Chaste: Finite Element Implementations

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This document lists the finite element implementations used in various solvers in the Chaste codebase. Section 1 can be read as an introduction to the stages required in converting Poisson's equation and the heat equation into finite element linear systems, while the remaining sections can be used as references for the solvers.

Contents

1 Finite element solution of basic equations

1.1 Poisson's equation

Let $\Omega \subset \mathbb{R}^n$, and let $\partial\Omega^{\mathrm{dir}}$ and $\partial\Omega^{\mathrm{neu}}$ be two non-intersecting subsets of the boundary of Ω whose union is the entire boundary. Consider Poisson's equation with mixed Dirichlet-Neumann boundary conditions:

$$\begin{aligned} \nabla^2 u &= f(x) \qquad (1)\\ u &= u^*(x) \qquad \text{on } \partial\Omega^{\mathrm{dir}} \\ \boldsymbol{\nabla} u \cdot \mathbf{n} &= g(x) \qquad \text{on } \partial\Omega^{\mathrm{neu}} \end{aligned}$$

where $\mathbf{n}$ is the unit *outward-facing* normal.

The weak form of this equation is found by multiplying by a test function[1] satisfying $v(\partial\Omega^{\text{dir}}) = 0$ (i.e. v is zero on the Dirichlet part of the boundary), and integrating using the divergence theorem:

$$\begin{aligned} 0 &= -\int_\Omega \left(\nabla^2 u\right) v \,\mathrm{d}V + \int_\Omega f v \,\mathrm{d}V && \forall v \in V_0 \\ &= \int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v \,\mathrm{d}V - \int_{\partial\Omega} v \boldsymbol{\nabla} u \cdot \mathbf{n} \,\mathrm{d}S + \int_\Omega f v \,\mathrm{d}V && \forall v \in V_0 \\ &= \int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v \,\mathrm{d}V - \int_{\partial\Omega^{\text{dir}}} v \boldsymbol{\nabla} u \cdot \mathbf{n} \,\mathrm{d}S - \int_{\partial\Omega^{\text{neu}}} v \boldsymbol{\nabla} u \cdot \mathbf{n} \,\mathrm{d}S + \int_\Omega f v \,\mathrm{d}V && \forall v \in V_0 \end{aligned}$$

Using the facts that v is zero on $\partial\Omega^{\text{dir}}$ and $\boldsymbol{\nabla} u \cdot \mathbf{n} = g$ on $\partial\Omega^{\text{neu}}$, we have the weak form: find u such that $u = u^*$ on $\partial\Omega^{\text{dir}}$ satisfying:

$$\int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v \,\mathrm{d}V - \int_{\partial\Omega^{\text{neu}}} g v \,\mathrm{d}S + \int_\Omega f v \,\mathrm{d}V = 0 \qquad \forall v \in V_0$$

For simplicity we now just consider the case $u^* = 0$. The finite element discretisation is obtained by choosing a set of piecewise polynomial basis functions (such as linear basis functions), one for each node in $\Omega\backslash\partial\Omega^{\text{dir}}$, i.e. one for each node at which u is unknown: $\{\phi_1, \phi_2, \ldots, \phi_N\}$, where N is the number of nodes; and restricting the test functions v to just these basis functions, to obtain N equations:

$$\int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} \phi_i \,\mathrm{d}V - \int_{\partial\Omega^{\text{neu}}} g \phi_i \,\mathrm{d}S + \int_\Omega f \phi_i \,\mathrm{d}V \qquad i = 1, \ldots, N,$$

and then approximating u by $u = \sum_{j=1}^N U_j \phi_j$, where U_j is the approximation of $u(x_j)$. Since $\boldsymbol{\nabla} u$ is then equal to $\sum_{j=1}^N U_j \boldsymbol{\nabla} \phi_j$, this gives

$$\int_\Omega \sum_{j=1}^N U_j \boldsymbol{\nabla} \phi_j \cdot \boldsymbol{\nabla} \phi_i \,\mathrm{d}V - \int_{\partial\Omega^{\text{neu}}} g \phi_i \,\mathrm{d}S + \int_\Omega f \phi_i \,\mathrm{d}V \qquad i = 1, \ldots, N,$$

or

$$\sum K_{ij} U_j = b_i, \quad i = 1, \ldots, N,$$

where K is the *stiffness matrix*:

$$K_{ij} = \int_\Omega \boldsymbol{\nabla} \phi_i \cdot \boldsymbol{\nabla} \phi_j \,\mathrm{d}V, \tag{2}$$

and

$$b_i = \int_{\partial\Omega^{\text{neu}}} g \phi_i \,\mathrm{d}S - \int_\Omega f \phi_i \,\mathrm{d}V,$$

or in other words, the linear system

$$K\mathbf{U} = \mathbf{b}.$$

1.1.1 Applying Dirichlet boundary conditions

In practice, we allow the test functions to vary over *all* the nodes, and then apply the Dirichlet boundary conditions by altering the rows of the matrix K: zeroing the row and setting the diagonal to be one; and the

[1] From some suitable space V (actually the Sobolev space H^1). We write V_0 for $\{v \in V : v(\partial\Omega^{\text{dir}}) = 0\}$.

vector $\mathbf{b}$: setting its value to be the boundary condition value. If k corresponds to a node with a Dirichlet boundary condition, the new row of the linear system looks like:

$$\begin{bmatrix} 0\dots 0 & 1 & 0\dots 0 \end{bmatrix} \begin{bmatrix} \vdots \\ U_k \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ u^*(x_k) \\ \vdots \end{bmatrix}$$

(i.e. the equation $U_k = u^*(x_k)$ in matrix form). And actually, we then alter the matrix and right-hand-side vector again so that the k-th *column* of the matrix becomes zeroed with a one on the diagonal, in order to maintain symmetry.

1.2 The heat equation

Now consider the heat equation with mixed Dirichlet-Neumann boundary conditions and an initial condition: find $u(t,x)$ satisfying

$$\begin{aligned} \frac{\partial u}{\partial t} &= \nabla^2 u \\ u &= u^*(x) \qquad \text{on } \partial\Omega^{\text{dir}} \\ \boldsymbol{\nabla} u \cdot \mathbf{n} &= g(x) \qquad \text{on } \partial\Omega^{\text{neu}} \\ u(0,x) &= u_0(x) \end{aligned} \tag{3}$$

There are two possible time-discretisations: the explicit approach:

$$\frac{u^{m+1}-u^m}{\Delta t} = \nabla^2 u^m,$$

or the implicit approach

$$\frac{u^{m+1}-u^m}{\Delta t} = \nabla^2 u^{m+1}.$$

We choose the latter as it is unconditionally stable, and as with the finite element method (in contrast to the finite difference method), a linear system would still have to be solved if the explicit approach were taken. For the heat equation with a nonlinear source term (such as the monodomain equation—see later):

$$\frac{\partial u}{\partial t} = \nabla^2 u + f(u),$$

we choose a *semi-implicit* discretisation

$$\frac{u^{m+1}-u^m}{\Delta t} = \nabla^2 u^{m+1} + f(u^m), \tag{4}$$

since a fully-implicit discretisation would require the solution of a nonlinear system.

The weak form corresponding to (3) with an implicit time-discretisation is: given u^m, find u^{m+1} such that $u^{m+1} = u^*$ on $\partial\Omega^{\text{dir}}$ satisfying:

$$\frac{1}{\Delta t}\int_\Omega u^{m+1} v \,\mathrm{d}V + \int_\Omega \boldsymbol{\nabla} u^{m+1} \cdot \boldsymbol{\nabla} v \,\mathrm{d}V = \frac{1}{\Delta t}\int_\Omega u^m v \,\mathrm{d}V + \int_{\partial\Omega^{\text{neu}}} g v \,\mathrm{d}S \qquad \forall v \in V_0$$

Letting v be $\phi_1, \dots, \phi_N$ as before, and with $u = \sum U_j \phi_j$, we get the finite element approximation

$$\frac{1}{\Delta t} M\mathbf{U}^{m+1} + K\mathbf{U}^{m+1} = \frac{1}{\Delta t} M\mathbf{U}^m + \mathbf{b},$$

where M is the *mass matrix*

$$M_{ij} = \int_\Omega \phi_i \phi_j \, \mathrm{d}V,$$

where K is the stiffness matrix defined in (2), and here (since we have no source term), $\mathbf{b}$ is just

$$b_i = \int_{\partial\Omega^{\mathrm{neu}}} g\phi_i \, \mathrm{d}S.$$

Dirichlet boundary conditions are then applied as described in Section 1.1.1.

2 Chaste PDE solvers

2.1 `SimpleLinearEllipticSolver`

This takes in an `AbstractLinearEllipticPde` and boundary conditions, which overall are of the form

$$\begin{aligned}
\nabla \cdot (D(x)\boldsymbol{\nabla} u) + \alpha(x)u + c(x) &= 0 \\
u &= u^*(x) \qquad \text{on } \partial\Omega^{\mathrm{dir}} \\
(D(x)\boldsymbol{\nabla} u)\cdot \mathbf{n} &= g(x) \qquad \text{on } \partial\Omega^{\mathrm{neu}}
\end{aligned}$$

where $D(x)$ is a matrix-valued function, and α and c are scalar-valued functions, all provided by the user. *Note that the Neumman boundary condition the user provides is* $(D(x)\boldsymbol{\nabla} u)\cdot\mathbf{n}$, *not* $\boldsymbol{\nabla} u\cdot\mathbf{n}$. When D is the identity matrix and $\alpha \equiv 0$ this is just (1).

The weak form is: find u such that $u = u^*$ on $\partial\Omega^{\mathrm{dir}}$ satisfying:

$$\int_\Omega (D\boldsymbol{\nabla} u)\cdot\boldsymbol{\nabla} v \, \mathrm{d}V - \int_{\partial\Omega^{\mathrm{neu}}} gv\, \mathrm{d}S - \int_\Omega \alpha u v \, \mathrm{d}V - \int_\Omega cv\, \mathrm{d}V = 0 \qquad \forall v \in V_0$$

Letting v be $\phi_1, \dots, \phi_N$ and with $u = \sum U_j\phi_j$ as before, the finite element approximation is

$$K\mathbf{U} - M\mathbf{U} = \mathbf{b},$$

where here the stiffness matrix is now dependent on the diffusion tensor $D(x)$

$$K_{ij} = \int_\Omega \boldsymbol{\nabla}\phi_i \cdot (D\boldsymbol{\nabla}\phi_j) \, \mathrm{d}V, \tag{5}$$

and the mass-matrix is dependent on $\alpha(x)$

$$M_{ij} = \int_\Omega \alpha\phi_i\phi_j \, \mathrm{d}V,$$

and the right-hand-side vector is

$$b_i = \int_{\partial\Omega^{\mathrm{neu}}} g\phi_i \, \mathrm{d}S + \int_\Omega c\phi_i \, \mathrm{d}V.$$

Dirichlet boundary conditions are then applied as described in Section 1.1.1. (Note also that in the code we do not (currently) distinguish between the two matrices: the 'full' matrix to be assembled is $A = K - M$, so the linear system is $A\mathbf{U} = \mathbf{b}$).

2.2 SimpleLinearParabolicSolver

This solver is for parabolic problems defined by an `AbstractLinearParabolicPde` and boundary conditions, which overall are of the form

$$
\begin{aligned}
k(x)\frac{\partial u}{\partial t} &= \nabla\cdot(D(x)\boldsymbol{\nabla} u) + f(x,u) \qquad (6)\\
u &= u^*(x) \qquad \text{on } \partial\Omega^{\text{dir}}\\
\boldsymbol{\nabla} u\cdot\mathbf{n} &= g(x) \qquad \text{on } \partial\Omega^{\text{neu}}\\
u(0,x) &= u_0(x)
\end{aligned}
$$

where $D(x)$ is a matrix-valued function, and k and f are scalar-valued functions, all provided by the user. Again, the Neumman boundary condition the user provides is $(D(x)\boldsymbol{\nabla} u)\cdot\mathbf{n}$, not $\boldsymbol{\nabla} u\cdot\mathbf{n}$.

Using a semi-implicit discretisation as in (4), the weak form is find u^{m+1} such that $u^{m+1} = u^*$ on $\partial\Omega^{\text{dir}}$ satisfying:

$$
\begin{aligned}
&\frac{1}{\Delta t}\int_\Omega k u^{m+1} v \,\mathrm{d}V + \int_\Omega \left(D\boldsymbol{\nabla} u^{m+1}\right)\cdot\boldsymbol{\nabla} v\,\mathrm{d}V\\
=\;& \frac{1}{\Delta t}\int_\Omega k u^{m} v\,\mathrm{d}V + \int_\Omega f(x,u^m)v\,\mathrm{d}V + \int_{\partial\Omega^{\text{neu}}} g v\,\mathrm{d}S \qquad \forall v\in V_0
\end{aligned}
$$

The finite element approximation is therefore given by

$$
\frac{1}{\Delta t}M\mathbf{U}^{m+1} + K\mathbf{U}^{m+1} = \frac{1}{\Delta t}M\mathbf{U}^m + \mathbf{c},
$$

where K is the diffusion-tensor dependent stiffness matrix given by (5), the mass matrix depends on $k(x)$

$$
M_{ij} = \int_\Omega k\phi_i\phi_j\,\mathrm{d}V,
$$

and $\mathbf{c}$ depends on the solution at the previous time

$$
c_i = \int_\Omega f(x,u^m)\phi_i\,\mathrm{d}V + \int_{\partial\Omega^{\text{neu}}} g\phi_i\,\mathrm{d}S.
$$

Dirichlet boundary conditions are then applied as described in Section 1.1.1. Again, in the code we do not (currently) distinguish between the two matrices: the 'full' matrix to be assembled is $A = K + M/\Delta t$, and the 'full' right-hand-side vector is $\mathbf{b} = \frac{1}{\Delta t}M\mathbf{U}^m + \mathbf{c}$; and we then solve $A\mathbf{U} = \mathbf{b}$.

2.3 SimpleNonlinearEllipticSolver

This takes in an `AbstractNonlinearEllipticPde` and boundary conditions, which overall are of the form

$$
\begin{aligned}
\nabla\cdot(D(x,u)\boldsymbol{\nabla} u) + f(x,u) &= 0\\
u &= u^*(x) \qquad \text{on } \partial\Omega^{\text{dir}}\\
(D(x,u)\boldsymbol{\nabla} u)\cdot\mathbf{n} &= g(x) \qquad \text{on } \partial\Omega^{\text{neu}}
\end{aligned}
$$

The weak form is: find u such that $u = u^*$ on $\partial\Omega^{\text{dir}}$ satisfying:

$$
\int_\Omega (D(x,u)\boldsymbol{\nabla} u)\cdot\boldsymbol{\nabla} v\,\mathrm{d}V - \int_{\partial\Omega^{\text{neu}}} g v\,\mathrm{d}S - \int_\Omega f(x,u)v\,\mathrm{d}V = 0 \qquad \forall v\in V_0
$$

The *nonlinear* finite element problem is then: find the solution $\mathbf{U}$ of the nonlinear set of equations: $\mathbf{f}(\mathbf{U}) = 0$, where

$$f_i(\mathbf{U}) = \int_\Omega \left(D\left(x, \sum U_j\phi_j\right)\boldsymbol{\nabla}u\right)\cdot\boldsymbol{\nabla}\phi_i\,\mathrm{d}V - \int_{\partial\Omega^{\text{neu}}} g\phi_i\,\mathrm{d}S - \int_\Omega f\left(x, \sum U_j\phi_j\right)\phi_i\,\mathrm{d}V = 0$$

(using $u = \sum U_j\phi_j$), together with the Dirichlet boundary conditions. This can be solved using the Newton (or a Newton-like) method. $\mathbf{f}$ is the residual vector, and the matrix that is computed is the Jacobian, $\frac{\partial f_i}{\partial U_j}$.

3 Cardiac electrophsiology

3.1 The monodomain equations

The monodomain equations are

$$\begin{aligned} \chi\left(\mathcal{C}\frac{\partial V}{\partial t} + I_{\text{ion}}(\mathbf{u}, V)\right) - \nabla\cdot(\sigma\boldsymbol{\nabla}V) + I^{(\text{vol})} &= 0, & (7)\\ \frac{\partial\mathbf{u}}{\partial t} &= \mathbf{f}(\mathbf{u}, V), & (8)\end{aligned}$$

where $\sigma(x)$ is an effective conductivity[2], χ is the surface-area-to-volume ratio, $\mathcal{C}$ is the capacitance across the membrane, $I^{(\text{vol})}(x)$ the stimulus current (per unit volume) and $I_{\text{ion}}(\mathbf{u}, V)$ the ionic current (per unit area) provided by the cell model.

This is exactly the form given by (6), with $k = \chi\mathcal{C}$ (constant), $D = \sigma$ and $f(x, u) = -I^{(\text{vol})} - \chi I_{\text{ion}}(\mathbf{u}, V)$. We usually take the Neumman boundary condition to be zero for monodomain problems, although we can also use an surface stimulus, in which case $g = I^{(\text{surf})}(x)$. The weak form and finite element discretisation are therefore those given in Section 2.2, but for easy comparison with the source code we write this out fully. The weak form is: find V^{m+1} satisfying

$$\begin{aligned} &\frac{\chi\mathcal{C}}{\Delta t}\int_\Omega V^{m+1}v\,\mathrm{d}^3\mathbf{x} + \int_\Omega\left(\sigma\boldsymbol{\nabla}V^{m+1}\right)\cdot\boldsymbol{\nabla}v\,\mathrm{d}^3\mathbf{x}\\ = &\frac{\chi\mathcal{C}}{\Delta t}\int_\Omega V^{m}v\,\mathrm{d}^3\mathbf{x} - \int_\Omega\left(I^{(\text{vol})} + \chi I_{\text{ion}}(\mathbf{u}, V^m)\right)v\,\mathrm{d}^3\mathbf{x}\\ &+ \int_{\partial\Omega^{\text{neu}}} I^{(\text{surf})}v\,\mathrm{d}S \qquad \forall v \in V_0\end{aligned}$$

(having used $\mathrm{d}^3\mathbf{x}$ rather than $\mathrm{d}V$ as V denotes voltage), giving the FE problem

$$\left(\frac{\chi\mathcal{C}}{\Delta t}M + K\right)\mathbf{V}^{m+1} = \frac{\chi\mathcal{C}}{\Delta t}M\mathbf{V}^m + \mathbf{c},$$

where $M_{ij} = \int\phi_i\phi_j\,\mathrm{d}^3\mathbf{x}$, $K_{ij} = \int\boldsymbol{\nabla}\phi_i\cdot(\sigma\boldsymbol{\nabla}\phi_j)\,\mathrm{d}^3\mathbf{x}$ and

$$c_i = -\int_\Omega\left(I^{(\text{vol})} + \chi I_{\text{ion}}(\mathbf{u}, V^m)\right)\phi_i\,\mathrm{d}^3\mathbf{x} + \int_{\partial\Omega^{\text{neu}}} I^{(\text{surf})}\phi_i\,\mathrm{d}S.$$

The only complication is that the cell model ODEs are given at the nodes (not quadrature points), so $I_{\text{ion}}(\mathbf{u}, V)$ is only initially known at the nodes, and has to be interpolated onto the quadrature points

[2]The monodomain equations apply if the extracellular conductivity σ_e is a multiple of the intracellular conductivity σ_i: $\sigma_e = \lambda\sigma_i$ say. The effective conductivity for the monodomain equation is then $\sigma = \frac{\lambda}{1+\lambda}\sigma_i$.

3.2 The bidomain equations

The bidomain problem in full generality is: find $V(t,x)$ and $\phi_e(t,x)$ satisfying:

$$\begin{aligned}\chi\left(\mathcal{C}\frac{\partial V}{\partial t}+I_{\text{ion}}(\mathbf{u},V)\right)-\nabla\cdot\left(\sigma_i\boldsymbol{\nabla}\left(V+\phi_e\right)\right) &= -I_i^{(\text{vol})}, && (9)\\ \nabla\cdot\left(\sigma_i\boldsymbol{\nabla}V+\left(\sigma_i+\sigma_e\right)\boldsymbol{\nabla}\phi_e\right) &= I_{\text{total}}^{(\text{vol})}, && (10)\\ \frac{\partial\mathbf{u}}{\partial t} &= \mathbf{f}\left(\mathbf{u},V\right),\end{aligned}$$

where $I_{\text{total}}^{(\text{vol})}=I_i^{(\text{vol})}+I_e^{(\text{vol})}$, with boundary conditions

$$\begin{aligned}\mathbf{n}\cdot\left(\sigma_i\boldsymbol{\nabla}\left(V+\phi_e\right)\right) &= I_i^{(\text{surf})}, && (11)\\ \mathbf{n}\cdot\left(\sigma_e\boldsymbol{\nabla}\phi_e\right) &= I_e^{(\text{surf})}. && (12)\end{aligned}$$

There are now two PDEs, so there are two equations the in the weak form: find V, ϕ_e satisfying

$$\begin{aligned}&\frac{\chi\mathcal{C}}{\Delta t}\int_\Omega V^{m+1}v\,\mathrm{d}^3\mathbf{x}+\int_\Omega\left(\sigma_i\boldsymbol{\nabla}(V^{m+1}+\phi_e^{m+1}\right)\cdot\boldsymbol{\nabla}v\,\mathrm{d}^3\mathbf{x}\\ =\;&\frac{\chi\mathcal{C}}{\Delta t}\int_\Omega V^m v\,\mathrm{d}^3\mathbf{x}-\int_\Omega\left(I_i^{(\text{vol})}+\chi I_{\text{ion}}(\mathbf{u},V^m)\right)v\,\mathrm{d}^3\mathbf{x}\\ &+\int_{\partial\Omega^{\text{neu}}}I_i^{(\text{surf})}v\,\mathrm{d}S\qquad\forall v\in V_0 &&(13)\end{aligned}$$

and

$$\begin{aligned}&\int_\Omega\left(\sigma_i\boldsymbol{\nabla}V+\left(\sigma_i+\sigma_e\right)\boldsymbol{\nabla}\phi_e\right)\cdot\boldsymbol{\nabla}v\,\mathrm{d}^3\mathbf{x}\\ =\;&-\int_\Omega I_{\text{total}}^{(\text{vol})}v\,\mathrm{d}^3\mathbf{x}+\int_{\partial\Omega^{\text{neu}}}I_{\text{total}}^{(\text{surf})}v\,\mathrm{d}S\qquad\forall v\in V_0 &&(14)\end{aligned}$$

(where $I_{\text{total}}^{(\text{surf})}$ is obviously $I_i^{(\text{surf})}+I_e^{(\text{surf})}$).

For the finite element discretisation, we set choose a set of basis functions $\psi_1,\psi_2,\ldots,\psi_N$ (now using ψ instead of ϕ for basis functions as the latter denotes electrical potential), set $V=\sum V_k\psi_k$ and $\phi_e=\sum\Phi_k\psi_k$ (now avoiding the use of i as a subscript, since it denotes 'intracellular'), and set $v=\psi_j$ in turn in (13) and (14) to obtain $2N$ equations. For any particular conductivity σ, let us define the stiffness matrix $K[\sigma]$ by

$$\left(K[\sigma]\right)_{jk}=\int_\Omega\boldsymbol{\nabla}\psi_j\cdot\left(\sigma\boldsymbol{\nabla}\psi_k\right)\,\mathrm{d}^3\mathbf{x}. \tag{15}$$

The first N equations are:

$$\frac{\chi\mathcal{C}}{\Delta t}M\mathbf{V}^{m+1}+K[\sigma_i]\mathbf{V}^{m+1}+K[\sigma_i]\boldsymbol{\Phi}_e^{m+1}=\frac{\chi\mathcal{C}}{\Delta t}M\mathbf{V}^m+\mathbf{c}^{(1)},$$

(here $\boldsymbol{\Phi}_e=(\Phi_1,\ldots,\Phi_N)$), where

$$c_j^{(1)}=\int_\Omega-\left(I_i^{(\text{vol})}+\chi I_{\text{ion}}(\mathbf{u},V^m)\right)\psi_j\,\mathrm{d}^3\mathbf{x}+\int_{\partial\Omega^{\text{neu}}}I_i^{(\text{surf})}\psi_j\,\mathrm{d}S. \tag{16}$$

The second N equations are:

$$K[\sigma_i]\mathbf{V}^{m+1}+K[\sigma_i+\sigma_e]\boldsymbol{\Phi}_e^{m+1}=\mathbf{c}^{(2)},$$

where

$$c_j^{(2)}=-\int_\Omega I_{\text{total}}^{(\text{vol})}\psi_j\,\mathrm{d}^3\mathbf{x}+\int_{\partial\Omega^{\text{neu}}}I_e^{(\text{surf})}\psi_j\,\mathrm{d}S.$$

Note: in the code, we do not allow the direct specification of $I_e^{(\mathrm{vol})}$, and in order for compatibility conditions to be satisfied[3], force $I_{\mathrm{total}}^{(\mathrm{vol})}$ to be zero (i.e. implicitly choose $I_e^{(\mathrm{vol})} = I_i^{(\mathrm{vol})}$), so that actually

$$c_j^{(2)} = \int_{\partial\Omega^{\mathrm{neu}}} I_{\mathrm{total}}^{(\mathrm{surf})} \psi_j \,\mathrm{d}S$$

only[4].

Overall, we have the $2N$ equations

$$\begin{pmatrix} \frac{\chi\mathcal{C}}{\Delta t}M + K[\sigma_i] & K[\sigma_i] \\ K[\sigma_i] & K[\sigma_i+\sigma_e] \end{pmatrix} \begin{pmatrix} \mathbf{V}^{m+1} \\ \mathbf{\Phi}_e^{m+1} \end{pmatrix} = \begin{pmatrix} \frac{\chi\mathcal{C}}{\Delta t}M\mathbf{V}^m + \mathbf{c}^{(1)} \\ \mathbf{c}^{(2)} \end{pmatrix}$$

3.3 The bidomain equations with a perfusing bath

For the bidomain problem with a perfusing bath, the implementation quickly becomes more difficult to write, so for clarity let us temporarily take all the stimuli to be zero, and also take $\chi = \mathcal{C} = 1$. We will also occasionally write ϕ_i instead of $V + \phi_e$, again for clarity.

We suppose there are two disjoint domains, Ω (tissue) and Ω_b (the bath), with interface $\partial\Omega$ (the boundary of the tissue). In this problem ϕ_i (and therefore V) is only defined in Ω, but ϕ_e is defined throughout $\Omega \cup \Omega_b$.

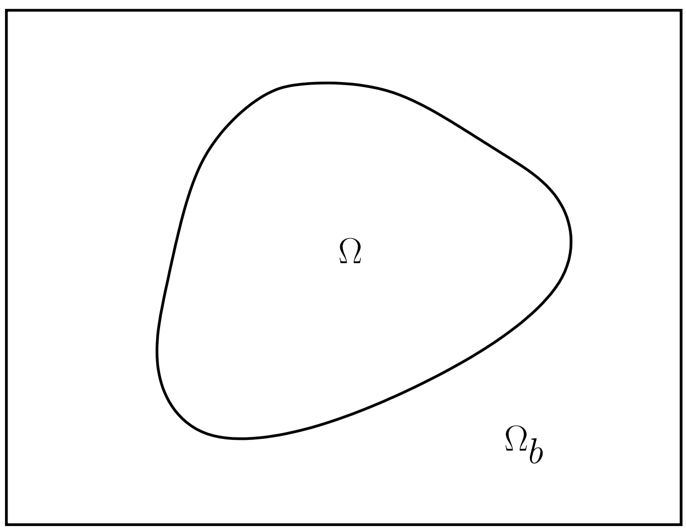

Figure 1: Domains in a model of cardiac tissue contained in a conductive bath.

The problem to be solved is: find $V \in H^1(\Omega)$ and $\phi_e \in H^1(\Omega \cup \Omega_b)$ satisfying

$$\begin{aligned} \frac{\partial V}{\partial t} - \nabla\cdot(\sigma_i \boldsymbol{\nabla}\phi_i) + I_{\mathrm{ion}} &= 0, \qquad \text{in } \Omega && (17)\\ \nabla\cdot(\sigma_i\boldsymbol{\nabla}\phi_i + \sigma_e\boldsymbol{\nabla}\phi_e) &= 0, \qquad \text{in } \Omega && (18)\\ \nabla\cdot(\sigma_b\boldsymbol{\nabla}\phi_e) &= 0, \qquad \text{in } \Omega_b && (19)\\ \frac{\partial \mathbf{u}}{\partial t} &= \mathbf{f}(\mathbf{u}, V), \end{aligned}$$

[3]See numerics paper.

[4]$\int_{\partial\Omega^{\mathrm{neu}}} I_{\mathrm{total}}^{(\mathrm{surf})}\,\mathrm{d}S$ also needs to be zero (if no Dirichlet boundary conditions), so the electrodes class makes sure $I_e^{(\mathrm{surf})}$ takes equal and opposite values on the opposite faces of the bath.

with boundary conditions:

$$\begin{aligned}
\mathbf{n}\cdot(\sigma_i \boldsymbol{\nabla}\phi_i) &= 0, \qquad \text{on } \partial\Omega \text{ (i.e. tissue boundary)} && (20)\\
\mathbf{n}\cdot(\sigma_b \boldsymbol{\nabla}\phi_e) &= 0, \qquad \text{on } \partial\Omega_b\backslash\partial\Omega \text{ (i.e. bath boundary)} && (21)
\end{aligned}$$

and suitable initial conditions. An interface boundary condition is also required: it is

$$\mathbf{n}\cdot(\sigma_e \boldsymbol{\nabla}\phi_e)\big|_{\Omega\to\partial\Omega} + \mathbf{n}\cdot(\sigma_b \boldsymbol{\nabla}\phi_e)\big|_{\Omega_b\to\partial\Omega} = 0 \qquad \text{on } \partial\Omega \tag{22}$$

(where $\big|_{\Omega\to\partial\Omega}$ denotes the limit as $\mathbf{x}\in\Omega$ tends to $\partial\Omega$), and $\big|_{\Omega_b\to\partial\Omega}$ denotes the limit as $\mathbf{x}\in\Omega_b$ tends to $\partial\Omega$). This is the condition which will arise naturally in the weak form (see below).

The first equation of weak form is found by multiplying (17) by $v\in H^1(\Omega)$ and integrating using the divergence theorem:

$$\begin{aligned}
0 &= \int_\Omega \frac{\partial V}{\partial t} v\,\mathrm{d}^3\mathrm{x} + \int_\Omega (\sigma_i \boldsymbol{\nabla}\phi_i)\cdot\boldsymbol{\nabla}v\,\mathrm{d}^3\mathrm{x} - \int_{\partial\Omega} v\,(\sigma_i \boldsymbol{\nabla}\phi_i)\cdot\mathbf{n}\,\mathrm{d}S + \int_\Omega I_{\text{ion}} v\,\mathrm{d}^3\mathrm{x} \qquad \forall v\in H^1(\Omega)\\
&= \int_\Omega \frac{\partial V}{\partial t} v\,\mathrm{d}^3\mathrm{x} + \int_\Omega (\sigma_i \boldsymbol{\nabla}\phi_i)\cdot\boldsymbol{\nabla}v\,\mathrm{d}^3\mathrm{x} + \int_\Omega I_{\text{ion}} v\,\mathrm{d}^3\mathrm{x} \qquad \forall v\in H^1(\Omega)
\end{aligned}$$

the boundary integral vanishing due to (20).

The second equation in the weak form is found by multiplying (18) and (19) (essentially one equation over the whole domain $\Omega\cup\Omega_b$) by $w\in H^1(\Omega\cup\Omega_b)$ (note the larger domain) and integrating using the divergence theorem:

$$\begin{aligned}
0 = \quad & \int_\Omega (\sigma_i \boldsymbol{\nabla}\phi_i + \sigma_e \boldsymbol{\nabla}\phi_e)\cdot\boldsymbol{\nabla}w\,\mathrm{d}^3\mathrm{x} - \int_{\partial\Omega} w\,(\sigma_i \boldsymbol{\nabla}\phi_i + \sigma_e \boldsymbol{\nabla}\phi_e)\cdot\mathbf{n}\big|_{\Omega\to\partial\Omega}\,\mathrm{d}S\\
& + \int_{\Omega_b} (\sigma_b \boldsymbol{\nabla}\phi_e)\cdot\boldsymbol{\nabla}w\,\mathrm{d}^3\mathrm{x} - \int_{\partial\Omega} w\,(\sigma_b \boldsymbol{\nabla}\phi_e)\cdot\mathbf{n}\big|_{\Omega_b\to\partial\Omega}\,\mathrm{d}S - \int_{\partial\Omega_b} w\,(\sigma_b \boldsymbol{\nabla}\phi_e)\cdot\mathbf{n}\,\mathrm{d}S \quad \forall w\in H^1(\Omega\cup\Omega_b)
\end{aligned}$$

Here, the last boundary integral vanishes due to the boundary condition (21), as does the first part of the first boundary integral, $\int_{\partial\Omega} w\,(\sigma_i \boldsymbol{\nabla}\phi_i)\cdot\mathbf{n}\big|_{\Omega\to\partial\Omega}\,\mathrm{d}S$, due to (20). The remaining boundary terms are

$$-\int_{\partial\Omega} w\,(\sigma_e \boldsymbol{\nabla}\phi_e)\cdot\mathbf{n}\big|_{\Omega\to\partial\Omega}\,\mathrm{d}S - \int_{\partial\Omega} w\,(\sigma_b \boldsymbol{\nabla}\phi_e)\cdot\mathbf{n}\big|_{\Omega_b\to\partial\Omega}\,\mathrm{d}S$$

Now, $w\in H^1(\Omega\cup\Omega_b)$, so w continuous across the interface, i.e. $w\big|_{\Omega\to\partial\Omega} = w\big|_{\Omega_b\to\partial\Omega}$, so the above is equal to

$$-\int_{\partial\Omega} w\left((\sigma_i \boldsymbol{\nabla}\phi_i)\cdot\mathbf{n}\big|_{\Omega\to\partial\Omega} + (\sigma_b \boldsymbol{\nabla}\phi_e)\cdot\mathbf{n}\big|_{\Omega_b\to\partial\Omega}\right)\mathrm{d}S$$

which is zero due to the interface condition (22). Hence all the surface-integrals in the second equation of the weak form also vanish.

The full weak problem is therefore: find $V\in H^1(\Omega)$ and $\phi_e\in H^1(\Omega\cup\Omega_b)$ satisfying (initial conditions and):

$$\int_\Omega \frac{\partial V}{\partial t} v\,\mathrm{d}^3\mathrm{x} + \int_\Omega (\sigma_i \boldsymbol{\nabla}\phi_i)\cdot\boldsymbol{\nabla}v\,\mathrm{d}^3\mathrm{x} + \int_\Omega I_{\text{ion}} v\,\mathrm{d}^3\mathrm{x} = 0 \quad \forall v\in H^1(\Omega) \tag{23}$$

and

$$\int_\Omega (\sigma_i \boldsymbol{\nabla}\phi_i + \sigma_e \boldsymbol{\nabla}\phi_e)\cdot\boldsymbol{\nabla}w\,\mathrm{d}^3\mathrm{x} + \int_{\Omega_b} (\sigma_b \boldsymbol{\nabla}\phi_e)\cdot\boldsymbol{\nabla}w\,\mathrm{d}^3\mathrm{x} = 0 \quad \forall w\in H^1(\Omega\cup\Omega_b) \tag{24}$$

For the finite element discretisation, assume for convenience that Ω and Ω_b are open (i.e. $\partial\Omega$ is not contained in either Ω or Ω_b. Let $K<N<N+M$, and suppose there are K nodes in the interior of Ω, $N-K$ nodes on the boundary $\partial\Omega$, and M nodes in Ω_b:

$$\begin{aligned}
\mathbf{x}_1,\ldots,\mathbf{x}_K &\in \Omega \qquad \text{and therefore} \notin \partial\Omega\\
\mathbf{x}_{K+1},\ldots,\mathbf{x}_N &\in \partial\Omega\\
\mathbf{x}_{N+1},\ldots,\mathbf{x}_{N+M} &\in \Omega_b \qquad \text{and therefore} \notin \partial\Omega
\end{aligned}$$

as shown in Figure***

The basis functions are then

$$\underbrace{\psi_1, \ldots, \psi_K}_{=0 \text{ in } \Omega_b}, \underbrace{\psi_{K+1}, \ldots, \psi_N}_{\neq 0 \text{ in } \Omega \text{ or } \Omega_b}, \underbrace{\psi_{N+1}, \ldots, \psi_{N+M}}_{=0 \text{ in } \Omega}$$

We can write $V = \sum_{j=1}^{N} V_j \psi_j$. This technically would give V non-zero in a small band outside Ω, where V isn't defined, so this has to be understood to apply only for $\mathbf{x} \in \Omega \cup \partial\Omega\ (= \overline{\Omega})$. Also, $\phi_e = \sum_{j=1}^{N+M} \Phi_j \psi_j$. Let $\mathbf{V} = (V_1, \ldots, V_N)$, $\mathbf{\Phi} = (\Phi_1, \ldots, \Phi_{N+M})$ and define $\mathbf{\Phi}_{(1)} = (\Phi_1, \ldots, \Phi_N)$, i.e. the first N components of $\mathbf{\Phi}$.

The final finite element linear system will of size $2N + M$. The first N equations are given by setting $v = \psi_j$, $j = 1, \ldots, N$ in (23). Since $\psi_{N+1}, \ldots, \psi_{N+M}$ are zero in $\Omega \cup \partial\Omega$, this equation is only dependent on $\Phi_1, \ldots, \Phi_N$, i.e. on $\mathbf{\Phi}_{(1)}$ rather than the full $\mathbf{\Phi}$. We get, as in Section 3.2,

$$\frac{1}{\Delta t} M \mathbf{V}^{m+1} + K[\sigma_i]\left(\mathbf{V}^{m+1} + \mathbf{\Phi}_{(1)}^{m+1}\right) = \frac{1}{\Delta t} M \mathbf{V}^m + \mathbf{c}^{(1)} \tag{25}$$

where M in the $N \times N$ mass stiffness, and $K[\sigma_i]$ is the $N \times N$ stiffness matrix using conductivity σ_i.

The remaining $N + M$ equations are obtained by setting $w = \psi_1, \ldots, \psi_{N+M}$ in (24). This gives

$$\begin{aligned} 0 \;=\; & \sum_{k=1}^{N} V_k \int_\Omega (\sigma_i \nabla \psi_k) \cdot \nabla \psi_j \, \mathrm{d}^3\mathbf{x} \\ & + \sum_{k=1}^{N+M} \Phi_k \left(\int_\Omega ((\sigma_i + \sigma_e) \nabla \psi_k) \cdot \nabla \psi_j \, \mathrm{d}^3\mathbf{x} + \int_{\Omega_b} (\sigma_b \nabla \psi_k) \cdot \nabla \psi_j \, \mathrm{d}^3\mathbf{x} \right) \qquad j = 1, \ldots, N+M \end{aligned} \tag{26}$$

The first term here is: $K[\sigma_i]\mathbf{V}$ for equations $j = 1, \ldots, N$; and zero for equations $j = N+1, \ldots, N+M$ (as then $\psi_j = 0$ in Ω), i.e.

$$\begin{pmatrix} K[\sigma_i]\mathbf{V} \\ \mathbf{0} \end{pmatrix} \begin{array}{l} \}\text{ size } N \\ \}\text{ size } M \end{array}$$

The second term can be written as the product $\mathcal{K}\mathbf{\Phi}$, where $\mathcal{K}$ is the $(N+M) \times (N+M)$ matrix:

$$\mathcal{K}_{jk} = \int_\Omega ((\sigma_i + \sigma_e) \nabla \psi_k) \cdot \nabla \psi_j \, \mathrm{d}^3\mathbf{x} + \int_{\Omega_b} (\sigma_b \nabla \psi_k) \cdot \nabla \psi_j \, \mathrm{d}^3\mathbf{x} \tag{27}$$

which we write in 2 by 2 block matrix form

$$\mathcal{K} = \begin{pmatrix} \mathcal{K}_{(1,1)} & \mathcal{K}_{(1,2)} \\ \mathcal{K}_{(2,1)} & \mathcal{K}_{(2,2)} \end{pmatrix} \begin{array}{l} \}\text{ size } N \\ \}\text{ size } M \end{array}$$

So overall we have that (26) in matrix form is:

$$\begin{bmatrix} K[\sigma_i] & \mathcal{K}_{(1,1)} & \mathcal{K}_{(1,2)} \\ 0 & \mathcal{K}_{(2,1)} & \mathcal{K}_{(2,2)} \end{bmatrix} \begin{bmatrix} \mathbf{V}^{m+1} \\ \mathbf{\Phi}_{(1)}^{m+1} \\ \mathbf{\Phi}_{(2)}^{m+1} \end{bmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix} \begin{array}{l} \}\text{ first } N \text{ equations of (26)} \\ \}\text{ next } M \text{ equations of (26)} \end{array} \tag{28}$$

Finally, we put together (25) and (28) to get the full finite element system

$$\begin{bmatrix} \frac{1}{\Delta t} M + K[\sigma_i] & K[\sigma_i] & 0 \\ K[\sigma_i] & \mathcal{K}_{(1,1)} & \mathcal{K}_{(1,2)} \\ 0 & \mathcal{K}_{(2,1)} & \mathcal{K}_{(2,2)} \end{bmatrix} \begin{bmatrix} \mathbf{V}^{m+1} \\ \mathbf{\Phi}_{(1)}^{m+1} \\ \mathbf{\Phi}_{(2)}^{m+1} \end{bmatrix} = \begin{bmatrix} \frac{1}{\Delta t} M \mathbf{V}^m + \mathbf{c}^{(1)} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{array}{l} \}\text{ size } N \\ \}\text{ size } N \\ \}\text{ size } M \end{array}$$

Note that $\mathcal{K}_{(1,2)} = \mathcal{K}_{(2,1)}$ and is nearly all zero—it is only non-zero at values corresponding to nodes on or near $\partial\Omega$.

In practice, for implementation/parallelisation reasons, we introduce a set of dummy voltages values at the bath nodes, $V_{N+1}, \ldots, V_{N+M}$, and also include the equations

$$V_j = 0, \qquad j = N+1, \ldots, N+M.$$

Letting $\mathbf{V}_{(1)} = \mathbf{V}$, and $\mathbf{V}_{(2)} = (V_{N+1}, \ldots, V_{N+M})$ (i.e. the vector of dummy values), and letting I_M denote the M by M identity matrix, we have

$$\begin{bmatrix} \frac{1}{\Delta t}M + K[\sigma_i] & 0 & K[\sigma_i] & 0 \\ 0 & I_M & 0 & 0 \\ K[\sigma_i] & 0 & \mathcal{K}_{(1,1)} & \mathcal{K}_{(1,2)} \\ 0 & 0 & \mathcal{K}_{(2,1)} & \mathcal{K}_{(2,2)} \end{bmatrix} \begin{bmatrix} \mathbf{V}^{m+1}_{(1)} \\ \mathbf{V}^{m+1}_{(2)} \\ \mathbf{\Phi}^{m+1}_{(1)} \\ \mathbf{\Phi}^{m+1}_{(2)} \end{bmatrix} = \begin{bmatrix} \frac{1}{\Delta t}M\mathbf{V}^m + \mathbf{c}^{(1)} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{matrix} \}\text{ size } N \\ \}\text{ size } M \\ \}\text{ size } N \\ \}\text{ size } M \end{matrix}$$

3.3.1 The bidomain problem with a bath, including stimuli and parameters

We know re-state the above without the simplications. The problem to be solved is: find $V \in H^1(\Omega)$ and $\phi_e \in H^1(\Omega \cup \Omega_b)$ satisfying

$$\begin{aligned} \chi\mathcal{C}\frac{\partial V}{\partial t} - \nabla \cdot (\sigma_i \boldsymbol{\nabla}\phi_i) + \chi I_{\text{ion}} + I_i^{(\text{vol})} &= 0, && \text{in } \Omega \\ \nabla \cdot (\sigma_i \boldsymbol{\nabla}\phi_i + \sigma_e \boldsymbol{\nabla}\phi_e) &= 0, && \text{in } \Omega \\ \nabla \cdot (\sigma_b \boldsymbol{\nabla}\phi_e) &= 0, && \text{in } \Omega_b \\ \frac{\partial \mathbf{u}}{\partial t} &= \mathbf{f}(\mathbf{u}, V), \end{aligned}$$

with boundary conditions:

$$\begin{aligned} \mathbf{n} \cdot (\sigma_i \boldsymbol{\nabla}\phi_i) &= I_i^{(\text{surf})}, && \text{on } \partial\Omega \text{ (i.e. tissue boundary)} \\ \mathbf{n} \cdot (\sigma_b \boldsymbol{\nabla}\phi_e) &= I_e^{(\text{surf})}, && \text{on } \partial\Omega_b \backslash \partial\Omega \text{ (i.e. bath boundary)} \end{aligned}$$

and interface boundary condition

$$\mathbf{n} \cdot (\sigma_e \boldsymbol{\nabla}\phi_e)\big|_{\Omega \to \partial\Omega} + \mathbf{n} \cdot (\sigma_b \boldsymbol{\nabla}\phi_e)\big|_{\Omega_b \to \partial\Omega} = 0 \qquad \text{on } \partial\Omega$$

Note: we are assuming $I_{\text{total}}^{(\text{vol})} = 0$ in the 2nd PDE, as described in the end of Section 3.2, i.e. implicitly choosing $I_e^{(\text{vol})} = -I_i^{(\text{vol})}$; we have not allowed a volume bath stimulus; and $I_e^{(\text{surf})}$, acting on the bath boundary only, corresponds to electrodes.

The finite element problem is

$$\begin{bmatrix} \frac{\chi\mathcal{C}}{\Delta t}M + K[\sigma_i] & 0 & K[\sigma_i] & 0 \\ 0 & I_M & 0 & 0 \\ K[\sigma_i] & 0 & \mathcal{K}_{(1,1)} & \mathcal{K}_{(1,2)} \\ 0 & 0 & \mathcal{K}_{(2,1)} & \mathcal{K}_{(2,2)} \end{bmatrix} \begin{bmatrix} \mathbf{V}^{m+1}_{(1)} \\ \mathbf{V}^{m+1}_{(2)} \\ \mathbf{\Phi}^{m+1}_{(1)} \\ \mathbf{\Phi}^{m+1}_{(2)} \end{bmatrix} = \begin{bmatrix} \frac{\chi\mathcal{C}}{\Delta t}M\mathbf{V}^m + \mathbf{c}^{(1)} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{c}^{(2)} \end{bmatrix} \begin{matrix} \}\text{ size } N \\ \}\text{ size } M \\ \}\text{ size } N \\ \}\text{ size } M \end{matrix}$$

where $M_{jk} = \int \psi_j \psi_k \,\mathrm{d}^3\mathbf{x}$ is the standard mass matrix, $K[\sigma]$ is defined by (15), $\mathcal{K}$ is defined by (27), and

$$\begin{aligned} c_j^{(1)} &= \int_\Omega -\left(I_i^{(\text{vol})} + \chi I_{\text{ion}}(\mathbf{u}, V^m)\right)\psi_j \,\mathrm{d}^3\mathbf{x} + \int_{\partial\Omega} I_i^{(\text{surf})}\psi_j \,\mathrm{d}S, \\ c_j^{(2)} &= \int_{\partial\Omega_b} I_e^{(\text{surf})}\psi_{j+N} \,\mathrm{d}S. \end{aligned}$$

4 Mechanics

4.1 Nonlinear elasticity

We now describe how to solve solid mechanics problems using the finite element method. We assume the material in question: undergoes large deformations, which means that nonlinear elasticity (also known as finite elasticity) has to be used; is incompressible; and is hyperelastic, which means there exists a strain-energy function (to be defined shortly).

Let $\Omega_0 \subset \mathbb{R}^3$ denote a body in its undeformed, stress-free configuration, and let $\mathbf{X}$ be a point in Ω_0. Let the deformed configuration, under some given loads, be given by Ω, and let $\mathbf{x}(\mathbf{X}) \in \Omega$ be the corresponding point in a deformed configuration.

The important deformation-based quantities are the deformation gradient and deformation tensor. The deformation gradient is defined to be

$$F = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \qquad \text{i.e.} \qquad F_{iM} = \frac{\partial x_i}{\partial X_M},$$

from which the Green deformation tensor is defined to be

$$C = F^{\mathrm{T}} F \qquad \text{i.e.} \qquad C_{MN} = F_{iM} F_{iN},$$

The Lagrangian strain tensor is $E = \frac{1}{2}(C - I)$ but it is easier to work with C rather than E.

There are three important stress tensors: the *Cauchy stress*, σ or σ_{ij}, which is a measure of the true stress in the body, the force acting on a surface in the deformed body, per unit deformed area; the first Piola-Kirchhoff tensor, S or S_{Mi}, which measures the force acting on a surface in the deformed body per unit *undeformed* area; and the *second Piola-Kirchhoff stress*, T, or T_{MN}, which is a transformed (non-physical) stress, the force 'acting' on a surface in the *undeformed* body, per unit *undeformed* area. σ and T are symmetric. The relationship between the stresses are

$$\sigma = \frac{1}{\det F} F S, \qquad T = S F^{-\mathrm{T}}, \qquad \sigma = \frac{1}{\det F} F T F^{\mathrm{T}}$$

To link stress and strain (or stress and deformation), a material-law is required, which is a nonlinear functional relationship between stress and deformation-gradient: $T \equiv T(C)$ (or alternatively, $T \equiv T(E)$, $S \equiv S(F)$, $\sigma = \sigma(F)$, etc). The material law is material-dependent and can only be determined by experiment.

The definition of hyperelasticity is that there exists a strain energy function $W \equiv W(E)$, from which the 2nd Piola-Kirchhoff stress is determined by $T = \frac{\partial W}{\partial E}$. Equivalently, $W \equiv W(C)$ and $T = 2\frac{\partial W}{\partial C}$. In the *isotropic* case, the strain energy becomes dependent on, rather than all the components of C, just the three *principal invariants* of C, which are $I_1 = \mathrm{tr}(C)$, $I_2 = \frac{1}{2}((\mathrm{tr}(C))^2 - \mathrm{tr}(C^2))$, and $I_3 = \det C$. An example of a simple (compressible) isotropic strain energy is $W(C) = c_1(I_1 - 3) + c_2(I_2 - 3) + c_3(I_3 - 1)$, which gives the stress to be[5] $T = 2\frac{\partial W}{\partial C} = c_1 I + c_2(I_1 I - C) + c_3 I_3 C^{-1}$

In compressible elasticity, the equations of static equilibrium which determine the new configuration $\mathbf{x}(\mathbf{X})$ given a material law $T \equiv T(C(\mathbf{x}))$ is

$$\frac{\partial}{\partial X_M}\left(T_{MN}(\mathbf{x}) F_{iN}(\mathbf{x})\right) + \rho_0 b_i = 0 \qquad \text{in } \Omega_0, \tag{29}$$

where $\rho_0 b_i$ is the applied body force, defined below, with appropriate boundary conditions, also defined below. Since $T_{MN} F_{iN}$ is just the first Piola-Kirchhoff stress S_{Mi}, this equation is just $\nabla \cdot S + \rho_0 \mathbf{b} = 0$—"divergence of stress plus body force equals zero."

[5]Some useful formulae: for an matrix A, $\frac{\partial(\det(A))}{\partial A_{pq}} = \det(A)(A^{-1})_{qp}$ and $\frac{\partial A^{-1}_{MN}}{\partial A_{PQ}} = -A^{-1}_{MP} A^{-1}_{QN}$ (differentiate $A^{-1}A = I$); for $I_1(A)$, $\frac{\partial I_1}{\partial A_{MN}} = \delta_{MN}$ and $\frac{\mathrm{d}^2 I_1}{\mathrm{d}A_{MN} \partial A_{PQ}} = 0$; for $I_2(A)$, $\frac{\partial I_2}{\partial A_{MN}} = I_1 \delta_{MN} - A_{MN}$ and $\frac{\partial^2 I_2}{\partial A_{MN} \partial A_{PQ}} = \delta_{MN}\delta_{PQ} - \delta_{MP}\delta_{NQ}$.

In incompressible elasticity, we have in addition the constraint of incompressibility, which is $\det F = 1$. Since this is equivalent to $I_3 = 1$, the form of the (isotropic) material law changes to

$$W(I_1, I_2, I_3) = W^{\text{mat}}(I_1, I_2) - \frac{p}{2}(I_3 - 1),$$

where W^{mat} is material-dependent and determined by experimentation, and p is the pressure—a Lagrange multiplier corresponding to the constraint $I_3 = 1$ which has to be computed together with the deformation. This material law gives the 2nd Piola-Kirchhoff stress to be $T = 2\frac{\partial W}{\partial C} = 2\frac{\partial W^{\text{mat}}}{\partial C} - pC^{-1}$, for which the second term here corresponds to a Cauchy stress of $\sigma_{ij} = -p\delta_{ij}$, hence the interpretation of p as a pressure.

The full problem in the incompressible problem case is to find $\mathbf{x} \equiv \mathbf{x}(\mathbf{X})$ and $p \equiv p(\mathbf{X})$ given a material law $T \equiv T(C(\mathbf{x}), p)$ satisfying

$$\begin{aligned} \frac{\partial}{\partial X_M}\left(T_{MN}(\mathbf{x}, p)F_{iN}(\mathbf{x})\right) + \rho_0 b_i &= 0, \qquad (30)\\ \det F &= 1, \qquad (31) \end{aligned}$$

$\mathbf{b}$ is the body force per unit mass (generally equal to $(0, 0, -g)$ if the effect of gravity is not neglected, or zero otherwise), and ρ_0 is the density. Suitable boundary conditions are the specification of the deformation on part of the boundary of Ω_0 and surface traction on the remainder of $\partial\Omega_0$:

$$\begin{aligned} \mathbf{x} &= \mathbf{x}^* \qquad \text{on } \partial\Omega_0^{\text{disp}}\\ TF^{\mathrm{T}}\mathbf{N} &= \mathbf{s} \qquad \text{on } \partial\Omega_0^{\text{trac}} \end{aligned}$$

where $\mathbf{x}^*$ is the specified deformation, $\mathbf{N}$ is the undeformed unit normal, $\mathbf{s}$ is a specified surface traction (force per unit area), and $\partial\Omega_0^{\text{disp}}$ and $\partial\Omega_0^{\text{trac}}$ are disjoint subsets of $\partial\Omega_0$ whose union makes up $\partial\Omega_0$.

For the weak form, we use the notation $\delta\mathbf{x}$ for the test functions (one vector-valued function rather than, say, three function v_1, v_2, v_3). The appropriate choice of function space for nonlinear elasticity is far more complex than for the previous problems, so will just set $\mathcal{V}$ to be a 'suitable' function space. Let $\mathcal{V}_0$ be the subspace of functions which are zero on $\partial\Omega_0^{\text{disp}}$, i.e. $\mathcal{V}_0 = \{\mathbf{y} \in \mathcal{V} : \mathbf{y}(\mathbf{X}) = 0 \text{ if } \mathbf{X} \in \partial\Omega_0^{\text{disp}}\}$.

The weak form for the compressible equilibrium equation (29) is obtained by taking the inner product of (29) with $\delta\mathbf{x}$ and integrating using the divergence theorem, from which we obtain: find $\mathbf{x} \in \mathcal{V}$ such $\mathbf{x} = \mathbf{x}^*$ on $\partial\Omega_0^{\text{disp}}$ and

$$\int_{\Omega_0} T_{MN}\frac{\partial x_i}{\partial X_N}\frac{\partial(\delta x_i)}{\partial X_M}\,\mathrm{d}V_0 = \int_{\Omega_0} \rho_0 b_i \delta x_i\,\mathrm{d}V_0 + \int_{\partial\Omega_0^{\text{trac}}} s_i \delta x_i\,\mathrm{d}S_0 \qquad \forall \delta\mathbf{x} \in \mathcal{V}_0 \qquad (32)$$

For the incompressible case, we also have the constraint equation, which we have to multiply with a test function δp, from a suitable space $\mathcal{W}$, and integrate. The full problem is therefore: find $\mathbf{x} \in \mathcal{V}$ and $p \in \mathcal{W}$ such $\mathbf{x} = \mathbf{x}^*$ on $\partial\Omega_0^{\text{disp}}$ and

$$\begin{aligned} \int_{\Omega_0} T_{MN}\frac{\partial x_i}{\partial X_N}\frac{\partial(\delta x_i)}{\partial X_M}\,\mathrm{d}V_0 - \int_{\Omega_0} \rho_0 b_i \delta x_i\,\mathrm{d}V_0 - \int_{\partial\Omega_0^{\text{trac}}} s_i \delta x_i\,\mathrm{d}S_0 &= 0 \qquad \forall \delta\mathbf{x} \in \mathcal{V}_0 \qquad (33)\\ \int_{\Omega_0} \delta p\,(\det F - 1)\,\mathrm{d}V_0 &= 0 \qquad \forall \delta p \in \mathcal{W} \qquad (34) \end{aligned}$$

For the finite element implementation, suppose we have a mesh in which $\mathbf{x}$ will be solved at $\mathcal{N}$ nodes and p will be solved for at $\mathcal{M}$ nodes. For example, when using a quadratic mesh, with quadratic interpolation for displacement (i.e. for $\mathbf{x}$), and linear interpolation for pressure[6], then $\mathcal{N}$ is the total number of nodes, and $\mathcal{M}$ is the number of vertices. Now, the total number of unknowns is $3\mathcal{N} + \mathcal{M}$ (assuming a 3D problem). Let $\phi_1, \phi_2, \ldots, \phi_{\mathcal{N}}$ by the bases used for displacement (in this example, quadratic bases), and $\psi_1, \psi_2, \ldots, \psi_{\mathcal{M}}$ those for pressure (in this example, linear bases).

[6]The order of polynomial interpolation for pressure must be lower than that for displacement.

Let the unknown $\mathbf{x}$-values at the nodes be denoted $\boldsymbol{\mathcal{X}}_I = ((\mathcal{X}_I)_1, (\mathcal{X}_I)_2, (\mathcal{X}_I)_3) = (\mathcal{X}_I, \mathcal{Y}_I, \mathcal{Z}_I)$, so that $\mathbf{x} = \sum_{I=1}^{\mathcal{N}} \boldsymbol{\mathcal{X}}_I \phi_I$. Similarly, let the unknown pressures be $\mathcal{P}_1, \dots, \mathcal{P}_{\mathcal{M}}$, so $p = \sum_{I=1}^{\mathcal{M}} \mathcal{P}_I \psi_I$. Let us write the vector of all the unknowns as

$$\boldsymbol{\mathcal{A}} = (\mathcal{X}_1, \dots, \mathcal{X}_{\mathcal{N}}, \mathcal{Y}_1, \dots, \mathcal{Y}_{\mathcal{N}}, \mathcal{Z}_1, \dots, \mathcal{Z}_{\mathcal{N}}, \mathcal{P}_1, \dots, \mathcal{P}_{\mathcal{M}}).$$

Now, suppose $\mathcal{I}$ is an index into $\boldsymbol{\mathcal{A}}$, in others words, that $1 \le \mathcal{I} \le 3\mathcal{N} + \mathcal{M}$. Clearly $\mathcal{A}_{\mathcal{I}}$ is either a spatial variable, $(\mathcal{X}_I)_d$ for some $d = 1, 2$ or 3 and some $I \le \mathcal{N}$; or a pressure variable, $\mathcal{P}_I$ for some $I \le \mathcal{M}$. Let us introduce the notation

$$\mathcal{I} = \mathrm{disp}(I, d)$$

if $\mathcal{I}$ corresponds to a spatial unknown and $\mathcal{A}_{\mathcal{I}} = (\mathcal{X}_I)_d$, and

$$\mathcal{I} = \mathrm{pressure}(I)$$

if $\mathcal{I}$ corresponds to a pressure unknown and $\mathcal{A}_{\mathcal{I}} = \mathcal{P}_I$. For example, for small I, if $\mathcal{I} = I$ then $\mathcal{I} = \mathrm{disp}(I, 1)$; if $\mathcal{I} = 2\mathcal{N} + I$ then $\mathcal{I} = \mathrm{disp}(I, 3)$, if $\mathcal{I} = 3\mathcal{N} + I$ then $\mathcal{I} = \mathrm{pressure}(I)$.

$$\boldsymbol{\mathcal{A}} = \left(\underbrace{\mathcal{X}_1, \dots, \mathcal{X}_{\mathcal{N}}}_{\mathcal{I}=\mathrm{disp}(I,1)}, \underbrace{\mathcal{Y}_1, \dots, \mathcal{Y}_{\mathcal{N}}}_{\mathcal{I}=\mathrm{disp}(I,2)}, \underbrace{\mathcal{Z}_1, \dots, \mathcal{Z}_{\mathcal{N}}}_{\mathcal{I}=\mathrm{disp}(I,3)}, \underbrace{\mathcal{P}_1, \dots, \mathcal{P}_{\mathcal{M}}}_{\mathcal{I}=\mathrm{pressure}(I)} \right).$$

There will be $3\mathcal{N} + \mathcal{M}$ nonlinear equations in the finite element problem. The first $3\mathcal{N}$ equations are obtained by setting $\delta\mathbf{x} = (\phi_I, 0, 0)$ in (33) for $I = 1, \dots, \mathcal{N}$, then $\delta\mathbf{x} = (0, \phi_I, 0)$, then $\delta\mathbf{x} = (0, 0, \phi_I)$; and the next $\mathcal{M}$ equations obtained by setting $\delta p = \psi_I$ in (34), $I = 1, \dots, \mathcal{M}$. Overall, we have: solve $\boldsymbol{\mathcal{F}}(\boldsymbol{\mathcal{A}}) = 0$, where

$$\mathcal{F}_{\mathcal{I}}(\boldsymbol{\mathcal{A}}) = \begin{cases} \int_{\Omega_0} T_{MN} F_{dN} \frac{\partial \phi_I}{\partial X_M}\, \mathrm{d}V_0 - \int_{\Omega_0} \rho_0 b_d \phi_I \,\mathrm{d}V_0 - \int_{\partial\Omega_0^{\mathrm{trac}}} s_d \phi_I \,\mathrm{d}S_0 & \text{if } \mathcal{I} = \mathrm{disp}(I, d) \\ \int_{\Omega_0} \psi_I (\det F - 1)\, \mathrm{d}V_0 & \text{if } \mathcal{I} = \mathrm{pressure}(I) \end{cases}$$

In this equation T and F should be considered as functions of $\boldsymbol{\mathcal{A}}$, through $T \equiv T(C(\mathbf{x}), p)$ with $\mathbf{x} = \sum_{I=1}^{\mathcal{N}} \boldsymbol{\mathcal{X}}_I \phi_I$ and $p = \sum_{I=1}^{\mathcal{M}} \mathcal{P}_I \psi_I$.

This equation has to be solved using a nonlinear solver such as Newton's method. We use Newton's method with damping, for which we need to compute the Jacobian, $\frac{\partial \mathcal{F}_{\mathcal{I}}}{\partial \mathcal{A}_{\mathcal{J}}}$. After some calculation, the Jacobian can be shown to be

$$\frac{\partial \mathcal{F}_{\mathcal{I}}}{\partial \mathcal{A}_{\mathcal{J}}} = \begin{cases} \int_{\Omega_0} \frac{\partial T_{MN}}{\partial C_{PQ}} \left(F_{eQ} \frac{\partial \phi_J}{\partial X_P} + F_{eP} \frac{\partial \phi_J}{\partial X_Q} \right) F_{dN} \frac{\partial \phi_I}{\partial X_M} + T_{MN} \delta_{de} \frac{\partial \phi_J}{\partial X_N} \frac{\partial \phi_I}{\partial X_M}\, \mathrm{d}V_0 & \text{if } \mathcal{I} = \mathrm{disp}(I, d),\ \mathcal{J} = \mathrm{disp}(J, e) \\ \int_{\Omega_0} -\psi_J C^{-1}_{MN} F_{dN} \frac{\partial \phi_I}{\partial X_M}\, \mathrm{d}V_0 & \text{if } \mathcal{I} = \mathrm{disp}(I, d),\ \mathcal{J} = \mathrm{pressure}(J) \\ \int_{\Omega_0} \psi_I (\det F) F^{-1}_{Me} \frac{\partial \phi_J}{\partial X_M}\, \mathrm{d}V_0 & \text{if } \mathcal{I} = \mathrm{pressure}(I),\ \mathcal{J} = \mathrm{disp}(J, e) \\ 0 & \text{if } \mathcal{I} = \mathrm{pressure}(I),\ \mathcal{J} = \mathrm{pressure}(J) \end{cases}$$

which can be simplified further to (here, we write the first term using the symmetrisation of $\frac{\partial T}{\partial C}$ so that a smaller number of contractions (i.e. tensor-matrix multiplications) is required, which significantly reduces the computational cost)

$$\mathrm{Jac}_{\mathcal{I}\mathcal{J}} = \begin{cases} \int_{\Omega_0} \left(\frac{\partial T_{MN}}{\partial C_{PQ}} + \frac{\partial T_{MN}}{\partial C_{QP}} \right) F_{dN} F_{eQ} \frac{\partial \phi_J}{\partial X_P} \frac{\partial \phi_I}{\partial X_M} + T_{MN} \delta_{de} \frac{\partial \phi_J}{\partial X_N} \frac{\partial \phi_I}{\partial X_M}\, \mathrm{d}V_0 & \text{if } \mathcal{I} = \mathrm{disp}(I, d),\ \mathcal{J} = \mathrm{disp}(J, e) \\ \int_{\Omega_0} -\psi_J F^{-1}_{Md} \frac{\partial \phi_I}{\partial X_M}\, \mathrm{d}V_0 & \text{if } \mathcal{I} = \mathrm{disp}(I, d),\ \mathcal{J} = \mathrm{pressure}(J) \\ \int_{\Omega_0} \psi_I (\det F) F^{-1}_{Me} \frac{\partial \phi_J}{\partial X_M}\, \mathrm{d}V_0 & \text{if } \mathcal{I} = \mathrm{pressure}(I),\ \mathcal{J} = \mathrm{disp}(J, e) \\ 0 & \text{if } \mathcal{I} = \mathrm{pressure}(I),\ \mathcal{J} = \mathrm{pressure}(J) \end{cases} \tag{35}$$

$\frac{\partial T}{\partial C}$ has to be provided by the user (through the material law).

Rewriting slightly, we have

$$\text{Jac}_{\mathcal{I}\mathcal{J}} = \begin{cases} \int_{\Omega_0} \left(\left(\frac{\partial T_{MP}}{\partial C_{NQ}} + \frac{\partial T_{MP}}{\partial C_{QN}} \right) F_{dP} F_{eQ} + T_{MN}\delta_{de} \right) \frac{\partial \phi_J}{\partial X_N} \frac{\partial \phi_I}{\partial X_M} \, \mathrm{d}V_0 & \text{if } \mathcal{I} = \text{disp}(I,d),\ \mathcal{J} = \text{disp}(J,e) \\ \int_{\Omega_0} -\psi_J F^{-1}_{Md} \frac{\partial \phi_I}{\partial X_M} \, \mathrm{d}V_0 & \text{if } \mathcal{I} = \text{disp}(I,d),\ \mathcal{J} = \text{pressure}(J) \\ \int_{\Omega_0} \psi_I (\det F) F^{-1}_{Me} \frac{\partial \phi_J}{\partial X_M} \, \mathrm{d}V_0 & \text{if } \mathcal{I} = \text{pressure}(I),\ \mathcal{J} = \text{disp}(J,e) \\ 0 & \text{if } \mathcal{I} = \text{pressure}(I),\ \mathcal{J} = \text{pressure}(J) \end{cases} \tag{36}$$

Note that the term multiplying the basis gradients is just $\frac{\partial S}{\partial F}$ written in terms of $\frac{\partial T}{\partial E}$ and T

$$\frac{\partial S_{Mi}}{\partial F_{jN}} = \left(\frac{\partial T_{MP}}{\partial C_{NQ}} + \frac{\partial T_{MP}}{\partial C_{QN}} \right) F_{iP} F_{jQ} + T_{MN}\delta_{ij}$$

If we had used S in the weak form rather than TF^{T} than this $\frac{\partial S}{\partial F}$ term would have dropped out immediately. Overall, we have

$$\text{Jac}_{\mathcal{I}\mathcal{J}} = \begin{cases} \int_{\Omega_0} \frac{\partial S_{Md}}{\partial F_{eN}} \frac{\partial \phi_J}{\partial X_N} \frac{\partial \phi_I}{\partial X_M} \, \mathrm{d}V_0 & \text{if } \mathcal{I} = \text{disp}(I,d),\ \mathcal{J} = \text{disp}(J,e) \\ \int_{\Omega_0} -\psi_J F^{-1}_{Md} \frac{\partial \phi_I}{\partial X_M} \, \mathrm{d}V_0 & \text{if } \mathcal{I} = \text{disp}(I,d),\ \mathcal{J} = \text{pressure}(J) \\ \int_{\Omega_0} \psi_I (\det F) F^{-1}_{Me} \frac{\partial \phi_J}{\partial X_M} \, \mathrm{d}V_0 & \text{if } \mathcal{I} = \text{pressure}(I),\ \mathcal{J} = \text{disp}(J,e) \\ 0 & \text{if } \mathcal{I} = \text{pressure}(I),\ \mathcal{J} = \text{pressure}(J) \end{cases} \tag{37}$$

Note that the Jacobian has a natural 2×2 block structure

$$\text{Jac} = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & 0 \end{pmatrix} \begin{array}{l} \}\ _{\text{displacement}} \\ \}\ _{\text{pressure}} \end{array}$$

J_{11} is not in general symmetric, and J_{12} is not in general equal to $-J_{21}$. (It would be if we set $\det F = 1$ in the third equation in (37), but although $\det F$ must be 1 for the solution, it may not be of the current Newton guess).

4.2 Cardiac electro-mechanics

4.2.1 Formulation

In cardiac electro-mechanical problems, the monodomain/bidomain equations are amended slightly to take into account the deformation, an extra set of ODE systems—*the contraction model*, which model active force generation on the cell-level—are introduced, and this active force is added to the nonlinear elasticity equations.

Physiologically, the mechanical response in the cell is dependent on the electrical activity largely through the *intracellular calcium concentration*, $[\mathrm{Ca}^{2+}]$, and therefore most contraction models take this as input[7]. Now, let $\mathbf{m}$ denote the undeformed unit fibre direction. The *fibre-stretch* (stretch in the fibre-direction) is then given by $\mathbf{m}^{\mathrm{T}} C \mathbf{m}$ (C is the standard deformation tensor defined in Section 4). The contraction model can also be dependent on the fibre-stretch, as well as possibly on the fibre-stretch-rate, $\dot{\lambda}$. Let $\mathbf{w}$ be a vector of internal state variables for the contraction model. The contraction model is a set of ODEs determining how the state variables evolve and an equation which provides the *active tension*, σ_a. Despite the name, this is actually a stress not a force; a scalar stress generated at the cellular level in the fibre direction in response to excitation.

$$\frac{\mathrm{d}\mathbf{w}}{\mathrm{d}t} = \mathbf{g}(\mathbf{w}; [\mathrm{Ca}^{2+}], \lambda, \dot{\lambda}), \tag{38}$$

$$\sigma_a \equiv \sigma_a(\mathbf{w}; [\mathrm{Ca}^{2+}], \lambda, \dot{\lambda}). \tag{39}$$

[7]Some simpler models are instead dependent on the voltage and some also possibly explicitly on time.

Note that we have denoted active tension as σ_a rather than the more common T_a. This is to emphasise the fact that the active tension is likely to be a *Cauchy* (true) stress, rather than a Piola-Kirchhoff stress. This is will be the case if the deformed cross-sectional area (rather than undeformed cross-sectional area) was used in the experiments used to fit contraction model parameters.

The equations of nonlinear elasticity are amended to take into account the active response of the tissue by introducing a third term to the stress which depends on the active tension[8]

$$T = 2\frac{\partial W}{\partial C} - pC^{-1} + \frac{\sigma_a}{\mathbf{m}^{\mathrm{T}} C \mathbf{m}} \mathbf{m}\mathbf{m}^{\mathrm{T}}, \tag{40}$$

or

$$T = T^{\text{passive}} + T^{\text{active}}, \tag{41}$$

where

$$\begin{aligned} T^{\text{passive}} &= 2\frac{\partial W^{\text{mat}}}{\partial C} - pC^{-1}, \\ T^{\text{active}} &= \frac{\sigma_a}{\lambda^2}\mathbf{m}\mathbf{m}^{\mathrm{T}}. \end{aligned} \tag{42}$$

T^{active} is the active (tensor) stress corresponding to the cellular active tension that is induced in the fibre direction. The denominator just scales the active tension for the undeformed state (see cardiac electromechanics papers).

We assume the tissue is always instantaneously in equilibrium and that that inertial effects can be neglected (i.e. quasi-steady), which means the static equilibrium equations, (30) and (31), are used. We also take zero body force (i.e. neglect gravity), so the equations of equilibrium are:

$$\frac{\partial}{\partial X_M}\left(T_{MN}F_{iN}\right) = 0, \tag{43}$$

$$\det(F) = 1. \tag{44}$$

where T is now the total stress, with zero traction boundary conditions $\partial\Omega_0^{\text{trac}}$. It is not clear what a suitable choice of $\partial\Omega_0^{\text{disp}}$ and $\mathbf{x}^*$ is.

The deformation affects the electrical activity in two ways. First, the deformation of the tissue alters the geometry over which the voltage propagates, altering the spatial derivatives in (7); and secondly, the cell-model can be dependent on fibre-stretch through the so-called 'stretch-activated channels'. Equations (7) and (8) become

$$\chi C_m \frac{\partial V}{\partial t} = \nabla\cdot(F^{-1}\sigma F^{-\mathrm{T}}\nabla V) - \chi I_{\text{ion}}(\mathbf{u}, V, \lambda), \tag{45}$$

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{f}(\mathbf{u}, V, \lambda). \tag{46}$$

(Note: $F^{-1}\sigma F^{-\mathrm{T}} = C^{-1}\sigma$ if σ is isotropic, i.e. if fibre directions are not being used in the electrical simulation). The code currently has C^{-1} replaced with the identity, as in the case of simple propagation it has been shown that this approximation gives very little error (essentially because, when there is diffusion of the voltage occurring, there is little deformation).

[8]This equation can be understood better if we consider the Cauchy stress counterpart, and assume the fibres are in the X-direction. This the corresponding total Cauchy stress is

$$\underline{\underline{\sigma}}^{\text{total}} = \underline{\underline{\sigma}}^{\text{mat}} - pI + \begin{bmatrix} \sigma_a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

4.2.2 Implicit or explicit schemes

Consider evaluating a stress $T \equiv T(C)$. T is dependent on σ_a, which is dependent on C through possibly being dependent on λ and $\dot{\lambda}$. One possibility is to use the previous value of λ and $\dot{\lambda}$ for computing σ_a (so using both the current and previous value of C in evaluating T). This is the commonly-used *explicit method*, and has the advantage that the contraction models ODEs need only be solved once per timestep (per node/quadrature point). However, this can have serious stability/accuracy issues (see cardiac electromechanics paper). The alternative is to evaluate σ_a using the current value of C, which is the *implicit method*. This has no stability issues, but requires the contraction models ODEs to be re-integrated every time a stress is evaluated (which is several times during the nonlinear solve). Letting C^n be the value of C at the previous timestep, etc, the two schemes evaluate T using:

$$T = 2\frac{\partial W}{\partial C}(C^{n+1}) - p(C^{n+1})^{-1} + \frac{\sigma_a(\lambda^n, \dot{\lambda}^n)}{(\lambda^{n+1})^2}\mathbf{m}\mathbf{m}^{\mathrm{T}}, \tag{47}$$

in the explicit method, and

$$T = 2\frac{\partial W}{\partial C}(C^{n+1}) - p(C^{n+1})^{-1} + \frac{\sigma_a(\lambda^{n+1}, \dot{\lambda}^{n+1})}{(\lambda^{n+1})^2}\mathbf{m}\mathbf{m}^{\mathrm{T}}, \tag{48}$$

in the implicit method.

The weak form, finite element residual $\boldsymbol{\mathcal{F}}$ and finite element Jacobian are all unchanged, they just need to be computing using the *total* stress, using both passive and active parts. This introduces an extra term in the $\frac{\partial T}{\partial C}$ term used in 36). In the implicit case, this term can be computed to be

$$\frac{\partial T^{\text{active}}_{MN}}{\partial C_{PQ}} = \left(-\frac{\sigma_a}{\lambda^4} + \frac{\partial\sigma_a/\partial\lambda + \frac{1}{\Delta t}\partial\sigma_a/\partial\dot{\lambda}}{\lambda^3}\right) m_M m_N m_P m_Q.$$

The derivatives of σ_a need to be approximated numerically.

4.2.3 Anisotropic passive material laws

Finally, a note on the implementation of anisotropic passive material laws, in particular cardiac material laws which depend on the fibre, sheet and normal directions[9]. An example is the pole-zero material law, which has terms of the form $k_{ff}E_{ff}$, where k_{ff} is a parameter and $E_{ff} = \mathbf{m}^{\mathrm{T}}E\mathbf{m}$. Let us write $\mathbf{m}_f$ (=$\mathbf{m}$), $\mathbf{m}_s$ and $\mathbf{m}_n$ for the fibre, sheet and normal directions. The material law implementations take in C and the change of basis matrix P, defined by

$$P = [\mathbf{m}_f \ \mathbf{m}_s \ \mathbf{m}_n].$$

The stress is computed by assuming the fibres are parallel to the X-axis, and the sheet in the XY plane, by transforming C to the fibre-sheet basis prior to the calculating the stress ($C \to C^*$) and transforming the resultant T^* after it has been computed. Also, the material law will return $\frac{\mathrm{d}T^*}{\mathrm{d}C^*}$, which has to be transformed as well. The appropriate computations are

$$C^* = P^{\mathrm{T}}CP \qquad T^* \equiv T^*(C^*) \qquad T = PT^*P^{\mathrm{T}}$$

and

$$\frac{\mathrm{d}T_{MN}}{\mathrm{d}C_{PQ}} = P_{Mm}P_{Nn}P_{Pp}P_{Qq}\frac{\mathrm{d}T^*_{mn}}{\mathrm{d}C^*_{pq}}.$$

[9] More precisely, these are three orthonormal directions at each point, the first being the fibre direction, the second being a vector in the sheet orthogonal to the fibre, the third being normal to the sheet.