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# FINITE DIFFERENCE SCHEMES FOR CALCIUM DIFFUSION EQUATIONS

S. M. CHOO

ABSTRACT. Finite difference schemes are considered for a $Ca^{2+}$ diffusion equations, which discribe $Ca^{2+}$ buffering by using stationary and mobile buffers. Stability and $L^\infty$ error estimates of approximate solutions for the corresponding schemes are obtained using the extended Lax-Richtmyer equivalence theorem.

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## 1. Introduction

We consider the $Ca^{2+}$ buffer reactions in cells

$$B_i + Ca^{2+} \underset{k_i^-}{\overset{k_i^+}{\rightleftarrows}} CaB_i$$

where $Ca^{2+}$ is free Calcium ion, buffer $B_i$ is stationary buffer $B_s$ or mobile buffer $B_m$, and $CaB_i$ represents $Ca^{2+}$ bound to a buffer site. $Ca^{2+}$ concentrations are buffered in living cells([1],[11]). Wagner and Keizer[13] have described the $Ca^{2+}$ buffering as the following partial differential equations without explicit initial and boundary conditions.

$$\frac{\partial[Ca^{2+}]}{\partial t} = D_{Ca}\frac{\partial^2[Ca^{2+}]}{\partial x^2} - k_s^+[Ca^{2+}][B_s] + k_s^-[CaB_s] \qquad (1)$$

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

For the completeness of the modeling, we need one condition about the state variable $[B_s]$. Assume that the total concentration of the stationary buffer $[B_s]_{tot}$ is conserved: for a constant $[B_s]_{tot}$,

$$[B_s] = [B_s]_{tot} - [CaB_s]. \tag{2}$$

The initial conditions are

$$
\begin{aligned}
&[Ca^{2+}](x,0) = [Ca^{2+}]_0(x), \quad [B_m](x,0) = [B_m]_0(x), \\
&[CaB_m](x,0) = [CaB_m]_0(x), \quad [CaB_s](x,0) = [CaB_s]_0(x)
\end{aligned} \tag{3}
$$

and boundary conditions are

$$\frac{\partial u}{\partial x}(x,t) = 0, \quad x \in \{0,\ell\}, t \in (0,T] \tag{4}$$

where $u$ is $[Ca^{2+}]$,$[B_m]$, $[CaB_m]$ or $[CaB_s]$.

There is no analysis of numerical schemes for the $Ca^{2+}$ dynamics such as $Ca^{2+}$ buffering as far as we know. The studies on the 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]). Following the finite difference approaches in [3]–[4], we can analysis numerical schemes for the $Ca^{2+}$ buffering.

In this paper, we consider estimates of approximate solutions for finite difference methods. In Section 2, we introduce the finite difference schemes for (1)–(4) and show that the finite difference scheme can satisfy the conservation of the concentration of the mobile buffer. In Sections 3, we briefly recall the Lax-Richtmyer equivalence theorem and obtain stability and error estimates for the equation by following the idea in Lopez-Marcos and Sanz-Serna[9] and 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 $\Omega_h$, define the difference operators as for $0 \le i \le \mathcal{M}$,

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

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

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

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)–(4) are defined as solutions of

$$\begin{aligned} \partial_t [C]_i^n &= D_1 \nabla^2 [C]_i^{n+\frac{1}{2}} - k_s^+ [C]_i^{n+\frac{1}{2}} [S]_i^{n+\frac{1}{2}} + k_s^- [CS]_i^{n+\frac{1}{2}} \\ &\quad - k_m^+ [C]_i^{n+\frac{1}{2}} [M]_i^{n+\frac{1}{2}} + k_m^- [CM]_i^{n+\frac{1}{2}}, \\ \partial_t [M]_i^n &= D_2 \nabla^2 [M]_i^{n+\frac{1}{2}} - k_m^+ [C]_i^{n+\frac{1}{2}} [M]_i^{n+\frac{1}{2}} + k_m^- [CM]_i^{n+\frac{1}{2}}, \\ \partial_t [CM]_i^n &= D_3 \nabla^2 [CM]_i^{n+\frac{1}{2}} + k_m^+ [C]_i^{n+\frac{1}{2}} [M]_i^{n+\frac{1}{2}} - k_m^- [CM]_i^{n+\frac{1}{2}}, \\ \partial_t [CS]_i^n &= k_s^+ [C]_i^{n+\frac{1}{2}} [S]_i^{n+\frac{1}{2}} - k_s^- [CS]_i^{n+\frac{1}{2}}, \\ [S]_i^{n+1} &= [B_s]_{tot} - [CS]_i^{n+1} \end{aligned} \tag{5}$$

with the initial conditions

$$\begin{aligned} [C]_i^0 &= [Ca^{2+}]_0(x_i), \quad [M]_i^0 = [B_m]_0(x_i), \\ [CM]_i^0 &= [CaB_m]_0(x_i), \quad [CS]_i^0 = [CaB_s]_0(x_i) \end{aligned} \tag{6}$$

and the Neumann boundary conditions

$$\frac{\nabla_+ + \nabla_-}{2} U_i^n = 0, \quad U \in \{[C], [M], [CM], [CS]\}, \quad i \in \{0, \mathcal{M}\}, \ 1 \le n \le N \tag{7}$$

Here $D_1 = D_{Ca}$, $D_2 = D_{B_m}$, and $D_3 = D_{CaB_m}$.

Note that the discretized Neumann boundary conditions (7) 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 $\Omega_h$

$$(V, W)_h = h \sum_{i=0}^{\mathcal{M}}{}'' V_i W_i = h\{(V_0 W_0 + V_{\mathcal{M}} W_{\mathcal{M}})/2 + \sum_{i=1}^{\mathcal{M}-1} V_i W_i\}, \|V\|_h = (V, V)_h^{1/2}$$

for functions $V$ and $W$ satisfying the boundary condition (7). 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 $\Omega_h$ and satisfying the boundary condition (7), the following identity and inequality hold.*

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

(2) $\max\{\|\nabla_+ V\|^2, \|\nabla_- V\|^2\} \le -2(\nabla^2 V, V)$.

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

**Lemma 2.** *For $V$ defined on $\Omega_h$, the following inequalities hold.*

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

*where* $\bar{\nabla} = (\nabla_- + \nabla_+)/2$.

**Remark 1.** The concentration of the total mobile buffer is conserved like the stationary buffer: for $0 < t \le T$,

$$\frac{d}{dt}\int_0^\ell \Big\{[B_m](x,t) + [CaB_m](x,t)\Big\}dx = 0.$$

It follows from (5) and (7) that the corresponding numerical solutions also satisfy the conservation: for $0 \le n \le N-1$

$$\partial_t \sum_{i=0}^{\mathcal{M}}{}'' ([M]_i^n + [CM]_i^n) = 0.$$

## 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 $\Omega_h$. Let $U_h$ be an approximate solution of $u$, which is obtained by solving the discrete equation

$$\Phi_h(U_h) = 0, \tag{8}$$

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 (8) is said to be convergent if (8) has a solution $U_h$ such that $\lim_{h\to 0} \|U_h - u_h\|_{\mathbf{X}_h} = 0$. The discretization (8) is said to be consistent if $\lim_{h\to 0}\|\Phi_h(u_h)\|_{\mathbf{Y}_h}=0$. The scheme (8) is said to be stable in the threshold $R_h$ if there exists a positive constant $\Theta$ such that for an open ball $B(u_h,R_h)\subset \mathbf{X}_h$,

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

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 (8) is consistent and stable in the threshold $R_h$. If $\Phi_h$ is continuous in $B(u_h,R_h)$ and $\|\Phi_h(u_h)\|_{\mathbf{Y}_h}=o(R_h)$ as $h\to 0$, then (8) has a unique solution $U_h$ in $B(u_h,R_h)$ and there exists a constant $\Theta$ such that*

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

According to Theorem 1, we have only to show that (8) 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 $\Omega_h$ satisfying the discretized Neumann boundary condition (7) at time level $n$ $(0\le n\le N)$. We take $\mathbf{X}_h = \mathbf{Y}_h = \left(\prod_{n=0}^{N} Z_h^n\right)^4$ and define a mapping $\Phi_h : \mathbf{X}_h \to \mathbf{Y}_h$ by $\Phi_h(\mathbf{U}) = \widetilde{\mathbf{U}}$, where for $n=0,\cdots,N-1$

$$\begin{aligned}
\widetilde{[U_1]}_i^{n+1} &= \partial_t[U_1]_i^n - D_1\nabla^2[U_1]_i^{n+\frac12} + k_s^+[U_1]_i^{n+\frac12}\left([B_s]_{tot} - [U_4]_i^{n+\frac12}\right) \\
&\quad - k_s^-[U_4]_i^{n+\frac12} + k_m^+[U_1]_i^{n+\frac12}[U_2]_i^{n+\frac12} - k_m^-[U_3]_i^{n+\frac12}, \\
\widetilde{[U_2]}_i^{n+1} &= \partial_t[U_2]_i^n - D_2\nabla^2[U_2]_i^{n+\frac12} + k_m^+[U_1]_i^{n+\frac12}[U_2]_i^{n+\frac12} - k_m^-[U_3]_i^{n+\frac12}, \\
\widetilde{[U_3]}_i^{n+1} &= \partial_t[U_3]_i^n - D_3\nabla^2[U_3]_i^{n+\frac12} - k_m^+[U_1]_i^{n+\frac12}[U_2]_i^{n+\frac12} + k_m^-[U_3]_i^{n+\frac12}, \\
\widetilde{[U_4]}_i^{n+1} &= \partial_t[U_4]_i^n - k_s^+[U_1]_i^{n+\frac12}\left([B_s]_{tot} - [U_4]_i^{n+\frac12}\right) + k_s^-[U_4]_i^{n+\frac12}
\end{aligned} \tag{9}$$

and

$$\begin{aligned}
&\widetilde{[U_1]}_i^0 = [U_1]_i^0 - [Ca^{2+}]_0(x_i), \quad \widetilde{[U_2]}_i^0 = [U_2]_i^0 - [B_m]_0(x_i), \\
&\widetilde{[U_3]}_i^0 = [U_3]_i^0 - [CaB_m]_0(x_i), \quad \widetilde{[U_4]}_i^0 = [U_4]_i^0 - [CaB_s]_0(x_i).
\end{aligned} \tag{10}$$

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

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

and

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

The consistency of the scheme (5)–(7) is obtained using Taylor's Theorem and the Mean Value Theorem.

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

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

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

**Theorem 3.** *Let* $\Phi_h(\mathbf{U}) = \widetilde{\mathbf{U}}$, $\Phi_h(\mathbf{V}) = \widetilde{\mathbf{V}}$ *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* $\Theta$ *such that for any* $\mathbf{U}$ *and* $\mathbf{V}$ *in* $B(u_h, R_h)$,

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

*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 (9) by $[V_j]^n$ and $[\widetilde{V_j}]^n$, respectively, and subtracting these results from (9), we obtain

$$\begin{aligned}
&\partial_t e_1^n - D_1\nabla^2 e_1^{n+\frac{1}{2}} + k_s^+[B_s]_{tot}e_1^{n+\frac{1}{2}} \qquad (11)\\
&\quad = k_s^+\left(e_1^{n+\frac{1}{2}}[U_4]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_4^{n+\frac{1}{2}}\right) + k_s^- e_4^{n+\frac{1}{2}}\\
&\qquad - k_m^+\left(e_1^{n+\frac{1}{2}}[U_2]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_2^{n+\frac{1}{2}}\right) + k_m^- e_3^{n+\frac{1}{2}} + \widetilde{K}_1^{n+1},\\
&\partial_t e_2^n - D_2\nabla^2 e_2^{n+\frac{1}{2}}\\
&\quad = -k_m^+\left(e_1^{n+\frac{1}{2}}[U_2]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_2^{n+\frac{1}{2}}\right) + k_m^- e_3^{n+\frac{1}{2}} + \widetilde{K}_2^{n+1},\\
&\partial_t e_3^n - D_3\nabla^2 e_3^{n+\frac{1}{2}} + k_m^- e_3^{n+\frac{1}{2}}\\
&\quad = k_m^+\left(e_1^{n+\frac{1}{2}}[U_2]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_2^{n+\frac{1}{2}}\right) + \widetilde{K}_3^{n+1},\\
&\partial_t e_4^n + k_s^- e_4^{n+\frac{1}{2}} = k_s^+[B_s]_{tot}e_1^{n+\frac{1}{2}} - k_s^+\left(e_1^{n+\frac{1}{2}}[U_4]^{n+\frac{1}{2}} + [U_1]^{n+\frac{1}{2}}e_4^{n+\frac{1}{2}}\right) + \widetilde{K}_4^{n+1}.
\end{aligned}$$

Taking inner products between (11) and $e_j^{n+\frac{1}{2}}$ and summing these results, we obtain for some constant $\Theta$

$$\sum_{j=1}^{4} \partial_t \|e_j^n\|^2 - \sum_{j=1}^{3} D_j \left(\nabla^2 e_j^{n+\frac{1}{2}}, e_j^{n+\frac{1}{2}}\right) + \sum_{j\in\{1,3,4\}} \tau_j \left\|e_j^{n+\frac{1}{2}}\right\|^2 \tag{12}$$
$$\leq \sum_{j=1}^{4} \left\|\widetilde{K}_j^{n+1}\right\|^2 + \Theta\left(\left\|e_3^{n+\frac{1}{2}}\right\| + \sum_{j\in\{1,2,4\}} \left\|e_j^{n+\frac{1}{2}}\right\|_\infty\right) \sum_{j=1}^{4} \left\|e_j^{n+\frac{1}{2}}\right\|$$

where $\tau_1 = k_s^+[B_s]_{tot}, \tau_3 = k_m^-$ and $\tau_4 = k_s^-$.
Applying Lemma 1–2 and the discrete Gronwall's inequality to (12), we obtain for $m \geq 0$,

$$\sum_{j=1}^{4} \|e_j^{m+1}\|^2 + k\sum_{n=0}^{m}\left\{-\sum_{j=1}^{3}\left(\nabla^2 e_j^{n+\frac{1}{2}}, e_j^{n+\frac{1}{2}}\right) + \sum_{j\in\{1,3,4\}} \left\|e_j^{n+\frac{1}{2}}\right\|^2\right\}$$
$$\leq \Theta \sum_{j=1}^{4}\left(\|e_j^0\|^2 + k\sum_{n=1}^{m+1}\|\widetilde{K}_j^n\|^2\right).$$

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. □

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

$$\frac{\|\Phi_h(u_h)\|_{\mathbf{Y}_h}}{R_h} = O(k^2 + h^2) \to 0 \quad \text{as} \quad h \to 0. \tag{13}$$

Hence, applying Theorems 2–3 and (13) to Theorem 1, we obtain the following error estimate for (5)–(7).

**Theorem 4.** *Suppose that hypotheses of Theorem 3 hold. Let* $\mathbf{U} = ([C],[M],[CM],[CS])$ *be a solution of (5)–(7). Then for* $k = O(h^\alpha)$ *and* $\alpha > 0$, *there exists a constant* $\Theta$ *such that*

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

**Remark 2.** If we restrict the $Ca^{2+}$ buffering model (1)–(4) to the cytoplasm of a cell, we need to modify the boundary condition of $Ca^{2+}$. But in the case of sarcoplasmic reticulum, we think the partial differential equations as well as the boundary conditions must be changed. These modifications are future studies.

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**S. M. Choo** received his degrees of B.S. and M.S. from Seoul National University. He earned his Ph.D. at Seoul National University under the direction of S.K. Chung. He has been at University of Ulsan since September, 2001. His research interest are numerical analysis and systems biology.

School of Electrical Engineering, University of Ulsan, Ulsan 680–749, Korea
e-mail:smchoo@ulsan.ac.kr