B^k be the matrix defined by blocks through

$$B^k = \left(\begin{array}{c|cccccc} 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ \hline 0 & \boxed{B_1^k} & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \boxed{B_2^k} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \boxed{B_{M-2}^k} & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \boxed{B_{M-1}^k} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 \end{array}\right).$$

Remarks

- B^k is a square matrix with $(M+1)(N+1)$ rows.
- Here, 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

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

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

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

$$A^{k+1} = \begin{pmatrix} I & -\nu I & 0 & 0 & \cdots & 0 & 0 & 0 \\ C_0^k & A_1^{k+1} & C_1^k & 0 & \cdots & 0 & 0 & 0 \\ 0 & C_1^k & A_2^{k+1} & C_2^k & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & C_{M-2}^k & A_{M-1}^{k+1} & C_{M-1}^k \\ 0 & 0 & 0 & 0 & \cdots & 0 & -\xi I & I \end{pmatrix}.$$

Method

The method is given by the recursive system of vector equations

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

- Here, $\mathbf{u}_0$ represents the vector of initial approximations.
- The vector equation is solved using the stabilized bi-conjugate gradient method.

Contents

By an *M-matrix* we mean a square, real matrix A which satisfies all of the following:

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.

Proposition

Every M-matrix is nonsingular, and all the entries of its inverse matrix are positive numbers. □

Definitions

- We say that $\mathbf{x} > 0$ if all its entries are positive numbers.
- We use the notation $\mathbf{x} < 1$ meaning that each of the components of this vector are less than 1. Evidently, $\mathbf{x} < 1$ if and only if $\mathbf{e} - \mathbf{x} > 0$, where $\mathbf{e} = (1, 1, \ldots, 1)$.
- The notation $0 < \mathbf{x} < 1$ represents the fact that $\mathbf{x} > 0$ and $\mathbf{x} < 1$.

Lemma

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

Proof.

Notice that the function D is positive in $(0, 1)$. Therefore, the off-diagonal elements of A^{k+1} are non-positive, and its diagonal elements are positive. The fact that this matrix is strictly diagonally dominant is immediate, also.

Proposition

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 $0 \geq \mathbf{u}^0 < 1$ and the inequality

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

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

Proof (positivity).

The conclusion is obviously true when $k = 0$. Suppose that $0 < \mathbf{u}^k < 1$, for some $k \in \overline{\mathbb{Z}}^+$. By the lemma, 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.

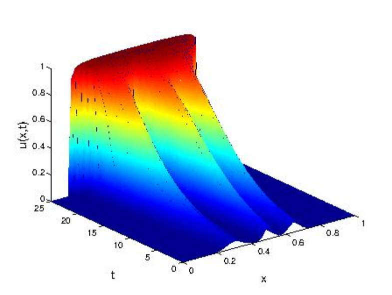
Proof (boundedness).

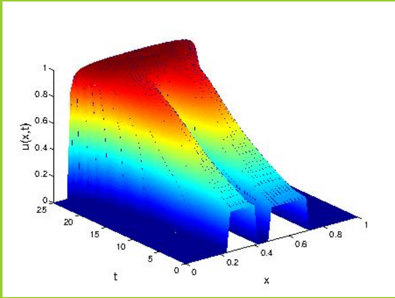
Let $\mathbf{w}^{k+1} = \mathbf{e} - \mathbf{u}^{k+1}$. A substitution in the vector form of the method yields

$$A^{k+1}\mathbf{w}^{k+1} = \mathbf{b}^{k+1},$$

where $\mathbf{b}^{k+1} = A^{k+1}\mathbf{e} - B^k \mathbf{u}^k$. The first and the last $N + 1$ rows of $\mathbf{b}^{k+1}$, 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 by hypothesis. 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.

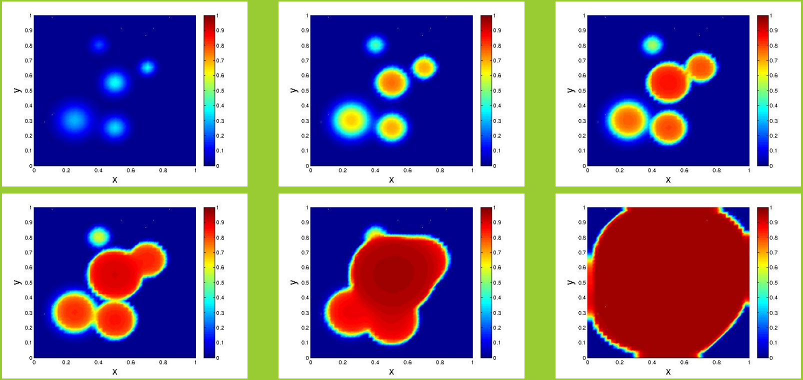
One-dimensional example





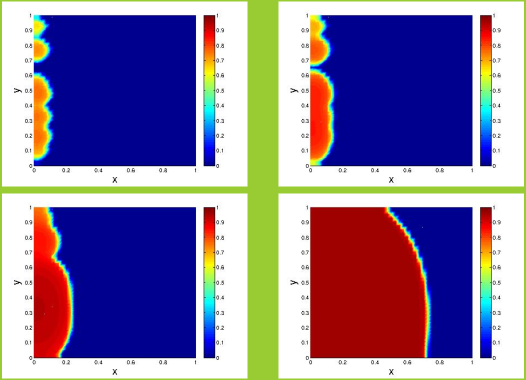
Two simulations of biofilm growth with $\delta = 1 \times 10^{-4}$, $\alpha = \beta = 2$, $r = 0.15$.
Computationally, $\Delta x = 0.005$, $\Delta t = 0.025$.

Two-dimensional example



Simulation of biofilm growth with $\delta = 1 \times 10^{-4}$, $\alpha = \beta = 2$, $r = 0.12$, at the times $t = 0, 8, 10, 11, 12, 13$. Computationally, $\Delta x = \Delta y = 0.025$, $\Delta t = 0.05$.

Two-dimensional example



Simulation of biofilm growth with $\delta = 1 \times 10^{-4}$, $\alpha = \beta = 2$, $r = 0.09$, at the times $t = 7, 9, 11, 13$. Computationally, $\Delta x = \Delta y = 0.025$, $\Delta t = 0.05$. The initial profile was nonzero at 10 random points (with random heights) on the left boundary.

A complex model

Contents

Nomenclature

- $\Omega \subset \mathbb{R}^n$ is open, bounded and connected.
- $\alpha, \beta \in \mathbb{R}$ such that $\alpha, \beta \geq 1$, and $d_1, d_2 \in \mathbb{R}$ satisfy $0 < d_1 \ll 1$ and $0 < d_2 \ll 1$. K_1, K_2, K_3 and K_4 are nonnegative constants.
- $D : [0, 1) \to \mathbb{R}$ is the function

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

Model

$u, s : \overline{\Omega} \times \mathbb{R}^+ \to \mathbb{R}$ are twice-differentiable functions satisfying

$$\begin{cases} \dfrac{\partial s}{\partial t}(\mathbf{x}, t) = d_1 \nabla^2 s(\mathbf{x}, t) - K_1 \dfrac{s(\mathbf{x}, t) u(\mathbf{x}, t)}{K_4 + s(\mathbf{x}, t)}, \\ \dfrac{\partial u}{\partial t}(\mathbf{x}, t) = d_2 \nabla \cdot (D(u(\mathbf{x}, t) \nabla u(\mathbf{x}, t)) - K_2 u + K_3 \dfrac{s(\mathbf{x}, t) u(\mathbf{x}, t)}{K_4 + s(\mathbf{x}, t)}. \\ s(\mathbf{x}, t) = 1, \ u(\mathbf{x}, t) = 0, \quad \forall \mathbf{x} \in \partial\Omega, \forall t \geq 0, \\ s(\mathbf{x}, 0) = s_0(\mathbf{x}), \ u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega, \end{cases}$$

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

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

Theorem

Let s_0 and u_0 satisfy the following conditions:

- $s_0 \in L^\infty(\Omega) \cap H^1(\Omega)$ and $0 \leq s_0(\mathbf{x}) \leq 1$ for every $\mathbf{x} \in \Omega$,
- $u_0 \in L^\infty(\Omega)$ and $F(u_o) \in H_0^1(\Omega)$,
- $u_0(\mathbf{x}) \geq 0$ for every $\mathbf{x} \in \Omega$, and $\|u_0\|_{L^\infty(\Omega)} < 1$.

Then, there exists a unique solution of our problem satisfying the following properties:

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

Dimensional restriction

We will restrict our attention to the $(2+1)$-dimensional case.

Nomenclature

- $\Omega = [a, b] \times [c, d] \subset \mathbb{R}^2$, for $a, b, c, d \in \mathbb{R}$ such that $a < b$ and $c < d$.
- Fix uniform partitions

$$\begin{aligned} a = x_0 < x_1 < \ldots < x_m < \ldots < x_M = b, \\ c = y_0 < y_1 < \ldots < y_n < \ldots < y_N = d. \end{aligned}$$

- Fix a uniform partition $0 = t_0 < t_1 < \ldots < t_k < \ldots$ of $[0, \infty)$.
- Let Δx, Δy and Δt be the respective step-sizes, let

$$\begin{aligned} u_{m,n}^k &\approx u(x_m, y_n, t_k), \\ s_{m,n}^k &\approx s(x_m, y_n, t_k). \end{aligned}$$

Nonstandard finite diferences

Define the operators

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

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

Numerical method

$$\begin{cases} \delta_t^{+} s_{m,n}^k = d_1(\delta_x^{(2)} + \delta_y^{(2)}) s_{m,n}^{k+1} - K_1 \dfrac{u_{m,n}^k s_{m,n}^{k+1}}{K_4 + s_{m,n}^k}, \\ \delta_t^{+} u_{m,n}^k = d_2(\epsilon_x + \epsilon_y) u_{m,n}^k - K_2 u_{m,n}^{k+1} + K_3 \dfrac{s_{m,n}^k u_{m,n}^{k+1}}{K_4 + s_{m,n}^k}, \\ s_{m,0}^k = s_{m,N}^k = s_{0,n}^k = s_{M,n}^k = 1, \\ u_{m,0}^k = u_{m,N}^k = u_{0,n}^k = u_{M,n}^k = 0, \\ s_{m,n}^0 = s_0(x_m, y_n), \; u_{m,n}^0 = u_0(x_m, y_n). \end{cases}$$

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

$$\begin{aligned}
\phi_{m,n}^k &= 1 + 2R_x^{(1)} + 2R_y^{(1)} + K_1 \Delta t \frac{u_{m,n}^k}{K_4 + s_{m,n}^k}, \\
\psi_{m,n,z}^{k,\pm} &= R_z^{(2)} D(\mu_z^{\pm} u_{m,n}^k), \\
\chi_{m,n}^k &= 1 + \sum_{z=x,y} \left(\psi_{m,n,z}^{k,+} + \psi_{m,n,z}^{k,-} \right) + K_2 \Delta t - K_3 \Delta t \frac{s_{m,n}^k}{K_4 + s_{m,n}^k}, \\
R_z^{(i)} &= d_i \frac{\Delta t}{(\Delta z)^2}, \quad i \in \{1, 2\}, z = x, y.
\end{aligned}$$

Implicit representation

$$\begin{cases}
-R_x^{(1)} s_{m-1,n}^{k+1} - R_y^{(1)} s_{m,n-1}^{k+1} + \phi_{m,n}^k s_{m,n}^{k+1} - R_y^{(1)} s_{m,n+1}^{k+1} - R_x^{(1)} s_{m+1,n}^{k+1} = s_{m,n}^{k+1}, \\
\psi_{m-1,n,x}^k u_{m-1,n}^{k+1} + \psi_{m,n-1,y}^k u_{m,n-1}^{k+1} + \phi_{m,n}^k u_{m,n}^{k+1} + \\
\quad \psi_{m,n,y}^k u_{m,n+1}^{k+1} + \psi_{m,n,x}^k u_{m+1,n}^{k+1} = \chi_{m,n}^k u_{m,n}^k.
\end{cases}$$

Contents

Vector notation

- Let $\mathbf{v}^k$ be the juxtaposition of the vectors

$$\begin{aligned}\mathbf{s}^k &= (s^k_{0,0}, s^k_{0,1}, \ldots, s^k_{0,N}, s^k_{1,0}, s^k_{1,1}, \ldots, s^k_{1,N}, \ldots, s^k_{M,0}, s^k_{M,1}, \ldots, s^k_{M,N}), \\ \mathbf{u}^k &= (u^k_{0,0}, u^k_{0,1}, \ldots, u^k_{0,N}, u^k_{1,0}, u^k_{1,1}, \ldots, u^k_{1,N}, \ldots, u^k_{M,0}, u^k_{M,1}, \ldots, u^k_{M,N}).\end{aligned}$$

- Similarly, let $\mathbf{v}^k_0$ be the juxtaposition of

$$\begin{aligned}\mathbf{t}^k &= (\underbrace{1, 1, \ldots, 1}_{N+1 \text{ entries}}, \underbrace{1, s^k_{1,1}, \ldots, s^k_{1,N-1}, 1}_{N+1 \text{ entries}}, \ldots \\ &\qquad \ldots, \underbrace{1, s^k_{M-1,1}, \ldots, s^k_{M-1,N-1}, 1}_{N+1 \text{ entries}}, \underbrace{1, 1, \ldots, 1}_{N+1 \text{ entries}}) \\ \mathbf{w}^k &= (\underbrace{0, 0, \ldots, 0}_{N+1 \text{ entries}}, \underbrace{0, u^k_{1,1}, \ldots, u^k_{1,N-1}, 0}_{N+1 \text{ entries}}, \ldots \\ &\qquad \ldots, \underbrace{0, u^k_{M-1,1}, \ldots, u^k_{M-1,N-1}, 0}_{N+1 \text{ entries}}, \underbrace{0, 0, \ldots, 0}_{N+1 \text{ entries}}).\end{aligned}$$

Let I represent 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

$$C = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -R_x^{(1)} & 0 & \cdots & 0 & 0 \\ 0 & 0 & -R_x^{(1)} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -R_x^{(1)} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

$$E_m^k = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -R_y^{(1)} & \phi_{m,1}^k & -R_y^{(1)} & 0 & \cdots & 0 & 0 & 0 \\ 0 & -R_y^{(1)} & \phi_{m,2}^k & -R_y^{(1)} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -R_y^{(1)} & \phi_{m,N-1}^k & -R_y^{(1)} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix}.$$

Define next the square matrix A^k as the block matrix given by

$$A^k = \left(\begin{array}{c|ccccccc} I & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ \hline C & E_1^k & C & 0 & \cdots & 0 & 0 & 0 \\ \hline 0 & C & E_2^k & C & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & C & E_{M-1}^k & C \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & I \end{array}\right).$$

Remarks

Let $k \in \{0, 1, \ldots, K\}$.

1. The off-diagonal elements of A^k are non-positive numbers: 0, $-R_x^{(1)}$ or $-R_y^{(1)}$.
2. If all the numbers $u_{m,n}^k$ and $s_{m,n}^k$ are non-negative, then the diagonal entries of A^k are either equal to 1 or equal to some $\phi_{m,n}^k$. In either case, the entry is positive.
3. A^k is strictly diagonally dominant when 2 above is satisfied.

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

$$F_{m,z}^{k,\pm} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\psi_{m,1,z}^{k,\pm} & 0 & \cdots & 0 & 0 \\ 0 & 0 & -\psi_{m,2,z}^{k,\pm} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -\psi_{m,N-1,z}^{k,\pm} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

$$G_m^k = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -\psi_{m,1,y}^{k,-} & \chi_{m,1}^k & -\psi_{m,1,y}^{k,+} & \cdots & 0 & 0 \\ 0 & -\psi_{m,2,y}^{k,-} & \chi_{m,2}^k & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \chi_{m,N-1}^k & -\psi_{m,N-1,y}^{k,+} \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}.$$

Define next the square matrix B^k as the block matrix given by

$$B^k = \begin{pmatrix} I & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ F_{1,x}^{k,-} & G_1^k & F_{1,x}^{k,+} & 0 & \cdots & 0 & 0 & 0 \\ 0 & F_{2,x}^{k,-} & G_2^k & F_{2,x}^{k,+} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & F_{M-1,x}^{k,-} & G_{M-1}^k & F_{M-1,x}^{k,+} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & I \end{pmatrix}.$$

Remarks

1. The off-diagonal entries of B^k are non-positive, being $-\psi_{m,n,z}^{k,\pm}$ for $z = x, y$, or 0.
2. Let $K_3 \Delta t < 1 + K_2 \Delta t$. The diagonal entries of B^k are 1 or equal to some
$$\chi_{m,n}^k \geq 1 + K_2 \Delta t - K_3 \Delta t \frac{s_{m,n}^k}{K_4 + s_{m,n}^k} \geq 1 + K_2 \Delta t - K_3 \Delta t > 0.$$
3. Finally, if the hypothesis of 2 holds then B^k is strictly diagonally dominant.

Define the block matrix M^k of size $[2(M+1)(N+1)] \times [2(M+1)(N+1)]$ through

$$M^k = \left(\begin{array}{c|c} A^k & 0 \\ \hline 0 & B^k \end{array} \right),$$

where the zeros represent zero matrices of sizes $(M+1)(N+1) \times (M+1)(N+1)$.

Method

The method is given by the recursive system of vector equations

$$M^k \mathbf{v}^{k+1} = \mathbf{v}_0^k,$$

- Here, $\mathbf{v}^0$ is just the vector of discrete, initial conditions.
- The technique proposed in this work is clearly implicit and linear.
- The vector equation is solved using the stabilized bi-conjugate gradient method.

Contents

By an *M-matrix* we mean a square, real matrix A which satisfies all of the following:

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.

Proposition

Every M-matrix is nonsingular, and all the entries of its inverse matrix are positive numbers. □

Definitions

- We say that $\mathbf{x} > 0$ (resp. $\mathbf{x} \geq 0$) if all its entries are positive (resp. non-negative) numbers.
- We use the notation $\mathbf{x} < 1$ (resp. $\mathbf{x} \leq 1$) meaning that each of the components of this vector are less than (resp. less than or equal to) 1.
- The notation $0 < \mathbf{x} < 1$ represents the fact that $\mathbf{x} > 0$ and $\mathbf{x} < 1$. Other statements involving the other inequality symbols have analogous meanings.

Lemma

Let $k \in \{0, 1, \ldots, K\}$ and $\mathbf{v}^k \geq 0$. If $K_3 \Delta t < 1 + K_2 \Delta t$ then M^k is an M-matrix. □

Proposition

Let $\mathbf{s}^0 \geq 0$ and $0 \leq \mathbf{u}^0 < 1$. If $K_3 \Delta t < 1 + K_2 \Delta t$ then $\mathbf{v}^k \geq 0$, for every $k \geq 0$. Moreover, every $\mathbf{v}^k$ is positive if $\mathbf{v}^0 > 0$.

Proof.

The vector $\mathbf{v}^0$ is non-negative by hypotheses. Suppose that $\mathbf{v}^k$ is also non-negative for some $k \in \{0, 1, \ldots, K-1\}$. The lemma guarantees that M^k is an M-matrix, so all the entries of its inverse are positive numbers. Observe also that $\mathbf{v}^k$ inherits the non-negativity to $\mathbf{v}_0^k$, whence we conclude that $\mathbf{v}^{k+1} = (M^k)^{-1} \mathbf{v}_0^k$ is a non-negative vector. The last statement of the proposition is analogous.

Proposition

Let $0 \leq \mathbf{v}^k \leq 1$ for some $k \in \{0, 1, \ldots, K-1\}$. If $1 + K_2\Delta t - K_3\Delta t - u^k_{m,n} > 0$ holds for every $m \in \{1, \ldots, M-1\}$ and $n \in \{1, \ldots, N-1\}$, then $0 \leq \mathbf{v}^{k+1} \leq 1$.

Proof.

Observe firstly that $K_3\Delta t < 1 + K_2\Delta t$ is satisfied under these hypotheses. Define

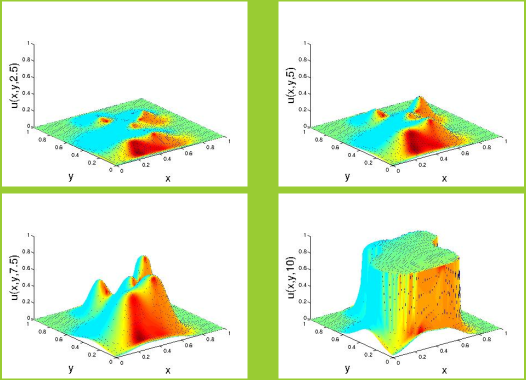
$$\mathbf{x}^{k+1} = \mathbf{e} - \mathbf{v}^{k+1},$$

where $\mathbf{e}$ is the vector of the same dimension as $\mathbf{v}^{k+1}$, all of whose components are equal to 1. In terms of $\mathbf{x}$, our method is rewritten as $M^k\mathbf{x}^{k+1} = \mathbf{b}^k$, where

$$\mathbf{b}^k = M^k\mathbf{e} - \mathbf{v}^k_0.$$

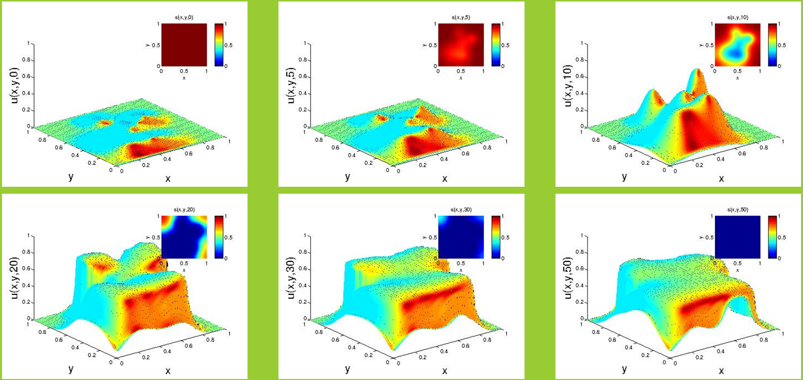
The conditions in the hypothesis guarantee that the vector $\mathbf{b}^k$ is non-negative. So, $\mathbf{x}^{k+1}$ is also non-negative or, equivalently, $\mathbf{v}^{k+1} \leq 1$. □

Constant substrate



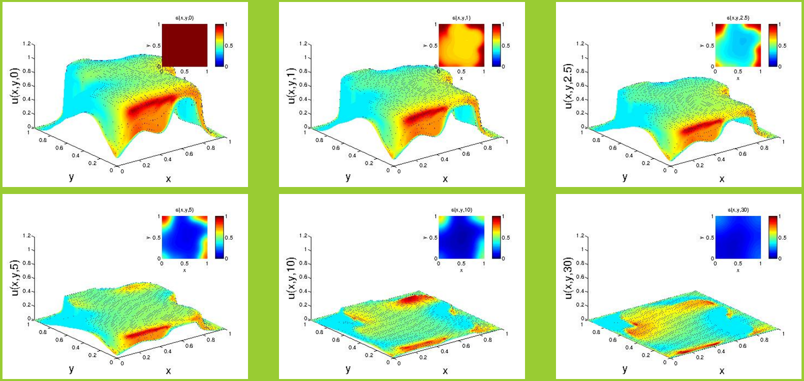
Simulation of biofilm growth with $\Omega = [0, 1] \times [0, 1]$, $d_1 = K_1 = K_2 = K_4 = 0$, $d_2 = 0.0001$, $K_3 = 0.4$, $\alpha = \beta = 4$; $\Delta x = \Delta y = 0.02$ and $\Delta t = 0.01$.

Variable substrate



Simulation of biofilm growth with $\Omega = [0, 1] \times [0, 1]$, $d_1 = 0.002$, $d_2 = 0.0001$, $K_1 = 0.85$, $K_2 = 0.0012$, $K_3 = 0.4$, $K_4 = 0.3$, $\alpha = \beta = 4$; $\Delta x = \Delta y = 0.02$ and $\Delta t = 0.01$.

Variable substrate



Simulation of biofilm growth with $\Omega = [0,1] \times [0,1]$, $d_1 = 0.0015$, $d_2 = 0.0001$, $K_1 = 0.65$, $K_2 = 0.36$, $K_3 = 0.2$, $K_4 = 0.3$, $\alpha = \beta = 4$; $\Delta x = \Delta y = 0.02$ and $\Delta t = 0.01$.

A nonlinear model

Contents

Problem

$$\begin{cases} \dfrac{\partial u}{\partial t} - \alpha u^p \dfrac{\partial u}{\partial x} - \dfrac{\partial^2 u}{\partial x^2} - f(u) = 0, \\ u(x,0) = u_0(x), \end{cases}$$

where

$$f(u) = u(1 - u^p).$$

Nomenclature

- $u : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$ is twice differentiable, and $u = u(x,t)$.
- Physically, x represents position and t denotes time.
- $\alpha \in \mathbb{R}$ is the advection/convection coefficient.
- $p \in \mathbb{R}$ satisfies $p \geq 1$.

The following are known exact solutions.

Burgers-Fisher

$$u(x,t) = \left(\frac{1}{2} + \frac{1}{2}\tanh\left[\frac{-\alpha p}{2(p+1)}\left(x - \left(\frac{\alpha}{p+1} + \frac{p+1}{\alpha}\right)t\right)\right]\right)^{1/p}.$$

Burgers-Fisher with $p = 2$, and $\alpha = 0$ (Newell-Whitehead-Segel)

$$u(x,t) = \frac{C_1 \exp(\frac{1}{\sqrt{2}}x) - C_2 \exp(-\frac{1}{\sqrt{2}}x)}{C_1 \exp(\frac{1}{\sqrt{2}}x) + C_2 \exp(-\frac{1}{\sqrt{2}}x) + C_3 \exp(-\frac{3}{2}t)}, \quad C_1, C_2, C_3 \in \mathbb{R}.$$

Remarks

- The first solutions is a traveling-wave front connecting $u = 0$ and $u = 1$.
- There are existence-and-uniqueness theorems that guarantee the the presence of traveling-wave solutions, but very few solutions known in exact form.

Conventions

- Fix a spatial domain $D = [a, b] \subset \mathbb{R}$.
- Fix uniform partitions and partition norms:

$$\begin{aligned} a = x_0 < x_1 < \ldots < x_N = b, &\quad \Delta x = (b-a)/N. \\ 0 = t_0 < t_1 < \ldots < t_k < \ldots < \infty, &\quad \Delta t > 0. \end{aligned}$$

- Let u_n^k represent an approximation to $u(x_n, t_k)$.

Define the linear operators

$$\delta_t u_n^k = \frac{u_n^{k+1} - u_n^k}{\Delta t}.$$

$$\delta_x^{(1)} u_n^k = \frac{u_{n+1}^k - u_{n-1}^k}{2\Delta x}.$$

$$\delta_x^{(2)} u_n^k = \frac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{(\Delta x)^2}.$$

Orders of consistency

- $u_t = \delta_t u_n^k + \mathcal{O}(\Delta t)$.
- $u_x = \delta_x^{(1)} u_n^k + \mathcal{O}((\Delta x)^2)$.
- $u_{xx} = \delta_x^{(2)} u_n^k + \mathcal{O}((\Delta x)^2)$.

Finite-difference scheme

$$\delta_t u_n^k - \alpha (u_n^{k+1})^p \delta_x^{(1)} u_n^k - \delta_x^{(2)} u_n^k - f(u_n^{k+1}) = 0, \quad \forall n \in \{1, \ldots, N-1\},$$
$$\text{such that} \begin{cases} u_n^0 = u_0(x_n), & \forall n \in \{1, \ldots, N-1\}, \\ u_0^k = \phi(t_k), & \forall k \in \mathbb{Z}^+, \\ u_N^k = \psi(t_k), & \forall k \in \mathbb{Z}^+. \end{cases}$$

- u_0 is the exact solution at $t = 0$.
- $\phi, \psi : [0, \infty) \to \mathbb{R}$ are the Dirichlet boundary conditions on D (exact solution for us).

Contents

Conventions

- The kth approximation is denoted by $\mathbf{u}^k = (u_0^k, u_1^k, \ldots, u_N^k)$.
- Introduce the constants $r = 0.5\Delta t/\Delta x$ and $R = \Delta t/(\Delta x)^2$.
- Let

$$\begin{aligned} a_n^k &= \alpha r(u_{n+1}^k - u_{n-1}^k), \\ b_n^k &= R u_{n+1}^k + (1-2R)u_n^k + R u_{n-1}^k. \end{aligned}$$

Equivalent formulation

The method may be rewritten as $F_{n,k}(u_n^{k+1}) = 0$ for every n and k, where

$$F_{n,k}(u) = (\Delta t)u^{p+1} - a_n^k u^p + (1-\Delta t)u - b_n^k.$$

Note: Thus, u_n^{k+1} represents geometrically a root of the function $F_{n,k}$.

Lemma

Suppose that $2R < 1$.

(A) If $\mathbf{u}^k$ is positive, then $F_{n,k}(0) < 0$ for every n.

(B) If $|\alpha|r < R$ and $\mathbf{u}^k < 1$, then $F_{n,k}(1) > 0$, for every n.

(C) If p is even, $|\alpha|r < R$ and $\mathbf{u}^k > -1$, then $F_{n,k}(-1) < 0$, for every n.

Proof.

Observe that $|\alpha|r < R$ if and only if $R + \alpha r > 0$ and $R - \alpha r > 0$.

(A) The conclusion follows from the facts that b_n^k is positive and $F_{n,k}(0) = -b_n^k$.

(B) After some calculations and using the fact that $\mathbf{u}^k < 1$, we obtain that $F_{n,k}(1) = 1 - (R + \alpha r)u_{n+1}^k - (1 - 2R)u_n^k - (R - \alpha r)u_{n-1}^k > 0$.

(C) In this case, $F_{n,k}(-1) = -1 - (R + \alpha r)u_{n+1}^k - (1 - 2R)u_n^k - (R - \alpha r)u_{n-1}^k$, which is negative. □

Lemma

Suppose that $2R < 1$ and $|\alpha| r < R$.

(A) If $0 < \mathbf{u}^k < 1$, then $F_{n,k}$ has a root in $(0, 1)$, for every n.

(B) If p is an even number and $-1 < \mathbf{u}^k < 1$, then $F_{n,k}$ has a root in $(-1, 1)$, for every n.

Proof.

The proof is an immediate consequence of the continuity of each of the functions $F_{n,k}$, the Intermediate Value Theorem and the previous lemma. □

Remark

This result proposes conditions under which $\mathbf{u}^{k+1}$ will be bounded within $(0, 1)$ or within $(-1, 1)$ when $\mathbf{u}^k$ is bounded within the same interval.

Proposition

Suppose $2R < 1$, and $|\alpha| r < R$.

(A) Let $0 < \mathbf{u}^0 < 1$. For every k, if $u_0^k, u_N^k \in (0, 1)$ then $0 < \mathbf{u}^k < 1$.

(B) Let p be an even number and $-1 < \mathbf{u}^k < 1$. For every k, if $u_0^k, u_N^k \in (-1, 1)$ then $-1 < \mathbf{u}^k < 1$.

Proof.

The proof is immediate. □

Remarks

- The condition $|\alpha| r < R$ holds if and only if $|\alpha| \Delta x < 2$.
- The conditions of the proposition assure that each $F_{n,k}$ has roots within $(0, 1)$ and $(-1, 1)$; however, they do not guarantee the uniqueness.
- To show uniqueness, it is enough to guarantee that each $F_{n,k}$ is increasing. □

Lemma

(A) If $\mathbf{u}^k \in (0,1)$ and $\Delta t + |\alpha| rp < 1$, then $F_{n,k}$ is increasing in $(0,1)$.

(B) If p is even, $\mathbf{u}^k \in (-1,1)$, $\Delta t + 2|\alpha| rp < 1$, then $F_{n,k}$ is increasing in $(-1,1)$.

Proof.

Suppose (A) or (B). Then $F'_{n,k}(u) \geq -|\alpha||u^k_{n+1} - u^k_{n-1}|rp + 1 - \Delta t$.
(A) $F'_{n,k}(u) \geq -|\alpha|rp + 1 - \Delta t > 0$, for every $u \in (0,1)$.
(B) $F'_{n,k}(u) \geq -2|\alpha|rp + 1 - \Delta t > 0$, for each $u \in (-1,1)$. □

Proposition

Let $2R < 1$, and $|\alpha| r < R$.

(A) Let $0 < \mathbf{u}^0 < 1$, $\Delta t + |\alpha| rp < 1$, and $u^k_0, u^k_N \in (0,1)$. There exists a unique sequence $\{\mathbf{u}^k\}_{k=0}^{\infty}$ bounded within $(0,1)$.

(B) Let p be even, $-1 < \mathbf{u}^0 < 1$ and $\Delta t + 2|\alpha| rp < 1$. Suppose that $u^k_0, u^k_N \in (-1,1)$. There exists a unique $\{\mathbf{u}^k\}_{k=0}^{\infty}$ bounded within $(-1,1)$. □

Contents

A method is *monotonicity-preserving* if for data $\mathbf{u}^0 < \mathbf{v}^0$, then $\mathbf{u}^k < \mathbf{v}^k$ for every k.

Lemma

Let $2R < 1$ and $|\alpha| r < R$. The method is monotonicity-preserving if either

(A) $\mathbf{u}^0$ and the boundary data lie within $I = (0, 1)$ and $\Delta t + |\alpha| rp < 1$, or

(B) $\mathbf{u}^0$ and the boundary data lie within $I = (-1, 1)$, p is even and $\Delta t + 2|\alpha| rp < 1$.

Proof.

By proposition, $\{\mathbf{u}^k\}_{k=0}^{\infty}, \{\mathbf{v}^k\}_{k=0}^{\infty} \subset I$. Let $\mathbf{u}^k < \mathbf{v}^k$ and let $w_n^k = v_n^k - u_n^k \in \mathbb{R}^+$. Let

$$c_n^k = \alpha r (v_{n+1}^k - v_{n-1}^k), \quad d_n^k = R v_{n+1}^k + (1 - 2R) v_n^k + R v_{n-1}^k.$$

Each v_n^{k+1} is the root of $G_{n,k}(v) = (\Delta t) v^{p+1} - c_n^k v^p + (1 - \Delta t) v - d_n^k$ in I. Let $H_{n,k} : I \to \mathbb{R}$ be given by $H_{n,k} = G_{n,k} - F_{n,k}$. It is readily checked that

$$H_{n,k}(w) = -(R + \alpha r w^p) w_{n+1}^k - (1 - 2R) w_n^k - (R - \alpha r w^p) w_{n-1}^k < 0,$$

for every $w \in I$. So $G_{n,k} < F_{n,k}$ over I, whence $u_n^{k+1} < v_n^{k+1}$ follows.

A method is *temporally increasing* (resp. *decreasing*) if $\mathbf{u}^k < \mathbf{u}^{k+1}$ (resp. $\mathbf{u}^k > \mathbf{u}^{k+1}$) is satisfied for every k whenever $\mathbf{u}^0 < \mathbf{u}^1$ (resp. $\mathbf{u}^0 > \mathbf{u}^1$)holds. A method which is temporally increasing and decreasing is *temporally monotone*.

Proposition

Let $2R < 1$, and $|\alpha|r < R$. The method is temporally monotone if either

(A) the initial and boundary conditions lie within $I = (0, 1)$ and $\Delta t + |\alpha|rp < 1$, or

(B) the initial and boundary conditions lie within $I = (-1, 1)$, p is an even integer and $\Delta t + 2|\alpha|rp < 1$.

Proof.

Suppose that $\mathbf{u}^0 < \mathbf{u}^1$ belong to I, and that the numbers $u_0^k, u_0^{k+1}, u_N^k, u_N^{k+1} \in I$ satisfy the inequalities $u_0^k < u_0^{k+1}$ y $u_N^k < u_N^{k+1}$, for each k. If we let $\mathbf{v}^k = \mathbf{u}^{k+1}$ for each k, the previous lemma implies that $\mathbf{u}^k < \mathbf{v}^k$ for each k. It follows that the method is temporally increasing. The fact that the method is temporally decreasing is proved analogously.

A vector $\mathbf{x} = (x_0, x_1, \ldots, x_N)$ is *spatially increasing* (resp. *decreasing*) when $x_n < x_{n+1}$ (resp. $x_n > x_{n+1}$) is satisfied for every n. A method is *spatially increasing* (resp. *decreasing*) if, for every spatially increasing (resp. decreasing) initial profile, the successive approximations are spatially increasing (resp. decreasing). A spatially increasing and decreasing method is called *spatially monotone*.

Proposition

Let $2R < 1$, and $|\alpha| r < R$. The method is spatially monotone if either

(A) the initial and boundary data lie within $I = (0,1)$ and $\Delta t + |\alpha| rp < 1$, or

(B) the initial and boundary data lie within $I = (-1,1)$, p is even and $\Delta t + 2|\alpha| rp < 1$.

Proof.

Let $\mathbf{u}^0$ be spatially increasing, and suppose that $u_0^k < u_1^k < u_{N-1}^k < u_N^k$, for every k. Let $\mathbf{v}^k = (u_0^k, u_1^k, \ldots, u_{N-1}^k)$ and $\mathbf{w}^k = (u_1^k, u_2^k, \ldots, u_N^k)$. Evidently, $\mathbf{v}^0 < \mathbf{w}^0$, and $v_0^k < w_0^k$ and $v_{N-1}^k < w_{N-1}^k$ hold for every k. We conclude by the lemma that $\mathbf{v}^k < \mathbf{w}^k$, for every k. Equivalently, each vector $\mathbf{u}^k$ is spatially increasing.

The following is a discrete form of the well-known Gronwall's inequality.

Lemma

Let $K > 1$, and suppose that A, B and C_k are nonnegative constants for each $k \in \{0, 1, \ldots, K\}$. If $(A + B)\Delta t \leq \frac{K-1}{2K}$ and if $\{w^k\}_{k=0}^{K}$ satisfies $w^k - w^{k-1} \leq A\Delta t w^k + B\Delta t w^{k-1} + C_k \Delta t$, for each $k = 1, \ldots, K$ then

$$\max_{1 \leq k \leq K} \left| w^k \right| \leq \left(w^0 + \Delta t \sum_{l=1}^{K} C_l \right) e^{2(A+B)T}.$$

We define now the vectors

$$\begin{aligned} \mathbf{z}^k &= (z_0^k, z_1^k, \ldots, z_K^k), \\ \mathbf{u}^k &= (u_0^k, u_1^k, \ldots, u_K^k), \end{aligned}$$

for each $k = 0, 1, \ldots, K$. Here, for every $n \in \{0, 1, \ldots, N\}$, we let $u_n^k = u(x_n, t_k)$, and z_n^k is the corresponding numerical approximation.

Proposition

Suppose that the following inequalities hold:

(C$_1$) $\Delta t - 2\dfrac{\Delta t}{(\Delta x)^2} < 1$,

(C$_2$) $\dfrac{1}{2\Delta x}|\alpha| < \dfrac{\Delta t}{(\Delta x)^2}$,

(C$_3$) $p\left(|\alpha|\dfrac{\Delta t}{2\Delta x}\right) < 1$.

Assume that the function $u \in C^{4,2}_{x,t}([a,b] \times [0,T])$ is a positive solution of the continuous problem such that $\|u\|_\infty < 1$. Then there exists a constant $\widetilde{C} \in \mathbb{R}^+$ which is independent of Δt and Δx, and there exists exactly one solution z of the finite-difference method which converges to u, and that satisfies

$$\max_{0 \le k \le K} \left\| \mathbf{u}^k - \mathbf{z}^k \right\|_\infty \le \widetilde{C}(\Delta t + (\Delta x)^2).$$

Feasibility of conditions

- The first and third conditions of the proposition may be equivalently restated as the inequalities

  (C'_1) $\left(1 - \frac{2}{(\Delta x)^2}\right) \Delta t < 1,$

  (C'_3) $p \left(\frac{|\alpha|}{2\Delta x}\right) \Delta t < 1$

  respectively, which are satisfied for sufficiently small values of Δt.
- The second condition of our main result is equivalent to the inequality

  (C'_2) $\frac{1}{2}|\alpha|\Delta x < \Delta t,$

  which is valid for sufficiently small values of the computational parameter Δx.

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M. A. Efendiev, H. J. Eberl, and S. V. Zelik,
Existence and longtime behavior of solutions of a nonlinear reaction-diffusion system arising in the modeling of biofilms.
RIMS Kokyuroko, **1258**:49–71, 2002.

H. J. Eberl, D. F. Parker, and M. C. M. van Loosdrecht,
A new deterministic spatiotemporal continuum model for biofilm development.
Comput. Math. Meth. Med. **3**:161–175, 2001.

J. E. Macías-Díaz *et al.*,
An efficient recursive algorithm in the computational simulation of the bounded growth of biological films.
Intern. J. Comput. Meth., **09**:1250050, 2012.

J. E. Macías-Díaz *et al.*,
A finite-difference scheme in the computational modeling of a coupled substrate-biomass system.
Intern. J. Comput. Math., in press, 2014.

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