1 Introduction

This document is relevant to the `bidomain_fhn` target.

We consider the Bidomain equations:

$$\begin{aligned}\chi C_{\mathrm{m}} \frac{\partial v}{\partial t} + \chi(I_{\mathrm{ion}}(v) + I_{\mathrm{stim}}) &= \nabla \cdot (\sigma_{\mathrm{i}} \nabla (v + u_{\mathrm{e}})) \\ 0 &= \nabla \cdot (\sigma_{\mathrm{i}} \nabla (v + u_{\mathrm{e}})) + \nabla \cdot (\sigma_{\mathrm{e}} \nabla u_{\mathrm{e}})\end{aligned}$$

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:

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

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

$$\begin{aligned}\chi C_{\mathrm{m}} \frac{\partial v}{\partial t} + \chi \varepsilon^{-1}(v - \frac{v^3}{3} - w) + \chi I_{\mathrm{stim}} &= \nabla \cdot (\sigma_{\mathrm{i}} \nabla (v + u_{\mathrm{e}})) \\ \frac{\partial w}{\partial t} &= \varepsilon(v + \beta - \gamma w) \\ 0 &= \nabla \cdot (\sigma_{\mathrm{i}} \nabla (v + u_{\mathrm{e}})) + \nabla \cdot (\sigma_{\mathrm{e}} \nabla u_{\mathrm{e}})\end{aligned}$$

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

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

And an implicit operator involving the Laplacian terms:

$$\begin{aligned}\chi C_{\mathrm{m}} \frac{\partial v}{\partial t} &= \nabla \cdot (\sigma_{\mathrm{i}} \nabla (v + u_{\mathrm{e}})) \\ \frac{\partial w}{\partial t} &= 0 \\ 0 &= \nabla \cdot (\sigma_{\mathrm{i}} \nabla (v + u_{\mathrm{e}})) + \nabla \cdot (\sigma_{\mathrm{e}} \nabla u_{\mathrm{e}})\end{aligned}$$

2 Spatial Discretization

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

$$\left\langle \boldsymbol{\Phi}_i \mid \begin{matrix} \chi C_\mathrm{m} \partial_t v \\ \partial_t w \\ 0 \end{matrix} \right\rangle = \left\langle \boldsymbol{\Phi}_i \mid \begin{matrix} -\chi\varepsilon^{-1}(v - \frac{v^3}{3} - w) - \chi I_\mathrm{stim} \\ \varepsilon(v + \beta - \gamma w) \\ 0 \end{matrix} \right\rangle$$
$$+ \left\langle \boldsymbol{\Phi}_i \mid \begin{matrix} \nabla \cdot (\sigma_\mathrm{i} \nabla (v + u_\mathrm{e})) \\ 0 \\ \nabla \cdot (\sigma_\mathrm{i} \nabla (v + u_\mathrm{e})) + \nabla \cdot (\sigma_\mathrm{e} \nabla u_\mathrm{e}) \end{matrix} \right\rangle$$

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 $u_\mathrm{e} = Q_j \varphi_{b_j} \delta_{3,c_j}$, 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:

$$\begin{aligned}
&\left\langle \boldsymbol{\Phi}_i \mid \begin{matrix} \chi C_\mathrm{m} \partial_t v \\ \partial_t w \\ 0 \end{matrix} \right\rangle \\
&= \delta_{1,c_i} \langle \varphi_{b_i} \mid \chi C_\mathrm{m} \partial_t v \rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid \partial_t w \rangle \\
&= \chi C_\mathrm{m} \delta_{1,c_i} \delta_{1,c_j} \left\langle \varphi_{b_i} \mid \dot{Q}_j \varphi_{b_j} \right\rangle + \delta_{2,c_i} \delta_{2,c_j} \left\langle \varphi_{b_i} \mid \dot{Q}_j \varphi_{b_j} \right\rangle \\
&= (\chi C_\mathrm{m} \delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \left\langle \varphi_{b_i} \mid \varphi_{b_j} \right\rangle \dot{Q}_j
\end{aligned}$$

$$\begin{aligned}
&\left\langle \boldsymbol{\Phi}_i \mid \begin{matrix} -\chi\varepsilon^{-1}(v - \frac{v^3}{3} - w) - \chi I_\mathrm{stim} \\ \varepsilon(v + \beta - \gamma w) \\ 0 \end{matrix} \right\rangle \\
&= \delta_{1,c_i} \left\langle \varphi_{b_i} \mid -\chi\varepsilon^{-1}(v - \frac{v^3}{3} - w) - \chi I_\mathrm{stim} \right\rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid \varepsilon(v + \beta - \gamma w) \rangle \\
&= (-\chi\varepsilon^{-1}\delta_{1,c_i} + \varepsilon\delta_{2,c_i}) \langle \varphi_{b_i} \mid v \rangle + (\chi\varepsilon^{-1}\delta_{1,c_i} - \varepsilon\gamma\delta_{2,c_i}) \langle \varphi_{b_i} \mid w \rangle \\
&\quad + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i} \left\langle \varphi_{b_i} \mid v^3 \right\rangle - \chi\delta_{1,c_i} \langle \varphi_{b_i} \mid I_\mathrm{stim} \rangle + \varepsilon\beta\delta_{2,c_i} \langle \varphi_{b_i} \mid 1 \rangle \\
&= (-\chi\varepsilon^{-1}\delta_{1,c_i} + \varepsilon\delta_{2,c_i})\delta_{1,c_j} \left\langle \varphi_{b_i} \mid Q_j \varphi_{b_j} \right\rangle + (\chi\varepsilon^{-1}\delta_{1,c_i} - \varepsilon\gamma\delta_{2,c_i})\delta_{2,c_j} \left\langle \varphi_{b_i} \mid Q_j \varphi_{b_j} \right\rangle \\
&\quad + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i} \left\langle \varphi_{b_i} \mid v^3 \right\rangle - \chi\delta_{1,c_i} \langle \varphi_{b_i} \mid I_\mathrm{stim} \rangle + \varepsilon\beta\delta_{2,c_i} \langle \varphi_{b_i} \mid 1 \rangle \\
&= (-\chi\varepsilon^{-1}\delta_{1,c_i}\delta_{1,c_j} + \varepsilon\delta_{2,c_i}\delta_{1,c_j} + \chi\varepsilon^{-1}\delta_{1,c_i}\delta_{2,c_j} - \varepsilon\gamma\delta_{2,c_i}\delta_{2,c_j}) \left\langle \varphi_{b_i} \mid \varphi_{b_j} \right\rangle Q_j \\
&\quad + \frac{1}{3}\chi\varepsilon^{-1}\delta_{1,c_i} \left\langle \varphi_{b_i} \mid v^3 \right\rangle - \chi\delta_{1,c_i} \langle \varphi_{b_i} \mid I_\mathrm{stim} \rangle + \varepsilon\beta\delta_{2,c_i} \langle \varphi_{b_i} \mid 1 \rangle
\end{aligned}$$

$$
\begin{aligned}
&\left\langle \boldsymbol{\Phi}_i \;\middle|\; \begin{matrix} \nabla\cdot(\sigma_{\mathrm{i}}\nabla(v+u_{\mathrm{e}})) \\ 0 \\ \nabla\cdot(\sigma_{\mathrm{i}}\nabla(v+u_{\mathrm{e}})) + \nabla\cdot(\sigma_{\mathrm{e}}\nabla u_{\mathrm{e}}) \end{matrix} \right\rangle \\
&\quad = \delta_{\{1,3\},c_i} \left\langle \varphi_{b_i} \mid \nabla\cdot(\sigma_{\mathrm{i}}\nabla(v+u_{\mathrm{e}}))\right\rangle + \delta_{3,c_i} \left\langle \varphi_{b_i} \mid \nabla\cdot(\sigma_{\mathrm{e}}\nabla u_{\mathrm{e}})\right\rangle \\
&\quad = -\delta_{\{1,3\},c_i} \left\langle \nabla\varphi_{b_i} \mid \sigma_i\nabla(v+u_{\mathrm{e}})\right\rangle - \delta_{3,c_i} \left\langle \nabla\varphi_{b_i} \mid \sigma_{\mathrm{e}}\nabla u_{\mathrm{e}}\right\rangle \\
&\quad = -\sigma_{\mathrm{i}}\delta_{\{1,3\},c_i} \left\langle \nabla\varphi_{b_i} \mid \nabla(Q_j\varphi_{b_j}\delta_{\{1,3\},c_j})\right\rangle - \sigma_{\mathrm{e}}\delta_{3,c_i} \left\langle \nabla\varphi_{b_i} \mid \nabla(Q_j\varphi_{b_j}\delta_{3,c_j})\right\rangle \\
&\quad = -(\sigma_{\mathrm{i}}\delta_{\{1,3\},c_i}\delta_{\{1,3\},c_j} + \sigma_{\mathrm{e}}\delta_{3,c_i}\delta_{3,c_j}) \left\langle \nabla\varphi_{b_i} \mid \nabla\varphi_{b_j}\right\rangle Q_j
\end{aligned}
$$

So, define:

$$
\begin{aligned}
M_{ij} &= (\chi C_{\mathrm{m}}\delta_{1,c_i}\delta_{1,c_j} + \delta_{2,c_i}\delta_{2,c_j}) \left\langle \varphi_{b_i} \mid \varphi_{b_j}\right\rangle \\
A_{ij} &= (-\chi\varepsilon^{-1}\delta_{1,c_i}\delta_{1,c_j} + \varepsilon\delta_{2,c_i}\delta_{1,c_j} + \chi\varepsilon^{-1}\delta_{1,c_i}\delta_{2,c_j} - \varepsilon\gamma\delta_{2,c_i}\delta_{2,c_j}) \left\langle \varphi_{b_i} \mid \varphi_{b_j}\right\rangle \\
f_i &= -\chi\delta_{1,c_i} \left\langle \varphi_{b_i} \mid I_{\mathrm{stim}}\right\rangle + \varepsilon\beta\delta_{2,c_i} \left\langle \varphi_{b_i} \mid 1\right\rangle \\
B_{ij} &= -(\sigma_{\mathrm{i}}\delta_{\{1,3\},c_i}\delta_{\{1,3\},c_j} + \sigma_{\mathrm{e}}\delta_{3,c_i}\delta_{3,c_j}) \left\langle \nabla\varphi_{b_i} \mid \nabla\varphi_{b_j}\right\rangle
\end{aligned}
$$

Then, we rewrite the monolithic equation as:

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

And, the split equations become:

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

3 Spatial Non-Discretization

Spatially discretizing the explicit operator performs poorly. Instead, we directly update the system using the formulas:

$$
\begin{aligned}
\frac{\partial V_i}{\partial t} &= \varepsilon^{-1}(V_i - \frac{1}{3}V_i^3 - W_i) + I_{\mathrm{stim}}(\boldsymbol{p}_i) \\
\frac{\partial W_i}{\partial t} &= \varepsilon(V_i + \beta - \gamma W_i)
\end{aligned}
$$

Where V_i and W_i are the DoFs associated with $\boldsymbol{v}$ and $\boldsymbol{w}$. This is a pointwise update for each DoF: for the `FE_Q` Lagrange finite element (and for certain other finite elements), each DoF i can be associated with a spatial point $\boldsymbol{p}_i$ at which the shape function $\varphi_i(\boldsymbol{p}_i) = 1$. So, a pointwise evaluation of this operator is justified. The deal.II function `VectorTools::interpolate` handles the evaluation of I_{stim} at these support points.

4 Time Integration

Time integration of the explicit operator is accomplished using an explicit Runge-Kutta method; the formulas from the previous section can be passed directly to a Runge-Kutta stepper since they are already in the required form.

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

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

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:

$$\begin{aligned} \dot{\boldsymbol{Q}} &= \boldsymbol{F}_{\mathrm{I}}(t, \boldsymbol{Q}) \\ &= \boldsymbol{M}^{-1}\boldsymbol{B}\boldsymbol{Q} \end{aligned}$$

For Backward Euler:

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

And, for Crank Nicolson:

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

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

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

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