

1 Introduction

We consider the Bidomain equations:

$$\begin{aligned}\chi C_m \frac{\partial v}{\partial t} + \chi(I_{\text{ion}}(v) + I_{\text{stim}}) &= \nabla \cdot (\sigma_i \nabla(v + u_e)) \\ 0 &= \nabla \cdot (\sigma_i \nabla(v + u_e)) + \nabla \cdot (\sigma_e \nabla u_e)\end{aligned}$$

We will be considering Neumann boundary conditions only. The domain is $\Omega = [0, 1]^n$.

We introduce a new state variable w , and the FitzHugh-Nagumo cell model:

$$\begin{aligned}I_{\text{ion}}(v, w) &= \varepsilon^{-1}(v - \frac{v^3}{3} - w) \\ \frac{\partial w}{\partial t} &= \varepsilon(v + \beta - \gamma w)\end{aligned}$$

When we add this cell model into the original equations, we have the new system:

$$\begin{aligned}\chi C_m \frac{\partial v}{\partial t} + \chi \varepsilon^{-1}(v - \frac{v^3}{3} - w) + \chi I_{\text{stim}} &= \nabla \cdot (\sigma_i \nabla(v + u_e)) \\ \frac{\partial w}{\partial t} &= \varepsilon(v + \beta - \gamma w) \\ 0 &= \nabla \cdot (\sigma_i \nabla(v + u_e)) + \nabla \cdot (\sigma_e \nabla u_e)\end{aligned}$$

We will be splitting the above system of equations into an explicit operator involving I_{ion} and I_{stim} :

$$\begin{aligned}\chi C_m \frac{\partial v}{\partial t} + \chi \varepsilon^{-1}(v - \frac{v^3}{3} - w) + \chi I_{\text{stim}} &= 0 \\ \frac{\partial w}{\partial t} &= \varepsilon(v + \beta - \gamma w) \\ 0 &= 0\end{aligned}$$

And an implicit operator involving the Laplacian terms:

$$\begin{aligned}\chi C_m \frac{\partial v}{\partial t} &= \nabla \cdot (\sigma_i \nabla(v + u_e)) \\ \frac{\partial w}{\partial t} &= 0 \\ 0 &= \nabla \cdot (\sigma_i \nabla(v + u_e)) + \nabla \cdot (\sigma_e \nabla u_e)\end{aligned}$$

2 Spatial Discretization

Consider the monolithic system of equations, and let $\mathbf{q} = \begin{bmatrix} v \\ w \\ u_e \end{bmatrix}$. We consider a set of basis functions $\Phi_i : \Omega \rightarrow \mathbb{R}^3$, where each $\Phi_i = \varphi_{b_i} \hat{\mathbf{e}}_{c_i}$ for some basis functions $\varphi_i : \Omega \rightarrow \mathbb{R}$. We make the approximation $\mathbf{q} = Q_j \Phi_j$ (Einstein summation) for a vector $\mathbf{Q} \in \mathbb{R}^N$, where N is the number of degrees of freedom. Also, we approximate $\frac{\partial \mathbf{q}}{\partial t} = \dot{Q}_j \Phi_j$. We multiply the monolithic system of equations by a test function Φ_i and integrate:

$$\begin{aligned} \left\langle \Phi_i \mid \begin{array}{c} \chi C_m \partial_t v \\ \partial_t w \\ 0 \end{array} \right\rangle &= \left\langle \Phi_i \mid \begin{array}{c} -\chi \varepsilon^{-1} (v - \frac{v^3}{3} - w) - \chi I_{\text{stim}} \\ \varepsilon (v + \beta - \gamma w) \\ 0 \end{array} \right\rangle \\ &+ \left\langle \Phi_i \mid \begin{array}{c} \nabla \cdot (\sigma_i \nabla (v + u_e)) \\ 0 \\ \nabla \cdot (\sigma_i \nabla (v + u_e)) + \nabla \cdot (\sigma_e \nabla u_e) \end{array} \right\rangle \end{aligned}$$

Using the fact that $v = Q_j \varphi_{b_j} \delta_{1,c_j}$, $w = Q_j \varphi_{b_j} \delta_{2,c_j}$, and $u_e = Q_j \varphi_{b_j} \delta_{3,c_j}$, as well as $\frac{\partial v}{\partial t} = \dot{Q}_j \varphi_{b_j} \delta_{1,c_j}$ and $\frac{\partial w}{\partial t} = \dot{Q}_j \varphi_{b_j} \delta_{2,c_j}$, we consider each of the forms above:

$$\begin{aligned} \left\langle \Phi_i \mid \begin{array}{c} \chi C_m \partial_t v \\ \partial_t w \\ 0 \end{array} \right\rangle &= \delta_{1,c_i} \langle \varphi_{b_i} \mid \chi C_m \partial_t v \rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid \partial_t w \rangle \\ &= \chi C_m \delta_{1,c_i} \delta_{1,c_j} \langle \varphi_{b_i} \mid \dot{Q}_j \varphi_{b_j} \rangle + \delta_{2,c_i} \delta_{2,c_j} \langle \varphi_{b_i} \mid \dot{Q}_j \varphi_{b_j} \rangle \\ &= (\chi C_m \delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \varphi_{b_i} \mid \varphi_{b_j} \rangle \dot{Q}_j \\ \left\langle \Phi_i \mid \begin{array}{c} -\chi \varepsilon^{-1} (v - \frac{v^3}{3} - w) - \chi I_{\text{stim}} \\ \varepsilon (v + \beta - \gamma w) \\ 0 \end{array} \right\rangle &= \delta_{1,c_i} \left\langle \varphi_{b_i} \mid -\chi \varepsilon^{-1} (v - \frac{v^3}{3} - w) - \chi I_{\text{stim}} \right\rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid \varepsilon (v + \beta - \gamma w) \rangle \\ &= (-\chi \varepsilon^{-1} \delta_{1,c_i} + \varepsilon \delta_{2,c_i}) \langle \varphi_{b_i} \mid v \rangle + (\chi \varepsilon^{-1} \delta_{1,c_i} - \varepsilon \gamma \delta_{2,c_i}) \langle \varphi_{b_i} \mid w \rangle \\ &\quad + \frac{1}{3} \chi \varepsilon^{-1} \delta_{1,c_i} \langle \varphi_{b_i} \mid v^3 \rangle - \chi \delta_{1,c_i} \langle \varphi_{b_i} \mid I_{\text{stim}} \rangle + \varepsilon \beta \delta_{2,c_i} \langle \varphi_{b_i} \mid 1 \rangle \\ &= (-\chi \varepsilon^{-1} \delta_{1,c_i} + \varepsilon \delta_{2,c_i}) \delta_{1,c_j} \langle \varphi_{b_i} \mid Q_j \varphi_{b_j} \rangle + (\chi \varepsilon^{-1} \delta_{1,c_i} - \varepsilon \gamma \delta_{2,c_i}) \delta_{2,c_j} \langle \varphi_{b_i} \mid Q_j \varphi_{b_j} \rangle \\ &\quad + \frac{1}{3} \chi \varepsilon^{-1} \delta_{1,c_i} \langle \varphi_{b_i} \mid v^3 \rangle - \chi \delta_{1,c_i} \langle \varphi_{b_i} \mid I_{\text{stim}} \rangle + \varepsilon \beta \delta_{2,c_i} \langle \varphi_{b_i} \mid 1 \rangle \\ &= (-\chi \varepsilon^{-1} \delta_{1,c_i} \delta_{1,c_j} + \varepsilon \delta_{2,c_i} \delta_{1,c_j} + \chi \varepsilon^{-1} \delta_{1,c_i} \delta_{2,c_j} - \varepsilon \gamma \delta_{2,c_i} \delta_{2,c_j}) \langle \varphi_{b_i} \mid \varphi_{b_j} \rangle Q_j \\ &\quad + \frac{1}{3} \chi \varepsilon^{-1} \delta_{1,c_i} \langle \varphi_{b_i} \mid v^3 \rangle - \chi \delta_{1,c_i} \langle \varphi_{b_i} \mid I_{\text{stim}} \rangle + \varepsilon \beta \delta_{2,c_i} \langle \varphi_{b_i} \mid 1 \rangle \end{aligned}$$

$$\begin{aligned}
& \left\langle \Phi_i \mid \begin{array}{c} \nabla \cdot (\sigma_i \nabla (v + u_e)) \\ 0 \\ \nabla \cdot (\sigma_i \nabla (v + u_e)) + \nabla \cdot (\sigma_e \nabla u_e) \end{array} \right\rangle \\
&= \delta_{\{1,3\},c_i} \langle \varphi_{b_i} \mid \nabla \cdot (\sigma_i \nabla (v + u_e)) \rangle + \delta_{3,c_i} \langle \varphi_{b_i} \mid \nabla \cdot (\sigma_e \nabla u_e) \rangle \\
&= -\delta_{\{1,3\},c_i} \langle \nabla \varphi_{b_i} \mid \sigma_i \nabla (v + u_e) \rangle - \delta_{3,c_i} \langle \nabla \varphi_{b_i} \mid \sigma_e \nabla u_e \rangle \\
&= -\sigma_i \delta_{\{1,3\},c_i} \langle \nabla \varphi_{b_i} \mid \nabla (Q_j \varphi_{b_j} \delta_{\{1,3\},c_j}) \rangle - \sigma_e \delta_{3,c_i} \langle \nabla \varphi_{b_i} \mid \nabla (Q_j \varphi_{b_j} \delta_{3,c_j}) \rangle \\
&= -(\sigma_i \delta_{\{1,3\},c_i} \delta_{\{1,3\},c_j} + \sigma_e \delta_{3,c_i} \delta_{3,c_j}) \langle \nabla \varphi_{b_i} \mid \nabla \varphi_{b_j} \rangle Q_j
\end{aligned}$$

So, define:

$$\begin{aligned}
M_{ij} &= (\chi C_m \delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \varphi_{b_i} \mid \varphi_{b_j} \rangle \\
A_{ij} &= (-\chi \varepsilon^{-1} \delta_{1,c_i} \delta_{1,c_j} + \varepsilon \delta_{2,c_i} \delta_{1,c_j} + \chi \varepsilon^{-1} \delta_{1,c_i} \delta_{2,c_j} - \varepsilon \gamma \delta_{2,c_i} \delta_{2,c_j}) \langle \varphi_{b_i} \mid \varphi_{b_j} \rangle \\
f_i &= -\chi \delta_{1,c_i} \langle \varphi_{b_i} \mid I_{\text{stim}} \rangle + \varepsilon \beta \delta_{2,c_i} \langle \varphi_{b_i} \mid 1 \rangle \\
B_{ij} &= -(\sigma_i \delta_{\{1,3\},c_i} \delta_{\{1,3\},c_j} + \sigma_e \delta_{3,c_i} \delta_{3,c_j}) \langle \nabla \varphi_{b_i} \mid \nabla \varphi_{b_j} \rangle
\end{aligned}$$

Then, we rewrite the monolithic equation as:

$$M\dot{Q} = A\mathbf{Q} + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i} \langle \varphi_{b_i} \mid v^3 \rangle + \mathbf{f} + B\mathbf{Q}$$

And, the split equations become:

$$\begin{aligned}
M\dot{Q} &= A\mathbf{Q} + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i} \langle \varphi_{b_i} \mid v^3 \rangle + \mathbf{f} \\
M\dot{Q} &= B\mathbf{Q}
\end{aligned}$$

3 Time Integration

As a DAE, complications arise when integrating the Bidomain equations because the mass matrix is singular. Our goal is to solve the first ("explicit") equation using an explicit method such as Forward Euler; we solve the second ("implicit") equation using an implicit method such as Backward Euler.

Recall that matrix form of the explicit equation from the previous section:

$$\mathbf{M}\dot{\mathbf{Q}} = \mathbf{A}\mathbf{Q} + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i}\langle\varphi_{b_i} \mid v^3\rangle + \mathbf{f}$$

To integrate this system, we write the equation as:

$$\begin{aligned}\dot{\mathbf{Q}} &= \mathbf{F}_E(t, \mathbf{Q}) \\ &= \mathbf{M}^{-1}(\mathbf{A}\mathbf{Q} + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i}\langle\varphi_{b_i} \mid v^3\rangle + \mathbf{f})\end{aligned}$$

The solution \mathbf{Q}_{t+1} at time step $t+1$ is then given by \mathbf{Q}_t plus a weighted sum of stages $\mathbf{F}_E(t^{(i)}, \mathbf{Q}_t^{(i)})$, where each $\mathbf{Q}_t^{(i)}$ is itself a weighted sum of previously computed stages. However, \mathbf{M} is singular (because no time derivatives of u_e appear in the Bidomain equations), and all components of the explicit equation's right-hand side are zero (because the operator has been split such that the explicit equation does not involve u_e).

Denote the set of all DoF indices by $\mathcal{I} = [0, N)$. Then, let $\mathcal{J} = \{i \in \mathcal{I} \mid c_i \in \{1, 2\}\}$ be the set of indices corresponding to the components v and w . Then:

$$\mathbf{M}_{\mathcal{J}}\dot{\mathbf{Q}}_{\mathcal{J}} = \mathbf{A}_{\mathcal{J}}\mathbf{Q}_{\mathcal{J}} + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i}\langle\varphi_{b_i} \mid v^3\rangle + \mathbf{f}_{\mathcal{J}}$$

Where a matrix or vector subscripted with \mathcal{J} denotes that only those elements with indices in \mathcal{J} are included. Because there are no longer elements corresponding to the u_e component of the system, $\mathbf{M}_{\mathcal{J}}$ is non-singular, and we may write:

$$\mathbf{F}_E(t, \mathbf{Q}_{\mathcal{J}}) = \mathbf{M}_{\mathcal{J}}^{-1}(\mathbf{A}_{\mathcal{J}}\mathbf{Q}_{\mathcal{J}} + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i}\langle\varphi_{b_i} \mid v^3\rangle + \mathbf{f}_{\mathcal{J}})$$

Now, we recall the matrix form of the implicit equation:

$$\mathbf{M}\dot{\mathbf{Q}} = \mathbf{B}\mathbf{Q}$$

Rather than formulating the solution of each time step as a sum of terms, we shall derive an explicit equation that can be solved, corresponding to the Backward Euler and Crank Nicolson methods. First, we again rearrange the equation:

$$\begin{aligned}\dot{\mathbf{Q}} &= \mathbf{F}_I(t, \mathbf{Q}) \\ &= \mathbf{M}^{-1}\mathbf{B}\mathbf{Q}\end{aligned}$$

For Backward Euler:

$$\begin{aligned}
\mathbf{Q}_{t+1} &= \mathbf{Q}_t + h\mathbf{F}_I(t+h, \mathbf{Q}_{t+1}) \\
\mathbf{Q}_{t+1} - \mathbf{Q}_t &= h\mathbf{M}^{-1}\mathbf{B}\mathbf{Q}_{t+1} \\
\mathbf{M}(\mathbf{Q}_{t+1} - \mathbf{Q}_t) &= h\mathbf{B}\mathbf{Q}_{t+1} \\
(\mathbf{M} - h\mathbf{B})\mathbf{Q}_{t+1} &= \mathbf{M}\mathbf{Q}_t
\end{aligned}$$

And, for Crank Nicolson:

$$\begin{aligned}
\mathbf{Q}_{t+1} &= \mathbf{Q}_t + \frac{h}{2}(\mathbf{F}_I(t, \mathbf{Q}_t) + \mathbf{F}_I(t+h, \mathbf{Q}_{t+1})) \\
\mathbf{Q}_{t+1} - \mathbf{Q}_t &= \frac{h}{2}(\mathbf{M}^{-1}\mathbf{B}\mathbf{Q}_t + \mathbf{M}^{-1}\mathbf{B}\mathbf{Q}_{t+1}) \\
\mathbf{M}(\mathbf{Q}_{t+1} - \mathbf{Q}_t) &= \frac{h}{2}(\mathbf{B}\mathbf{Q}_t + \mathbf{B}\mathbf{Q}_{t+1}) \\
(\mathbf{M} - \frac{h}{2}\mathbf{B})\mathbf{Q}_{t+1} &= (\mathbf{M} + \frac{h}{2}\mathbf{B})\mathbf{Q}_t
\end{aligned}$$

We generalize by picking some $\theta \in (0, 1]$:

$$(\mathbf{M} - \theta h\mathbf{B})\mathbf{Q}_{t+1} = (\mathbf{M} + (1 - \theta)h\mathbf{B})\mathbf{Q}_t$$

Where Backward Euler corresponds to $\theta = 1$ and Crank Nicolson corresponds to $\theta = \frac{1}{2}$.

Furthermore, we can pull the same trick as with the explicit equation and define $\mathcal{K} = \{i \in \mathcal{I} \mid c_i \in \{1, 3\}\}$. Note that in the implicit equation, the only involvement of w is the equation $\frac{\partial w}{\partial t} = 0$, so w components (with $c_i = 2$) can be safely ignored. This yields the update formula:

$$(\mathbf{M}_{\mathcal{K}} - \theta h\mathbf{B}_{\mathcal{K}})\mathbf{Q}_{\mathcal{K}, t+1} = (\mathbf{M}_{\mathcal{K}} + (1 - \theta)h\mathbf{B}_{\mathcal{K}})\mathbf{Q}_{\mathcal{K}, t}$$