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FINITE DIFFERENCE SCHEMES FOR A GENERALIZED CALCIUM DIFFUSION EQUATION

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Abstract. Finite difference schemes are considered for a Ca^{2+} diffusion equations with damping and convection terms, which describe Ca^{2+} buffering by using stationary and mobile buffers. Stability and L^{∞} error estimates of approximate solutions for the corresponding schemes are obtained using the extended Lax-Richtmyer equivalence theorem.

1. Introduction

Consider the Ca^{2+} diffusion equation in cells

$$
\begin{aligned}
\frac{\partial [Ca^{2+}]}{\partial t} &= D_{Ca}\frac{\partial^2 [Ca^{2+}]}{\partial x^2} - k_s^+[Ca^{2+}][B_s] + k_s^-[CaB_s] - k_m^+[Ca^{2+}][B_m] \\
&\quad + k_m^-[CaB_m] - \alpha_{Ca}[Ca^{2+}] - \beta_{Ca}\frac{\partial [Ca^{2+}]}{\partial x}, \\
\frac{\partial [B_m]}{\partial t} &= D_{B_m}\frac{\partial^2 [B_m]}{\partial x^2} - k_m^+[Ca^{2+}][B_m] + k_m^-[CaB_m] \\
&\quad - \alpha_{B_m}[B_m] - \beta_{B_m}\frac{\partial [B_m]}{\partial x}, \\
\frac{\partial [CaB_m]}{\partial t} &= D_{CaB_m}\frac{\partial^2 [CaB_m]}{\partial x^2} + k_m^+[Ca^{2+}][B_m] - k_m^-[CaB_m] \\
&\quad - \alpha_{CaB_m}[CaB_m] - \beta_{CaB_m}\frac{\partial [CaB_m]}{\partial x}, \\
\frac{\partial [CaB_s]}{\partial t} &= k_s^+[Ca^{2+}][B_s] - k_s^-[CaB_s], \\
[B_s] &= [B_s]_{tot} - [CaB_s], \quad x \in \Omega = (0,\ell),\ 0 < t \le T
\end{aligned} \tag{1}
$$

with initial conditions

$$
\begin{aligned}
(x,0) &= [Ca^{2+}]_0(x), \qquad [B_m](x,0) = [B_m]_0(x), \\
[CaB_m](x,0) &= [CaB_m]_0(x), \qquad [CaB_s](x,0) = [CaB_s]_0(x)
\end{aligned} \tag{2}
$$

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and boundary conditions

$$\frac{\partial u}{\partial x}(x,t) = 0, \quad x \in \{0, \ell\},\ t \in (0, T] \tag{3}$$

where $\alpha_i, \beta_i (i = Ca, B_m, CaB_m, CaB_s)$, $[\mathrm{Ca}^{2+}]$, $[\mathrm{B}_s]$, $[\mathrm{B}_m]$, $[\mathrm{CaB}_i]$ are damping term, convection term, concentrations of free Calcium ion, stationary and mobile buffers, and Ca^{2+} bounded to a buffer site ([1], [11]), respectively, and u is $[Ca^{2+}]$,$[B_m]$, $[CaB_m]$ or $[CaB_s]$. The total concentration of the stationary buffer $[B_s]_{tot}$ is constant, and D, k^+, k_- are diffusion, association, and dissociation constants, respectively and all constants are positive.

Studies on Calcium dynamics belong to the area of electrophysiology, in which almost all systems are described by ordinary differential equations ([2], [6]–[8]]) but recently some systems are modeled by partial differential equations having temporal and spatial terms ([5], [10], [12]). In the case of $\alpha_i = \beta_i = 0$, Wagner and Keizer [13] have described the Ca^{2+} buffering as the partial differential equations (1)–(3) without explicit initial and boundary conditions. There is no numerical analysis of the equations with damping and convection terms. Following the finite difference approaches in [3]–[4], we can analysis numerical schemes for the generalized Ca^{2+} buffering model.

In this paper, we consider estimates of approximate solutions for finite difference methods. In Section 2, we introduce the finite difference schemes for (1)–(3) and some lemmas necessary to obtain error estimates. In Section 3, we briefly recall the Lax-Richtmyer equivalence theorem [9] and obtain stability and error estimates for the equation by following the approaches in [3]–[4].

2. Finite difference schemes

Let $h = \ell/M$ be the uniform step size in the spatial direction for a positive integer $\mathcal{M}$ and $\Omega_h = \{x_i = ih | i = -1, 0, \cdots, \mathcal{M}, \mathcal{M}+1\}$. Let $k = T/N$ denote the uniform step size in the temporal direction for a positive integer N. Denote $V_i^n = V(x_i, t_n)$ for $t_n = nk, n = 0, 1, \cdots, N$. For a function V^n defined on Ω_h, define the difference operators as for $0 \le i \le \mathcal{M}$,

$$\nabla_+ V_i^n = \big(V_{i+1}^n - V_i^n\big)/h, \quad \nabla_- V_i^n = \nabla_+ V_{i-1}^n, \quad \nabla^2 V_i^n = \nabla_+(\nabla_- V_i^n).$$

Further, define operators $V^{n+\frac{1}{2}}$ and $\partial_t V^n$ as

$$V_i^{n+\frac{1}{2}} = \big(V_i^{n+1} + V_i^n\big)/2 \quad \text{and} \quad \partial_t V_i^n = \big(V_i^{n+1} - V_i^n\big)/k.$$

Then the approximate solutions $[C]_i^{n+1}, [M]_i^{n+1}, [CM]_i^{n+1}, [CS]_i^{n+1} (0 \le i \le \mathcal{M}, 0 \le n \le N-1)$ for (1)–(3) are defined as solutions of

$$
\begin{aligned}
\partial_t[C]_i^n &= D_1\nabla^2[C]_i^{n+\frac12} - k_s^+[C]_i^{n+\frac12}[S]_i^{n+\frac12} + k_s^-[CS]_i^{n+\frac12} \\
&\quad - k_m^+[C]_i^{n+\frac12}[M]_i^{n+\frac12} + k_m^-[CM]_i^{n+\frac12} - \alpha_1[C]_i^{n+\frac12} - \beta_1\bar{\nabla}[C]_i^{n+\frac12}, \\
\partial_t[M]_i^n &= D_2\nabla^2[M]_i^{n+\frac12} - k_m^+[C]_i^{n+\frac12}[M]_i^{n+\frac12} + k_m^-[CM]_i^{n+\frac12} \\
&\quad - \alpha_2[M]_i^{n+\frac12} - \beta_2\bar{\nabla}[M]_i^{n+\frac12}, \\
\partial_t[CM]_i^n &= D_3\nabla^2[CM]_i^{n+\frac12} + k_m^+[C]_i^{n+\frac12}[M]_i^{n+\frac12} - k_m^-[CM]_i^{n+\frac12} \\
&\quad - \alpha_3[CM]_i^{n+\frac12} - \beta_3\bar{\nabla}[CM]_i^{n+\frac12}, \\
\partial_t[CS]_i^n &= k_s^+[C]_i^{n+\frac12}[S]_i^{n+\frac12} - k_s^-[CS]_i^{n+\frac12}, \\
[S]_i^n &= [B_s]_{tot} - [CS]_i^n
\end{aligned} \tag{4}
$$

with the initial conditions

$$
\begin{aligned}
[C]_i^0 &= [Ca^{2+}]_0(x_i), \qquad & [M]_i^0 &= [B_m]_0(x_i), \\
[CM]_i^0 &= [CaB_m]_0(x_i), \qquad & [CS]_i^0 &= [CaB_s]_0(x_i)
\end{aligned} \tag{5}
$$

and the Neumann boundary conditions

$$
\frac{\nabla_+ + \nabla_-}{2} U_i^n = 0, \quad U \in \{[C],[M],[CM],[CS]\}, \quad i \in \{0, \mathcal{M}\},\ 1 \le n \le N \tag{6}
$$

where $\bar{\nabla} = (\nabla_- + \nabla_+)/2$, $D_1 = D_{Ca}$, $D_2 = D_{B_m}$, $D_3 = D_{CaB_m}$, $\alpha_1 = \alpha_{Ca}$, $\beta_1 = \beta_{Ca}$, $\alpha_2 = \alpha_{B_m}$, $\beta_2 = \beta_{B_m}$, and $\alpha_3 = \alpha_{CaB_m}$, $\beta_3 = \beta_{CaB_m}$.

Note that the discretized Neumann boundary conditions (6) are equal to $U_{-1}^n = U_1^n$ and $U_{\mathcal{M}+1}^n = U_{\mathcal{M}-1}^n$.

In order to consider the error estimates, we now introduce the discrete L^2-inner product and the corresponding discrete L^2-norm on Ω_h

$$
(V,W)_h = h\sum_{i=0}^{\mathcal{M}}{}'' V_iW_i = h\big\{(V_0W_0 + V_{\mathcal{M}}W_{\mathcal{M}})/2 + \sum_{i=1}^{\mathcal{M}-1} V_iW_i\big\},
$$

$$
\|V\|_h = (V,V)_h^{1/2}
$$

for functions V and W satisfying the boundary condition (6). For the maximum norm, we define

$$
\|V\|_\infty = \max_{0\le i\le \mathcal{M}} |V_i|.
$$

Hereafter, whenever there is no confusion, $(\cdot,\cdot)$ and $\|\cdot\|$ will denote $(\cdot,\cdot)_h$ and $\|\cdot\|_h$, respectively.

It follows from summation by parts and the definition of difference operators that Lemma 1 holds.

Lemma 1. *For functions V and W defined on Ω_h and satisfying the boundary condition (6), the following identity and inequality hold.*

(1) $(\nabla^2 V, W) = -h\sum_{i=1}^{\mathcal{M}}(\nabla_- V_i)(\nabla_- W_i)$.
(2) $\max\{\|\nabla_+ V\|^2, \|\nabla_- V\|^2\} \leq -2(\nabla^2 V, V)$.

Using Lemma 2.5 in [4] and Lemma 1, we obtain the following lemma.

Lemma 2. *For V defined on Ω_h, the following inequalities hold.*

$$\|V\|_\infty^2 \leq 3\|V\|^2 + 8\|V\|\|\bar{\nabla} V\|.$$

3. Convergence of approximate solution

We recall the extension of Lax-Richtmyer equivalence theorem in Lopez-Marcos and Sanz-Serna [9] which makes us avoid the difficulty of direct proof for convergence arising specially in nonlinear problems. Let u be a solution of a problem $\Phi(u) = 0$ and u_h be a discrete evaluation of u on Ω_h. Let U_h be an approximate solution of u, which is obtained by solving the discrete equation

$$\Phi_h(U_h) = 0, \tag{7}$$

where $\Phi_h : \mathbf{X}_h \to \mathbf{Y}_h$ is a continuous mapping and $\mathbf{X}_h, \mathbf{Y}_h$ are normed spaces having the same dimension. The scheme (7) is said to be convergent if (7) has a solution U_h such that $\lim_{h\to 0} \|U_h - u_h\|_{\mathbf{X}_h} = 0$. The discretization (7) is said to be consistent if $\lim_{h\to 0} \|\Phi_h(u_h)\|_{\mathbf{Y}_h} = 0$. The scheme (7) is said to be stable in the threshold R_h if there exists a positive constant Θ such that for an open ball $B(u_h, R_h) \subset \mathbf{X}_h$,

$$\|V_h - W_h\|_{\mathbf{X}_h} \leq \Theta\|\Phi_h(V_h) - \Phi_h(W_h)\|_{\mathbf{Y}_h}, \quad \forall\ V_h, W_h \in B(u_h, R_h).$$

The following theorem is the extended Lax-Richtmyer equivalence theorem which gives existence and convergence of approximate solutions. For the proof, see [9].

Theorem 1. *Assume that the discrete equation (7) is consistent and stable in the threshold R_h. If Φ_h is continuous in $B(u_h, R_h)$ and $\|\Phi_h(u_h)\|_{\mathbf{Y}_h} = o(R_h)$ as $h \to 0$, then (7) has a unique solution U_h in $B(u_h, R_h)$ and there exists a constant Θ such that*

$$\|U_h - u_h\|_{\mathbf{X}_h} \leq \Theta\|\Phi_h(u_h)\|_{\mathbf{Y}_h}.$$

According to Theorem 1, we have only to show that (7) is consistent and stable in the threshold in order to show the unique existence and convergence of approximate solutions.

Let Z_h^n be the set of all functions defined on Ω_h satisfying the discretized Neumann boundary condition (6) at time level n $(0 \leq n \leq N)$. We take $\mathbf{X}_h = \mathbf{Y}_h = \left(\prod_{n=0}^{N} Z_h^n\right)^4$ and define a mapping $\mathbf{\Phi}_h : \mathbf{X}_h \to \mathbf{Y}_h$ by $\mathbf{\Phi}_h(\mathbf{U}) = \widetilde{\mathbf{U}}$, where for $n = 0, \cdots, N-1$

$$
(8) \quad
\begin{aligned}
[\widetilde{U_1}]_i^{n+1} &= \partial_t [U_1]_i^n - D_1 \nabla^2 [U_1]_i^{n+\frac{1}{2}} + k_s^+ [U_1]_i^{n+\frac{1}{2}} \big([B_s]_{tot} - [U_4]_i^{n+\frac{1}{2}} \big) \\
&\quad - k_s^- [U_4]_i^{n+\frac{1}{2}} + k_m^+ [U_1]_i^{n+\frac{1}{2}} [U_2]_i^{n+\frac{1}{2}} - k_m^- [U_3]_i^{n+\frac{1}{2}} \\
&\quad + \alpha_1 [U_1]_i^{n+\frac{1}{2}} + \beta_1 \bar{\nabla} [U_1]_i^{n+\frac{1}{2}}, \\
[\widetilde{U_2}]_i^{n+1} &= \partial_t [U_2]_i^n - D_2 \nabla^2 [U_2]_i^{n+\frac{1}{2}} + k_m^+ [U_1]_i^{n+\frac{1}{2}} [U_2]_i^{n+\frac{1}{2}} - k_m^- [U_3]_i^{n+\frac{1}{2}} \\
&\quad + \alpha_2 [U_2]_i^{n+\frac{1}{2}} + \beta_2 \bar{\nabla} [U_2]_i^{n+\frac{1}{2}}, \\
[\widetilde{U_3}]_i^{n+1} &= \partial_t [U_3]_i^n - D_3 \nabla^2 [U_3]_i^{n+\frac{1}{2}} - k_m^+ [U_1]_i^{n+\frac{1}{2}} [U_2]_i^{n+\frac{1}{2}} + k_m^- [U_3]_i^{n+\frac{1}{2}} \\
&\quad + \alpha_3 [U_3]_i^{n+\frac{1}{2}} + \beta_3 \bar{\nabla} [U_3]_i^{n+\frac{1}{2}}, \\
[\widetilde{U_4}]_i^{n+1} &= \partial_t [U_4]_i^n - k_s^+ [U_1]_i^{n+\frac{1}{2}} \big([B_s]_{tot} - [U_4]_i^{n+\frac{1}{2}} \big) + k_s^- [U_4]_i^{n+\frac{1}{2}}
\end{aligned}
$$

and

$$
(9) \quad
\begin{aligned}
&[\widetilde{U_1}]_i^0 = [U_1]_i^0 - [Ca^{2+}]_0(x_i), \quad [\widetilde{U_2}]_i^0 = [U_2]_i^0 - [B_m]_0(x_i), \\
&[\widetilde{U_3}]_i^0 = [U_3]_i^0 - [CaB_m]_0(x_i), \quad [\widetilde{U_4}]_i^0 = [U_4]_i^0 - [CaB_s]_0(x_i).
\end{aligned}
$$

We take norms $\|\cdot\|_{\mathbf{X}_h}$ and $\|\cdot\|_{\mathbf{Y}_h}$ on $\mathbf{X}_h$ and $\mathbf{Y}_h$, respectively, such that

$$
\|\mathbf{U}\|_{\mathbf{X}_h}^2 = \max_{0 \le n \le N} \sum_{j=1}^{4} \|U_j^n\|^2 + k \sum_{n=0}^{N-1} \Big\{ - \sum_{j=1}^{3} \big(\nabla^2 U_j^{n+\frac{1}{2}}, U_j^{n+\frac{1}{2}} \big) + \sum_{j=1}^{4} \|U_j^{n+\frac{1}{2}}\|^2 \Big\}
$$

and

$$
\|\widetilde{\mathbf{U}}\|_{\mathbf{Y}_h}^2 = \sum_{j=1}^{4} \|\widetilde{U}_j^0\|^2 + k \sum_{n=1}^{N} \sum_{j=1}^{4} \|\widetilde{U}_j^n\|^2.
$$

The consistency of the scheme (4)–(6) is obtained using Taylor's Theorem and the Mean Value Theorem.

Theorem 2. *Let $u = \big([Ca^{2+}], [B_m], [CaB_m], [CaB_s]\big)$ be the solution of (1)–(3) with bounded derivatives $\frac{\partial^3 u_j}{\partial t^3}$ and $\frac{\partial^4 u_j}{\partial x^4} (1 \le j \le 4)$. Then there exists a constant Θ such that*

$$
\|\mathbf{\Phi}_h(u_h)\|_{\mathbf{Y}_h} \le \Theta(k^2 + h^2).
$$

We now consider the stability of the approximate solution in the threshold R_h.

Theorem 3. *Let $\mathbf{\Phi}_h(\mathbf{U}) = \widetilde{\mathbf{U}}$, $\mathbf{\Phi}_h(\mathbf{V}) = \widetilde{\mathbf{V}}$ and $B(u_h, R_h)$ be the ball with center u_h and radius $R_h = O(1)$. Assume that the conditions in* Theorem 2 *hold. Then there exists a constant Θ such that for any $\mathbf{U}$ and $\mathbf{V}$ in $B(u_h, R_h)$,*

$$
\|\mathbf{U} - \mathbf{V}\|_{\mathbf{X}_h} \le \Theta \|\mathbf{\Phi}_h(\mathbf{U}) - \mathbf{\Phi}_h(\mathbf{V})\|_{\mathbf{Y}_h}.
$$

Proof. Let $e_j^n = [U_j]^n - [V_j]^n$ and $\widetilde{K}_j^n = [\widetilde{U_j}]^n - [\widetilde{V_j}]^n$ with $1 \le j \le 4$. Replacing $[U_j]^n$ and $[\widetilde{U_j}]^n$ in (8) by $[V_j]^n$ and $[\widetilde{V_j}]^n$, respectively, and subtracting these results from (8), we obtain

$$
\begin{aligned}
&\partial_t e_1^n - D_1\nabla^2 e_1^{n+\frac{1}{2}} + (k_s^+[B_s]_{tot} + \alpha_1)e_1^{n+\frac{1}{2}} \\
&\qquad = k_s^+\big(e_1^{n+\frac{1}{2}}[U_4]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_4^{n+\frac{1}{2}}\big) + k_s^- e_4^{n+\frac{1}{2}} + k_m^- e_3^{n+\frac{1}{2}} \\
&\qquad\quad - k_m^+\big(e_1^{n+\frac{1}{2}}[U_2]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_2^{n+\frac{1}{2}}\big) + \beta_1\bar{\nabla} e_1^{n+\frac{1}{2}} + \widetilde{K}_1^{n+1} \\
&\partial_t e_2^n - D_2\nabla^2 e_2^{n+\frac{1}{2}} + \alpha_2 e_2^{n+\frac{1}{2}} \\
&\qquad = -k_m^+\big(e_1^{n+\frac{1}{2}}[U_2]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_2^{n+\frac{1}{2}}\big) + k_m^- e_3^{n+\frac{1}{2}} \\
&\qquad\quad + \beta_2\bar{\nabla} e_2^{n+\frac{1}{2}} + \widetilde{K}_2^{n+1}, \\
&\partial_t e_3^n - D_3\nabla^2 e_3^{n+\frac{1}{2}} + (k_m^- + \alpha_3)e_3^{n+\frac{1}{2}} \\
&\qquad = k_m^+\big(e_1^{n+\frac{1}{2}}[U_2]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_2^{n+\frac{1}{2}}\big) + \beta_3\bar{\nabla} e_3^{n+\frac{1}{2}} + \widetilde{K}_3^{n+1}, \\
&\partial_t e_4^n + k_s^- e_4^{n+\frac{1}{2}} = k_s^+[B_s]_{tot}e_1^{n+\frac{1}{2}} - k_s^+\big(e_1^{n+\frac{1}{2}}[U_4]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_4^{n+\frac{1}{2}}\big) \\
&\qquad + \widetilde{K}_4^{n+1}.
\end{aligned}
\tag{10}
$$

Taking inner products between (10) and $e_j^{n+\frac{1}{2}}$ and summing these results, we obtain for some constant Θ

$$
\begin{aligned}
&\sum_{j=1}^{4}\partial_t\|e_j^n\|^2 - \sum_{j=1}^{3} D_j(\nabla^2 e_j^{n+\frac{1}{2}}, e_j^{n+\frac{1}{2}}) + \sum_{j=1}^{4}\tau_j\|e_j^{n+\frac{1}{2}}\|^2 \\
&\qquad \le \Theta\bigg(\|e_3^{n+\frac{1}{2}}\| + \sum_{j=1}^{3}\|\bar{\nabla} e_j^{n+\frac{1}{2}}\| + \sum_{j\in\{1,2,4\}}\|e_j^{n+\frac{1}{2}}\|_\infty\bigg)\sum_{j=1}^{4}\|e_j^{n+\frac{1}{2}}\| \\
&\qquad\quad + \sum_{j=1}^{4}\|\widetilde{K}_j^{n+1}\|^2
\end{aligned}
\tag{11}
$$

where $\tau_1 = k_s^+[B_s]_{tot} + \alpha_1$, $\tau_2 = \alpha_2$, $\tau_3 = k_m^- + \alpha_3$ and $\tau_4 = k_s^-$.
Applying Lemma 1–2 and the discrete Gronwall's inequality to (11), we obtain for $0 \le m \le N-1$,

$$
\begin{aligned}
&\sum_{j=1}^{4}\|e_j^{m+1}\|^2 + k\sum_{n=0}^{m}\bigg\{-\sum_{j=1}^{3}(\nabla^2 e_j^{n+\frac{1}{2}}, e_j^{n+\frac{1}{2}}) + \sum_{j=1}^{4}\|e_j^{n+\frac{1}{2}}\|^2\bigg\} \\
&\qquad\qquad \le \Theta\sum_{j=1}^{4}\bigg(\|e_j^0\|^2 + k\sum_{n=1}^{m+1}\|\widetilde{K}_j^n\|^2\bigg).
\end{aligned}
$$

Since

$$e_j^0 = U_j^0 - V_j^0 = \widetilde{U}_j^0 - \widetilde{V}_j^0 = \widetilde{K}_j^0,$$

the desired result is obtained. $\square$

It follows from Theorem 1 that for $k = O(h^\alpha)$ and $\alpha > 0$,

$$\frac{\|\mathbf{\Phi}_h(u_h)\|_{\mathbf{Y}_h}}{R_h} = O(k^2 + h^2) \to 0 \quad \text{as} \quad h \to 0. \tag{12}$$

Hence, applying Theorems 2–3 and (12) to Theorem 1, we obtain the following error estimate for (4)–(6).

Theorem 4. *Suppose that hypotheses of Theorem 3 hold. Let* $\mathbf{U}$= ([C],[M],[CM], [CS]) *be a solution of (4)–(6). Then for* $k = O(h^\alpha)$ *and* $\alpha > 0$*, there exists a constant* Θ *such that*

$$\|\mathbf{U} - u_h\|_{\mathbf{X}_h} \le \Theta(k^2 + h^2).$$

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