CSPeskin 3/23/2018

Convergence of a numerical scheme for the Hodgkin-Huxley equations

We consider the system

$$(1) \quad \frac{\partial v}{\partial t} + a_{Na} s_1^3 s_2 (v - e_{Na}) + a_K s_3^4 (v - e_K)$$

$$+ a_L (v - e_L) = D \frac{\partial^2 v}{\partial x^2}$$

$$(2) \quad \tau_i(v) \frac{\partial s_i}{\partial t} = \sigma_i(v) - s_i \quad , \quad i = 1, 2, 3$$

on the spatial domain $0 \le x < x_0$ with periodic boundary conditions, and for $t > 0$. The initial conditions are

$$(3) \quad v(x,0) = v^{(0)}(x)$$

$$(4) \quad s_i(x,0) = s_i^{(0)}(x) \quad , \quad i = 1, 2, 3$$

The given constants a_{Na}, a_K, a_L, and D are all positive. In more conventional Hodgkin-Huxley notation

$$(5) \qquad a_{Na} = \frac{\bar{g}_{Na}}{C_m}, \quad a_K = \frac{\bar{g}_K}{C_m}, \quad a_L = \frac{\bar{g}_L}{C_m}$$

where $\bar{g}_{Na}$ is the maximum possible Na^+ conductance per unit area of membrane, $\bar{g}_K$ is the maximum possible K^+ conductance per unit area of membrane, and $\bar{g}_L$ is the constant leakage conductance per unit area of membrane. The constant C_m is the membrane capacitance per unit area. The constants a_{Na}, a_K, and a_L have units of reciprocal time. The constant D is given by

$$(6) \qquad D = \frac{r}{2\rho C_m}$$

in which r is the radius of the axon and ρ is the resistivity of the axoplasm. The units of D are length^2/time, which are those of a diffusion constant.

The constants e_{Na}, e_K, and e_L are the reversal potentials for the different types of ion channels. They satisfy

(7) $$e_K < e_L < 0 < e_{Na}$$

These constants have units of voltage.

The given functions $\sigma_i(v)$ and $\tau_i(v)$ are smooth, positive, and defined on the whole real line.

The σ_i are strictly monotonic and their range is $(0,1)$ with

(8) $$\sigma_1'(v) > 0 \,,\quad \sigma_2'(v) < 0 \,,\quad \sigma_3'(v) > 0$$

The functions τ_i are bell-shaped, which means that they each have a unique global maximum and are monotonic on either side of that maximum. The functions τ_i have units of time.

The unknown function $v(x,t)$ has units of voltage, and the unknown functions $s_i(x,t)$ for $i=1,2,3$ are dimensionless. In conventional Hodgkin-Huxley notation, the s_i are denoted m, h, n, respectively, and are called gating variables. Also the functions τ_i are denoted τ_m, τ_h, τ_n and the functions σ_i are denoted $m_\infty, h_\infty, n_\infty$.

An important restriction on the initial data is

$$v^{(0)}(x) \in (e_K, e_{Na}) \tag{9}$$

$$s_i^{(0)}(x) \in (0, 1), \quad i=1,2,3 \tag{10}$$

The initial data are also assumed to be smoothly periodic. Under these conditions, it is known that the Hodgkin-Huxley equations have a unique smooth periodic global solution with the property that

(11) $$v(x,t) \in (e_K, e_{Na})$$

(12) $$s_i(x,t) \in (0,1), \quad i=1,2,3$$

Because of (11), the values of the functions $\tau_i(v)$ and $\sigma_i(v)$ for $v \notin (e_K, e_{Na})$ are completely irrelevant. This gives us the freedom to alter these functions in any way that we like outside of the interval (e_K, e_{Na}). Such alteration may affect the computed solution if it goes outside of the interval (e_K, e_{Na}) but it will have no effect on the exact solution that the computed solution is supposed to approximate.

In the original Hodgkin-Huxley equations, the smooth bell-shaped functions $\tau_i(v)$ approach 0 as $v \to \pm\infty$. Here, we propose to modify these functions outside of the interval (e_K, e_{Na}) in such a manner that they are still smooth and bell-shaped but now are bounded from below by a positive constant τ_{min} (the same positive constant for all three of the τ_i). This can clearly be done without making any changes at all in the restriction of the functions τ_i to the interval (e_K, e_{Na}). Thus, in the following, we assume that

(13) $$\tau_i(v) > \tau_{min} > 0$$

for $i=1,2,3$ and for all $v \in (-\infty, \infty)$.

Now choose

(14) $$\Delta x = x_0 / J$$

where J is a positive integer, and also choose $\Delta t > 0$. Let

(15) $$v_j^{(n)} = v(j\Delta x, n\Delta t)$$

(16) $$S_{ij}^{(n+1/2)} = S_i(j\Delta x, (n+\tfrac{1}{2})\Delta t)$$

for $j = 0, 1, \ldots, J-1$ and for $n = 0, 1, \ldots$

Arithmetic on the index j will always be done modulo J to enforce periodicity.

Let the forward and backward spatial difference operators $d_x^{\pm}$ be defined by

(17) $$(d_x^+ \phi)_j = \frac{\phi_{j+1} - \phi_j}{\Delta x}$$

(18) $$(d_x^- \phi)_j = \frac{\phi_j - \phi_{j-1}}{\Delta x}$$

Then

(19) $$(d_x^+ d_x^- \phi)_j = (d_x^- d_x^+ \phi)_j$$

$$= \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{(\Delta x)^2}$$

We shall also make use of the discrete L2 inner product:

(20) $$(\phi, \psi) = \frac{1}{X} \sum_{j=0}^{J-1} \phi_j \psi_j (\Delta x) = \frac{1}{J} \sum_{j=0}^{J-1} \phi_j \psi_j$$

and the corresponding norm:

(21) $$\|\phi\| = \sqrt{\sum_{j=0}^{J-1} \phi_j^2 \frac{\Delta x}{x_0}} = \sqrt{\frac{1}{J}\sum_{j=0}^{J-1} \phi_j^2}$$

Note that

(22) $$x_0(\phi, d_x^+\psi) = \sum_{j=0}^{J-1} \phi_j(\psi_{j+1} - \psi_j)$$

$$= \sum_{j=0}^{J-1} \phi_j \psi_{j+1} - \sum_{j=0}^{J-1} \phi_j \psi_j$$

$$= \sum_{j=0}^{J-1} \phi_{j-1}\psi_j - \sum_{j=0}^{J-1} \phi_j \psi_j = -(d_x^-\phi, \psi)x_0$$

An immediate consequence of (22) is that

(23) $$-(\phi, d_x^+ d_x^- \phi) = (d_x^-\phi, d_x^-\phi) = \|d_x^-\phi\|^2 \geq 0$$

The first step in deriving a numerical method for the initial-value problem (1-4) is to notice that the exact solution of that initial value problem also satisfies exactly the following finite difference equation with residual:

$$\frac{v_j^{(n+1)} - v_j^{(n)}}{\Delta t} + a_{Na}\left(S_1^3 S_2\right)_j^{(n+1/2)}\left(\frac{v_j^{(n+1)} + v_j^{(n)}}{2} - e_{Na}\right) \tag{24}$$

$$+ a_K\left(S_3^4\right)_j^{(n+1/2)}\left(\frac{v_j^{(n+1)} + v_j^{(n)}}{2} - e_K\right)$$

$$+ a_L\left(\frac{v_j^{(n+1)} + v_j^{(n)}}{2} - e_L\right)$$

$$= D\left(d_x^+ d_x^- \frac{v^{(n+1)} + v^{(n)}}{2}\right)_j + \left(R_v\right)_j^{(n+1/2)}$$

for $n = 0, 1, 2, \cdots$, and

(25) $$\tau_i(v_j^{(n)}) \frac{S_{ij}^{(n+1/2)} - S_{ij}^{(n-1/2)}}{\Delta t}$$

$$= \sigma_i(v_j^{(n)}) - \frac{S_{ij}^{(n+1/2)} + S_{ij}^{(n-1/2)}}{2} + (R_s)_{ij}^{(n)}$$

for $n = 1, 2, \cdots$, with the following instead for $n = 0$:

(26) $$\tau_i(v_j^{(0)}) \frac{S_{ij}^{(1/2)} - S_{ij}^{(0)}}{(\Delta t/2)}$$

$$= \sigma_i(v_j^{(0)}) - S_{ij}^{(0)} + (R_s)_{ij}^{(0)}.$$

This can be shown by straightforward Taylor series analysis that exploits the smoothness and boundedness of the exact solution and also the smoothness and boundedness of the functions σ_i and τ_i. The results of this analysis are that

(27) $$\left(R_v\right)_j^{(n+1/2)} = O\left((\Delta t)^2\right) + O\left((\Delta x)^2\right)$$

for $n = 0, 1, \cdots$, and

(28) $$\left(R_s\right)_{ij}^{(n)} = \begin{cases} O\left(\Delta t\right), & n = 0 \\ O\left((\Delta t)^2\right), & n = 1, 2, \cdots \end{cases}$$

The constants in these relationships depend on the exact solution and its derivatives and are independent of n and j.

Now to get a numerical scheme, we simply drop the residual terms and denote the computed solution by

(29) $$\left(V, S_1, S_2, S_3\right)$$

Our scheme is therefore defined by

$$\frac{V_j^{(n+1)} - V_j^{(n)}}{\Delta t} + a_{Na}\left(S_1^3 S_2\right)_j^{(n+1/2)} \left(\frac{V_j^{(n+1)} + V_j^{(n)}}{2} - e_{Na}\right) \tag{30}$$

$$+ a_K\left(S_3^4\right)_j^{(n+1/2)} \left(\frac{V_j^{(n+1)} + V_j^{(n)}}{2} - e_K\right)$$

$$+ a_L\left(\frac{V_j^{(n+1)} + V_j^{(n)}}{2} - e_L\right)$$

$$= D\left(d_x^+ d_x^- \frac{V^{(n+1)} + V^{(n)}}{2}\right)_j$$

for $n = 0, 1, 2, \cdots$, and

(31) $$\tau_i\left(V_j^{(n)}\right)\frac{S_{ij}^{(n+1/2)}-S_{ij}^{(n-1/2)}}{\Delta t}$$

$$=\sigma_i\left(V_j^{(n)}\right)-\frac{S_{ij}^{(n+1/2)}+S_{ij}^{(n-1/2)}}{2}$$

for $n=1,2,\cdots$, with

(32) $$\tau_i\left(V_j^{(0)}\right)\frac{S_{ij}^{(1/2)}-S_{ij}^{(0)}}{(\Delta t/2)}$$

$$=\sigma_i\left(V_j^{(0)}\right)-S_{ij}^{(0)}$$

The initial conditions for the numerical scheme are

(33) $$V_j^{(0)}=v_j^{(0)}=v(j\Delta x,0)$$

(34) $$S_{ij}^{(0)}=s_{ij}^{(0)}=s(j\Delta x,0)$$

The order of operations for $n=0,1,2,\cdots$ is to evaluate $S_i^{(n+1/2)}$ (from (32) when $n=0$ and from (31) otherwise) and then to solve (30) for $V^{(n+1)}$.

Equation (32) gives the following formula for $S_{ij}^{(1/2)}$:

(35) $$S_{ij}^{(1/2)} = S_{ij}^{(0)}\left(1 - \frac{\Delta t}{2\tau_i(V_j^{(0)})}\right) + \frac{(\Delta t)}{2\tau_i(V_j^{(0)})}\,\sigma_i\left(V_j^{(0)}\right)$$

and equation (31) is easily solved for $S_{ij}^{(n+1/2)}$ with the following result:

(36)
$$S_{ij}^{(n+1/2)} = \frac{S_{ij}^{(n-1/2)}\left(1-\frac{\Delta t}{2\tau_i(V_j^{(n)})}\right)+\frac{\Delta t}{\tau_i(V_j^{(n)})}\sigma_i\left(V_j^{(n)}\right)}{1+\frac{\Delta t}{2\tau_i(V_j^{(n)})}}$$

which holds for $n = 1, 2, \cdots$

Now we impose the restriction

(37)
$$\Delta t \leq 2\tau_{min}$$

see (13) and the discussion leading up to (13).

With this restriction, the right-hand sides of (35) & (36) both have the form of weighted averages. Therefore, since $\sigma_i(v) \in (0,1)$ for all v, and since

$S_{ij}^{(0)} = s_i(j\Delta x, 0) \in (0,1)$, it follows

by induction that

(38) $$S_{ij}^{(n+1/2)} \in (0,1)$$

for $n = 0, 1, 2, \ldots$

Equation (30) is a linear system in the unknowns

(39) $$V_0^{(n+1)} \quad \ldots \quad V_{J-1}^{(n+1)}$$

Our numerical scheme is well-defined only if this linear system is non-singular.

To prove this, we consider the homogeneous system corresponding to (30), and call the unknown V. This homogeneous system is of the form

$$\left(I + \frac{\Delta t}{2} a - \frac{\Delta t}{2} D\, d_x^+ d_x^-\right) V = 0 \tag{40}$$

in which I is the identity operator and a denotes multiplication by

$$a_{Na}\left(S_1^3 S_2\right)_j^{(n+1/2)} + a_K\left(S_3^4\right)_j^{(n+1/2)} + a_L > 0 \tag{41}$$

Taking the inner product of both sides of (40) with V, and making use of (23), we get

$$\left(V, V\right) + \frac{\Delta t}{2}\left(V, aV\right) + \frac{D\Delta t}{2}\left(d_x^- V, d_x^- V\right) = 0 \tag{42}$$

Since the three terms on the left-hand side are non-negative and their sum is zero, it follows that each of them is separately equal to zero.

Thus, in particular,

(43) $$0 = (V, V) = \|V\|^2$$

and this implies that $V = 0$. It follows that the linear system (30) is non-singular and our scheme is well-defined.

We now turn to a consideration of the errors. Let

(44) $$\tilde{V} = V - v$$

(45) $$\tilde{S}_i = S_i - s_i$$

To obtain an evolution equation for $\tilde{V}$, we need to subtract (24) from (30), and to obtain an evolution equation for $\tilde{S}_i$, we need to subtract (25) from (31) and (26) from (31). In doing these subtractions, we handle products in the following way:

(46) $$PQ - pq = PQ - Pq + Pq - pq$$
$$= P(Q-q) + (P-p)q$$
$$= P\tilde{Q} + \tilde{P}q$$

Subtraction of (24) from (30) then gives the following:

(47) $$\frac{\tilde{V}_j^{(n+1)} - \tilde{V}_j^{(n)}}{\Delta t} + A_j^{(n+1/2)} \frac{\tilde{V}_j^{(n+1)} + \tilde{V}_j^{(n)}}{2}$$

$$- D\left(d_x^+ d_x^- \frac{\tilde{V}^{(n+1)} + \tilde{V}^{(n)}}{2}\right)_j =$$

$$- a_{Na}\left(\widetilde{S_1^3 S_2}\right)_j^{(n+1/2)} \left(\frac{v_j^{(n+1)} + v_j^{(n)}}{2} - e_{Na}\right)$$

$$- a_K\left(\widetilde{S_3^4}\right)_j^{(n+1/2)} \left(\frac{v_j^{(n+1)} + v_j^{(n)}}{2} - e_K\right)$$

$$- (Rv)_j^{(n+1/2)} =: Q_j^{(n+1/2)}$$

where

(48) $$A_j^{(n+1/2)} = a_{Na}\left(S_1^{\,3} S_2\right)_j^{(n+1/2)} + a_K\left(S_3^{\,4}\right)_j^{n+1/2} + a_L > 0$$

Subtraction of (25) from (31) gives

(49) $$\tau_i\left(V_j^{(n)}\right) \frac{\tilde{S}_{ij}^{(n+1/2)} - \tilde{S}_{ij}^{(n-1/2)}}{\Delta t}$$

$$+\left(\tau_i\left(V_j^{(n)}\right) - \tau_i\left(v_j^{(n)}\right)\right) \frac{S_{ij}^{(n+1/2)} - S_{ij}^{(n-1/2)}}{\Delta t}$$

$$= \sigma_i\left(V_j^{(n)}\right) - \sigma_i\left(v_j^{(n)}\right)$$

$$- \frac{\tilde{S}_{ij}^{(n+1/2)} + \tilde{S}_{ij}^{(n-1/2)}}{2} - \left(R_s\right)_{ij}^{(n)}$$

Subtraction of (26) from (32) is simpler because the values at $t=0$ are exact. We get

(50) $$\tau_i(v_j^{(0)})\,\frac{\tilde{S}_{ij}^{(1/2)}}{(\Delta t/2)} = -(R_s)_{ij}^{(0)}.$$

or

(51) $$\tilde{S}_{ij}^{(1/2)} = -\frac{(\Delta t)}{2\tau_i(v_j^{(0)})}(R_s)_{ij}^{(0)}$$

$$= O((\Delta t)^2)$$

as $\Delta t \to 0$, see (28).

The goal now is to derive bounds on the growth of the error.

Take the inner product of both sides of (47) with $(\tilde{V}^{(n+1)} + \tilde{V}^{(n)})/2$. This gives

(52) $$\frac{1}{2\Delta t}\left(\|\tilde{V}^{(n+1)}\|^2 - \|\tilde{V}^{(n)}\|^2\right)$$

$$+\left(\frac{\tilde{V}^{(n+1)}+\tilde{V}^{(n)}}{2}, A\,\frac{\tilde{V}^{(n+1)}+\tilde{V}^{(n)}}{2}\right)$$

$$-D\left(\frac{\tilde{V}^{(n+1)}+\tilde{V}^{(n)}}{2}, d_x^+ d_x^- \,\frac{\tilde{V}^{(n+1)}+\tilde{V}^{(n)}}{2}\right)$$

$$=\left(\frac{\tilde{V}^{(n+1)}+\tilde{V}^{(n)}}{2}, Q^{(n+1/2)}\right)$$

Now making use of (23) and the positivity of A on the left-hand side, and the Schwarz and triangle inequalities on the right-hand side, we see that this implies

(53) $$\frac{1}{\Delta t}\left(\|\tilde{V}^{(n+1)}\| - \|\tilde{V}^{(n)}\|\right)\frac{\|\tilde{V}^{(n+1)}\| + \|\tilde{V}^{(n)}\|}{2}$$

$$\leq \left\|\frac{\tilde{V}^{(n+1)} + \tilde{V}^{(n)}}{2}\right\| \left\|Q^{(n+1/2)}\right\|$$

$$\leq \frac{\|\tilde{V}^{(n+1)}\| + \|\tilde{V}^{(n)}\|}{2} \left\|Q^{(n+1/2)}\right\|$$

and then, dividing by $\left(\|\tilde{V}^{(n+1)}\| + \|\tilde{V}^{(n)}\|\right)/2$, we get

(54) $$\|\tilde{V}^{(n+1)}\| \leq \|\tilde{V}^{(n)}\| + (\Delta t)\left\|Q^{(n+1/2)}\right\|$$

We now need a bound on $\| Q^{(n+1/2)} \|$, see (47). Let $\overline{R_v}$ be such that

(55) $$\| R_v^{(n+1/2)} \| \leq \overline{R_v}$$

for all n. Such a bound exists because R_v depends only on the exact solution $v(x,t)$ and its derivatives, all of which are bounded.

Because of (11),

(56) $$\left| \frac{v_j^{(n+1)} + v_j^{(n)}}{2} - e_{Na} \right| < (e_{Na} - e_K)$$

(57) $$\left| \frac{v_j^{(n+1)} + v_j^{(n)}}{2} - e_K \right| < (e_{Na} - e_K)$$

Also, from (46),

(58) $$\|PQ - pq\| \leq \|P\tilde{Q}\| + \|\tilde{P}q\|$$

$$\leq \|P\|_{max}\|\tilde{Q}\| + \|\tilde{P}\|\,\|q\|_{max}$$

where

(59) $$\|\phi\|_{max} = \max_j |\phi_j|$$

Thus, if P_j and q_j are both in $(0,1)$ for all j, then

(60) $$\|PQ - pq\| \leq \|\tilde{Q}\| + \|\tilde{P}\|$$

Then, by induction

(61) $$\|\widetilde{S_1^3 S_2}\| \leq 3\|\tilde{S}_1\| + \|\tilde{S}_2\|$$

and

(62) $$\|\widetilde{S_3^4}\| \leq 4\|\tilde{S}_3\|$$

Putting everything together, we therefore get

(63) $$\|Q^{(n+1/2)}\| \leq$$

$$\overline{R_v} + (e_{Na} - e_K)\Big(a_{Na}\big(3\|\tilde{S}_1^{(n+1/2)}\| + \|\tilde{S}_2^{(n+1/2)}\|\big)$$

$$+ a_K 4 \|\tilde{S}_3^{(n+1/2)}\|\Big)$$

and this, together with (54), implies

(64) $$\|\tilde{V}^{(n+1)}\| \leq \|\tilde{V}^{(n)}\| + (\Delta t)\overline{R_v}$$

$$+ (\Delta t)(e_{Na} - e_K)\Big(a_{Na}\big(3\|\tilde{S}_1^{(n+1/2)}\| + \|\tilde{S}_2^{(n+1/2)}\|\big)$$

$$+ a_K 4 \|\tilde{S}_3^{(n+1/2)}\|\Big)$$

In exactly the same way, equation (49) implies

(65) $$\left\| \tilde{S}_i^{(n+1/2)} \right\| \leq \left\| \tilde{S}_i^{(n-1/2)} \right\| + \frac{\Delta t}{\tau_{min}} \left\| Q_i^{(n)} \right\|$$

where

(66) $$Q_{ij}^{(n)} = \sigma_i\left(V_j^{(n)}\right) - \sigma_i\left(v_j^{(n)}\right)$$

$$- \left(\tau_i\left(V_j^{(n)}\right) - \tau_i\left(v_j^{(n)}\right)\right) \frac{s_{ij}^{(n+1/2)} - s_{ij}^{(n-1/2)}}{\Delta t}$$

$$- \left(R_s\right)_{ij}^{(n)}$$

so

(67) $$\left\| Q_i^{(n)} \right\| \leq K \left\| \tilde{V}^{(n)} \right\| + \bar{R}_s$$

In equation (67)

(68) $$K = \max_i \left(\left(\max_v \left| \frac{\partial \sigma_i}{\partial v} \right| \right) + \left(\max_v \left| \frac{\partial \tau_i}{\partial v} \right| \right) \left(\max_{x,t} \left| \frac{\partial s_i}{\partial t} \right| \right) \right)$$

and $\overline{R_s}$ is such that

(69) $$\| R_{si}^{(n)} \| \leq \overline{R_s}$$

for all $n \geq 1$ and $i = 1,2,3$. Such a bound exists by the same reasoning as for $\overline{R_v}$, see below (55), except that here we are concerned with $s_i(x,t)$ and its derivates.

Note the restriction that $n \geq 1$, so we may choose

(70) $$\overline{R_s} = O((\Delta t)^2)$$

see (28).

Combining (65) & (67), we get

(71) $$\left\| \tilde{S}_i^{(n+1/2)} \right\| \leq \left\| \tilde{S}_i^{n-1/2} \right\| + \frac{\Delta t}{\tau_{min}} \left(K \left\| \tilde{V}^{(n)} \right\| + \overline{R_s} \right)$$

for $n = 1, 2, \cdots$

Now let

(72) $$\theta_v^{(n)} = \frac{\left\| \tilde{V}^{(n)} \right\|}{e_{Na} - e_K}$$

(73) $$\theta_s^{(n+1/2)} = \max_i \left\| \tilde{S}_i^{(n+1/2)} \right\|$$

Then (64) $\Rightarrow$

(74) $$\theta_v^{(n+1)} \leq \theta_v^{(n)} + (\Delta t)\left(a\,\theta_s^{(n+1/2)} + r_v\right)$$

for $n = 0, 1, \cdots$

where

(75) $$a = 4(a_{Na} + a_K)$$

(76) $$r_v = \frac{\overline{R_v}}{e_{Na} - e_K}$$

and (71) $\Rightarrow$

(77) $$\theta_s^{(n+1/2)} \leq \theta_s^{(n-1/2)} + (\Delta t)\left(b\,\theta_v^{(n)} + r_s\right)$$

$n = 1, 2, \cdots,$

where

(78) $$b = \frac{K(e_{Na} - e_K)}{\tau_{min}}$$

(79) $$r_s = \frac{\overline{R_s}}{\tau_{min}}$$

The initial conditions for the system of inequalities (74, 77) are

(80) $$\theta_v^{(0)} = 0$$

(81) $$\theta_S^{(1/2)} = c = O((\Delta t)^2)$$

see (51).

Now let $\overline{\theta}_v^{(n)}$ and $\overline{\theta}_S^{(n+1/2)}$ be defined by the corresponding equalities to (74) & (77), namely

(82) $$\overline{\theta}_v^{(n+1)} = \overline{\theta}_v^{(n)} + \Delta t\left(a\,\overline{\theta}_S^{(n+1/2)} + r_v \right)$$

for $n = 0, 1, \cdots$, and

(83) $$\overline{\theta}_S^{(n+1/2)} = \overline{\theta}_S^{(n-1/2)} + \Delta t\left(b\,\overline{\theta}_v^{(n)} + \hat{r}_S \right)$$

with the same initial conditions

(84) $$\overline{\theta}_v^{(0)} = 0$$

(85) $$\overline{\theta}_S^{(1/2)} = c$$

It is then obvious by induction that

(86) $$\theta_v^{(n)} \leq \overline{\theta}_v^{(n)}$$

(87) $$\theta_s^{(n+1/2)} \leq \overline{\theta}_s^{(n+1/2)}$$

for $n = 0, 1, 2, \ldots$

If we lower n by 1 in (82) and subtract the result from (82), and then use (83), we get

(88) $$\overline{\theta}_v^{(n+1)} - 2\overline{\theta}_v^{(n)} + \overline{\theta}_v^{(n-1)}$$

$$= a(\Delta t)^2 \left(b\,\overline{\theta}_v^{(n)} + r_s\right)$$

The initial conditions for this 2nd order difference equation are

(89) $$\overline{\theta}_v^{(0)} = 0$$

(90) $$\overline{\theta}_v^{(1)} = \Delta t\,(ac + r_v)$$

The general solution of (88) is of the form

(91) $$\bar{\theta}_v^{(n)} = -\frac{r_s}{b} + c_1 z_1^n + c_2 z_2^n$$

where z_1 and z_2 are the two solutions of

(92) $$z^2 - \left(2 + ab(\Delta t)^2\right) z + 1 = 0$$

which are

(93) $$z = 1 + \tfrac{1}{2} ab(\Delta t)^2 \pm \sqrt{\left(1 + \tfrac{1}{2} ab(\Delta t)^2\right)^2 - 1}$$

Thus, z_1 and z_2 are real and positive and their product is 1.

To find c_1 and c_2, we use the initial conditions (89-90), which become

(94) $$-\frac{r_s}{b} + c_1 + c_2 = 0$$

(95) $$-\frac{r_s}{b} + c_1 z_1 + c_2 z_2 = \Delta t\left(ac + r_v\right)$$

These equations can be rewritten as the pair

(96) $$\begin{cases} c_1(z_1-1) + c_2(z_2-1) = \Delta t\,(ac+r_v) \\ c_1 + c_2 = \dfrac{r_s}{b} \end{cases}$$

the solution of which is

(97) $$c_1 = \frac{(\Delta t)(ac+r_v) + (1-z_2)\frac{r_s}{b}}{z_1-z_2}$$

(98) $$c_2 = \frac{-(\Delta t)(ac+r_v) + (z_1-1)\frac{r_s}{b}}{z_1-z_2}.$$

Therefore

(99) $$\overline{D}_v^{(n)} = (ac+r_v)(\Delta t)\,\frac{z_1^n - z_2^n}{z_1-z_2} + \frac{r_s}{b}\left(\frac{(1-z_2)z_1^n + (z_1-1)z_2^n}{z_1-z_2} - 1\right)$$

From now on, let z_1 be the larger of the two roots, and recall that the product of the roots is 1, so $z_2 = 1/z_1$

We have

(100) $$z_1 - z_2 = 2\sqrt{\left(1 + \frac{1}{2}ab(\Delta t)^2\right)^2 - 1}$$

$$= 2\sqrt{ab(\Delta t)^2 + \frac{1}{4}(ab)^2(\Delta t)^4}$$

$$> 2\sqrt{ab}\,(\Delta t)$$

Also

(101) $$z_1 = 1 + \frac{1}{2}ab(\Delta t)^2 + \sqrt{ab}\,(\Delta t)\sqrt{1 + \frac{1}{4}ab(\Delta t)^2}$$

$$< 1 + \frac{1}{2}ab(\Delta t)^2 + \sqrt{ab}\,\Delta t\left(1 + \frac{1}{8}ab(\Delta t)^2\right)$$

$$= 1 + \sqrt{ab}\,\Delta t + \frac{1}{2}\left(\sqrt{ab}\,\Delta t\right)^2 + \frac{1}{8}\left(\sqrt{ab}\,\Delta t\right)^3$$

$$< e^{\sqrt{ab}\,\Delta t}$$

and it follows from this that

(102) $$z_2 = \frac{1}{z_1} > e^{-\sqrt{ab}\,\Delta t}$$

Combining (100-102), we get

(103) $$\frac{z_1^n - z_2^n}{z_1 - z_2} < \frac{e^{\sqrt{ab}\,n\Delta t} - e^{-\sqrt{ab}\,n\Delta t}}{2\sqrt{ab}\,\Delta t}$$

$$= \frac{\sinh\left(\sqrt{ab}\,n\Delta t\right)}{\sqrt{ab}\,\Delta t}$$

Also

(104) $$z_1 - 1 = \sqrt{ab}\,\Delta t\sqrt{1+\frac{1}{4}ab(\Delta t)^2} + \frac{1}{2}ab(\Delta t)^2$$

(105) $$1 - z_2 = \sqrt{ab}\,\Delta t\sqrt{1+\frac{1}{4}ab(\Delta t)^2} - \frac{1}{2}ab(\Delta t)^2$$

(106) $$z_1 - z_2 = 2\sqrt{ab}\,\Delta t\sqrt{1+\frac{1}{4}ab(\Delta t)^2}$$

and therefore

(107) $$\frac{z_1 - 1}{z_1 - z_2} = \frac{1}{2} + \frac{1}{4} \frac{\sqrt{ab}\ \Delta t}{\sqrt{1 + \frac{1}{4} ab (\Delta t)^2}}$$

(108) $$\frac{1 - z_2}{z_1 - z_2} = \frac{1}{2} - \frac{1}{4} \frac{\sqrt{ab}\ \Delta t}{\sqrt{1 + \frac{1}{4} ab (\Delta t)^2}}$$

(109) $$\frac{(1 - z_2) z_1^n + (z_1 - 1) z_2^n}{z_1 - z_2} - 1$$

$$= \frac{1}{2}\left(z_1^n - 2 + z_1^{-n}\right) - \frac{1}{4} \frac{\sqrt{ab}\,\Delta t}{\sqrt{1 + \frac{1}{4} ab (\Delta t)^2}} \left(z_1^n - z_1^{-n}\right)$$

$$< \frac{1}{2}\left(z_1^n - 2 + z_1^{-n}\right) = \frac{1}{2}\left(z_1^{n/2} - z_1^{-n/2}\right)^2$$

$$< \frac{1}{2}\left(e^{\frac{1}{2}\sqrt{ab}\, n \Delta t} - e^{-\frac{1}{2}\sqrt{ab}\, n \Delta t}\right)^2$$

$$= 2 \sinh^2\left(\tfrac{1}{2}\sqrt{ab}\ n \Delta t\right)$$

Now combining (99), (103), and (109), we get

$$(110) \qquad \overline{\theta}_v^{(n)} \leq (ac + r_v)\frac{\sinh(\sqrt{ab}\, n\Delta t)}{\sqrt{ab}}$$

$$+ \frac{2r_s}{b}\sinh^2\left(\frac{1}{2}\sqrt{ab}\, n\Delta t\right)$$

We still need a bound on $\overline{\theta}_s$. By repeated use of (83), we get

$$(111) \qquad \overline{\theta}_s^{(n+1/2)} = \overline{\theta}_s^{(1/2)} + \sum_{m=1}^{n}\left(b\overline{\theta}_v^{(m)} + r_s\right)\Delta t$$

$$= c + r_s n\Delta t + b\sum_{m=1}^{n}\overline{\theta}_v^{(m)}\Delta t$$

To bound the last term of (111), we can use (110) and then notice that the resulting sum can be thought of as a midpoint rule approximation to an integral over the interval $\left(\frac{\Delta t}{2}, (n+\frac{1}{2})\Delta t\right)$ of a convex function.

In the case of a convex function, the midpoint rule always gives a smaller value than the integral. Therefore

(112) $$\bar{\theta}_s^{(n+1/2)} \leq C + r_s n\Delta t + \frac{b(ac+r_v)}{\sqrt{ab}} \int_{\frac{\Delta t}{2}}^{(n+\frac{1}{2})\Delta t} \sinh(\sqrt{ab}\, t)\, dt + 2r_s \int_{\frac{\Delta t}{2}}^{(n+1/2)\Delta t} \sinh^2\left(\tfrac{1}{2}\sqrt{ab}\, t\right) dt$$

The term $r_s n\Delta t$ can be combined nicely with the last term of the foregoing, since

(113) $$n\Delta t = \int_{\frac{\Delta t}{2}}^{(n+1/2)\Delta t} dt$$

and since

(114) $$2\sinh^2\left(\tfrac{1}{2}\sqrt{ab}\,t\right) + 1$$

$$= 2\sinh^2\left(\tfrac{1}{2}\sqrt{ab}\,t\right) + \cosh^2\left(\tfrac{1}{2}\sqrt{ab}\,t\right) - \sinh^2\left(\tfrac{1}{2}\sqrt{ab}\,t\right)$$

$$= \sinh^2\left(\tfrac{1}{2}\sqrt{ab}\,t\right) + \cosh^2\left(\tfrac{1}{2}\sqrt{ab}\,t\right)$$

$$= \cosh\left(\sqrt{ab}\,t\right)$$

Thus (112) becomes

(115) $$\bar{\theta}_s^{(n+1/2)} \leq C + \frac{b(ac+r_{2r})}{\sqrt{ab}} \int_{\frac{\Delta t}{2}}^{(n+1/2)\Delta t} \sinh\left(\sqrt{ab}\,t\right) dt$$

$$+ r_s \int_{\frac{\Delta t}{2}}^{(n+1/2)\Delta t} \cosh\left(\sqrt{ab}\,t\right) dt$$

$$\leq c + \frac{b(ac + r_v)}{ab}\left(\cosh\left(\sqrt{ab}\,(n+\tfrac{1}{2})\Delta t\right) - 1\right)$$

$$+ \frac{r_s}{\sqrt{ab}} \sinh\left(\sqrt{ab}\,(n+\tfrac{1}{2})\Delta t\right)$$

$$= c + \left(c + \frac{r_v}{a}\right) 2\sinh^2\left(\tfrac{1}{2}\sqrt{ab}\,(n+\tfrac{1}{2})\Delta t\right)$$

$$+ \frac{r_s}{\sqrt{ab}} \sinh\left(\sqrt{ab}\,(n+\tfrac{1}{2})\Delta t\right)$$

Now we rewrite (110) & (115) in terms of the residuals of our difference scheme. From (51), we may set

(116) $$c = \frac{\Delta t}{2\,\tau_{min}} \overline{R}_s^{(0)}$$

where

(117) $$\overline{R}_s^{(0)} = \max_i \left\| (R_s)_i^{(0)} \right\|$$

Although $\bar{R}_S^{(0)} = O(\Delta t)$, $c = O((\Delta t)^2)$.

Recall also that (equation 76)

(118) $$\hat{r}_v = \frac{\bar{R}_v}{e_{Na} - e_K}$$

and

(119) $$\frac{r_s}{b} = \frac{\bar{R}_s}{K(e_{Na} - e_K)}$$

(120) $$r_s = \frac{\bar{R}_s}{T_{min}}$$

see (78-79). Therefore (110) & (115) become

(121) $$\bar{\theta}_v^{(n)} \le$$

$$\sqrt{\frac{a}{b}}\left(\frac{\Delta t}{2\tau_{min}}\bar{R}_s^{(0)} + \frac{\bar{R}_v}{a(e_{Na}-e_K)}\right)\sinh\left(\sqrt{ab}\,n\Delta t\right)$$

$$+\frac{\bar{R}_s}{K(e_{Na}-e_K)}\,2\sinh^2\left(\frac{1}{2}\sqrt{ab}\,n\Delta t\right)$$

(122) $$\bar{\theta}_s^{(n+1/2)} \le \frac{\Delta t}{2\tau_{min}}\bar{R}_s^{(0)}$$

$$+\left(\frac{\Delta t}{2\tau_{min}}\bar{R}_s^{(0)} + \frac{\bar{R}_v}{a(e_{Na}-e_K)}\right)2\sinh^2\left(\frac{1}{2}\sqrt{ab}\left(n+\frac{1}{2}\right)\Delta t\right)$$

$$+\frac{\bar{R}_s}{\sqrt{ab}\,\tau_{min}}\sinh\left(\sqrt{ab}\left(n+\frac{1}{2}\right)\Delta t\right)$$

The constants a, b in the foregoing error bounds are given by equations (75) and (78). They have units of 1/time.

The constant K is given by (68). It has units of 1/voltage, so the expression $K(e_{Na} - e_K)$ is dimensionless. (The subscript in "e_K" refers to the K^+ ion and has no connection with the constant K.)

The parameters Δt and T_{min} of course have units of time.

The residual R_s is dimensionless, see equations (25-26), but the residual R_v has units of voltage/time, see (24). Thus, the expression

(123) $$\frac{\overline{R_v}}{a(e_{Na} - e_K)}$$

is dimensionless, and indeed, all of the terms in (121-122) are dimensionless.

Now consider a computation that is restricted to some finite time interval $(0,t)$ so that

$$n\Delta t \le t \tag{124}$$

in (121), and

$$\left(n+\tfrac{1}{2}\right)\Delta t \le t \tag{125}$$

in (122). Then, since $\overline{R_S}^{(0)} = O(\Delta t)$, $\overline{R_S} = O((\Delta t)^2)$, and $\overline{R_{\varphi}} = O((\Delta t)^2) + O((\Delta x)^2)$, we have (recalling (72-73) and (86-87) as well as (121-122)):

$$\|\tilde{V}^{(n)}\| = O\left((\Delta t)^2\right) + O\left((\Delta x)^2\right) \tag{126}$$

$$\|\tilde{S}_i^{(n+1/2)}\| = O\left((\Delta t)^2\right) + O\left((\Delta x)^2\right) \tag{127}$$

for $i=1,2,3$,
and this is second-order convergence in the L2 norm.

An interesting consequence of the foregoing is convergence in the maximum norm. To see this, note that

(128) $$\|\phi\|_{max}^2 = \max_j \phi_j^2 \leq \sum_{j=0}^{J-1} \phi_j^2$$

$$= J\left(\frac{1}{J}\sum_{j=0}^{J-1}\phi_j^2\right) = J\|\phi\|^2 = \frac{x_0}{\Delta x}\|\phi\|^2$$

Thus, we have the inequality

(129) $$\|\phi\|_{max} \leq \left(\frac{x_0}{\Delta x}\right)^{1/2}\|\phi\|$$

Therefore, if we choose Δt proportional to Δx so that the right-hand sides of (126) & (127) become simply $O((\Delta x)^2)$, then (126-127) together with (129) imply

(130) $$\|\tilde{V}^{(n)}\|_{max} = O\left((\Delta x)^{3/2}\right)$$

(131) $$\|\tilde{S}_i^{(n+1/2)}\|_{max} = O\left((\Delta x)^{3/2}\right), \quad i=1,2,3$$

and this is pointwise convergence of order 3/2.

An important remark here is that the factor $(1/J)$, or equivalently $\Delta x / x_0$, in the definition of $\| \ \|^2$, see (21), cannot be omitted. If we tried to define $\| \ \|^2$ as simply the sum of the squares of the function values, then we would not have bounds on the norms of the residuals since these would increase without bound as $J \to \infty$.

In the above proof we have followed the outline or paradigm of the Lax equivalence theorem, which, in the forward direction says that

consistency + stability $\Rightarrow$ convergence

The consistency step is the proof that the exact solution of the continuous problem also satisfies a corresponding system of difference equations up to some residual terms, the orders of magnitude of which can be determined by Taylor series. We have not actually done the Taylor series analysis here but have simply stated the result.

The stability step is to study the evolution over time of the error and to show that it can be bounded over a finite time interval in terms of the residuals that were found in the consistency step. It is this part of the analysis that we have done in detail here.