1 Multidomain

The multidomain equations generalize the bidomain equation and have multiple compartments at each spatial point. Each compartment k describes one of the M_{mu} motor units. The electric potential in the extra-cellular space is designated by ϕ_e and the intra-cellular potential of motor unit k is desribed by ϕ_i. The transmembrane voltages are given by $V_m^k = \phi_i^k - \phi_e$.

The first multidomain equation balances current flow between intra and extra-cellular space:

$$\operatorname{div}\big(\boldsymbol{\sigma}_e \operatorname{grad}(\phi_e)\big) + \sum_{k=1}^{M_{\text{mu}}} f_r^k \operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(\underbrace{V_m^k + \phi_e}_{=\phi_i^k})\big) = 0. \tag{1}$$

It can be reformulated as:

$$\operatorname{div}\big((\underbrace{\boldsymbol{\sigma}_e + \sum_{k}^{M_{\text{mu}}} f_r^k \boldsymbol{\sigma}_i^k}_{=:\boldsymbol{\sigma}_i}) \operatorname{grad}(\phi_e)\big) + \sum_{k=1}^{M_{\text{mu}}} f_r^k \operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(V_m^k)\big) = 0. \tag{2}$$

The second multidomain equations describe flow over the membrane and hold for each compartment:

$$\operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(\underbrace{V_m^k + \phi_e}_{=\phi_i^k})\big) = A_m^k \left(C_m^k \frac{\partial V_m^k}{\partial t} + I_{\text{ion}}(V_m^k)\right) \qquad \forall\, k \in 1 \dots M_{\text{mu}} \tag{3}$$

The unknowns are the transmembrane voltages of compartment k, V_m^k and the extracellular potential, ϕ_e. $f_r^k \in [0,1]$ is a spatially varying factor of the presence of the compartment with $\sum_k f_i^k = 1$. $\boldsymbol{\sigma}_i^k$ and $\boldsymbol{\sigma}_e$ are the conductivity tensors of the intra- and extracellular spaces.

Solving (3) for $\partial V_m^k/\partial t$ yields:

$$\frac{\partial V_m^k}{\partial t} = \frac{1}{A_m^k\, C_m^k} \operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(V_m^k + \phi_e)\big) - \frac{1}{C_m^k}\; I_{\text{ion}}(V_m^k)$$

We solve using an operator splitting approach, e.g. Godunov splitting. The reaction term is solved with an explicit Euler scheme.

$$V_m^{k,(*)} = V_m^{k,(i)} - dt\, \frac{1}{C_m^k}\; I_{\text{ion}}(V_m^{k,(i)}).$$

The subcellular model provided by the CellML description computes $(-1/C_m^k\, I_{\text{ion}})$.

The diffusion term is solved using an implicit scheme, e.g. backward Euler.

$$V_m^{k,(i+1)} = V_m^{k,(*)} + dt\, \frac{1}{A_m^k\, C_m^k} \operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(V_m^{k,(i+1)} + \phi_e)\big) \tag{4}$$

$$\Leftrightarrow \quad V_m^{k,(i+1)} - \frac{dt}{A_m^k\, C_m^k} \operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(V_m^{k,(i+1)})\big) - \frac{dt}{A_m^k\, C_m^k} \operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(\phi_e)\big) = V_m^{k,(*)}$$

After discretizing the spatial terms with the Finite Element Method the following matrix equation is obtained:

$$\left[\begin{array}{ccc|c} \mathbf{A}^1_{V_m,V_m} & & & \mathbf{B}^1_{V_m,\phi_e} \\ & \ddots & & \vdots \\ & & \mathbf{A}^{M_\text{mu}}_{V_m,V_m} & \mathbf{B}^{M_\text{mu}}_{V_m,\phi_e} \\ \hline \mathbf{B}^1_{\phi_e,V_m} & \dots & \mathbf{B}^{M_\text{mu}}_{\phi_e,V_m} & \mathbf{B}_{\phi_e,\phi_e} \end{array}\right] \left[\begin{array}{c} V_m^{1,(i+1)} \\ \vdots \\ V_m^{M_\text{mu},(i+1)} \\ \hline \phi_{e,i} \end{array}\right] = \left[\begin{array}{c} \mathbf{b}^{1,(i+1)}_{V_m} \\ \vdots \\ \mathbf{b}^{M_\text{mu},(i+1)}_{V_m} \\ \hline \mathbf{0} \end{array}\right],$$

where

$$\begin{array}{lll} \mathbf{A}^k_{V_m,V_m} & \dots \quad \text{discretization of} & -\dfrac{dt}{A_m^k\,C_m^k}\,\text{div}\,\big(\boldsymbol{\sigma}_i^k\,\text{grad}\,(\cdot)\big) + (\cdot) \\ \mathbf{B}^k_{V_m,\phi_e} & \dots \quad \text{discretization of} & -\dfrac{dt}{A_m^k\,C_m^k}\,\text{div}\,\big(\boldsymbol{\sigma}_i^k\,\text{grad}\,(\cdot)\big) \\ \mathbf{B}^k_{\phi_e,V_m} & \dots \quad \text{discretization of} & f_r^k\,\text{div}\,\big(\boldsymbol{\sigma}_i^k\,\text{grad}\,(\cdot)\big) \\ \mathbf{B}_{\phi_e,\phi_e} & \dots \quad \text{discretization of} & \text{div}\,\big((\boldsymbol{\sigma}_e + \boldsymbol{\sigma}_i)\,\text{grad}\,(\cdot)\big) \end{array}$$

$$\mathbf{b}^{k,(i+1)}_{V_m} = V_m^{k,(*)} = V_m^{k,(i)} - \frac{dt}{C_m^k}\,I_\text{ion}(V_m^{k,(i)}) \quad (I_\text{ion}\text{ solved using splitting scheme})$$

The bidomain equation is the special case for $M_\text{mu} = 1$. It can also be used for computation of EMG (ϕ_e) from V_m in the fiber based model.

$$\text{div}\,\big((\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_e)\,\text{grad}\,\phi_e\big) = -\text{div}\,(\boldsymbol{\sigma}_i\,\text{grad}\,V_m)$$

1.1 Finite Element formulation

In this section the finite element formulation for the multidomain equation is derived. We start with an example problem.

1.1.1 Diffusion problem

In general, the weak form of a diffusion problem discretized with Crank-Nicolson,

$$\begin{aligned} &\Delta u = u_t, \qquad \frac{\partial u}{\partial \mathbf{n}} = f \quad \text{on } \Gamma_f, \qquad \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega\backslash\Gamma_f \\ \Rightarrow \quad &\int_\Omega \big(\theta\,\Delta u^{(i+1)} + (1-\theta)\,\Delta u^{(i)}\big)\,\phi\,\mathrm{d}\mathbf{x} = \frac{1}{dt}\int_\Omega (u^{(i+1)} - u^{(i)})\,\phi\,\mathrm{d}\mathbf{x}, \quad \forall \phi \in V_h \end{aligned} \tag{5}$$

Discretize in space with $u = \sum_j u_j\,\varphi_j, V_h = \text{span}\,\{\varphi_j | j = 1\dots N\}$ and using Divergence theorem

$$\begin{aligned} &\sum_{j=1}^N \big(\theta\,u_j^{(i+1)} + (1-\theta)\,u_j^{(i)}\big)\left(-\int_\Omega \nabla\varphi_j\cdot\nabla\varphi_k\,\mathrm{d}\mathbf{x} + \int_{\partial\Omega}(\nabla\varphi_j\cdot\mathbf{n})\varphi_k\,\mathrm{d}\mathbf{x}\right) \\ &\quad = \frac{1}{dt}\sum_{j=1}^N \big(u_j^{(i+1)} - u_j^{(i)}\big)\int_\Omega \varphi_j\,\varphi_k\,\mathrm{d}\mathbf{x}, \quad \forall k = 1\dots N. \end{aligned} \tag{6}$$

This can be written in matrix notation as

$$\mathbf{A}\,\mathbf{u}^{(i+1)} = \mathbf{b}(\mathbf{u}^{(i)}), \tag{7}$$

where

$$\begin{aligned} \mathbf{A} &= \theta\,(\mathbf{K}+\mathbf{B}) - \frac{1}{dt}\,\mathbf{M}, \\ \mathbf{b} &= \big((\theta-1)\,(\mathbf{K}+\mathbf{B}) - \frac{1}{dt}\,\mathbf{M}\big)\,\mathbf{u}^{(i)}, \end{aligned} \tag{8}$$

with

$$\begin{aligned} \mathbf{K}_{kj} &= -\int_\Omega \nabla\varphi_j \cdot \nabla\varphi_k \,\mathrm{d}\mathbf{x} \qquad \text{(note, the minus sign is correct for } +\Delta\text{)}, \\ \mathbf{B}_{kj} &= \int_{\Gamma_f} (\nabla\varphi_j \cdot \mathbf{n})\varphi_k \,\mathrm{d}\mathbf{x}, \\ \mathbf{M}_{kj} &= \int_\Omega \varphi_j\,\varphi_k \,\mathrm{d}\mathbf{x}, \end{aligned}$$

or written in component form:

$$\begin{aligned} \mathbf{A}_{kj} &= \theta\left(-\int_\Omega \nabla\varphi_j \cdot \nabla\varphi_k \,\mathrm{d}\mathbf{x} + \int_{\partial\Omega} (\nabla\varphi_j \cdot \mathbf{n})\varphi_k \,\mathrm{d}\mathbf{x}\right) - \frac{1}{dt}\ \int_\Omega \varphi_j\,\varphi_k \,\mathrm{d}\mathbf{x}, \\ \mathbf{b}_k &= \sum_{j=1}^N -(1-\theta)\,u_j^{(i)}\ \left(-\int_\Omega \nabla\varphi_j \cdot \nabla\varphi_k \,\mathrm{d}\mathbf{x} + \int_{\partial\Omega} (\nabla\varphi_j \cdot \mathbf{n})\varphi_k \,\mathrm{d}\mathbf{x}\right) + \frac{1}{dt}\sum_{j=1}^N -u_j^{(i)} \int_\Omega \varphi_j\,\varphi_k \,\mathrm{d}\mathbf{x}. \end{aligned}$$

So far we did not plug in the boundary conditions. For $f = 0$ we get $\mathbf{B} = \mathbf{0}$. The case $f \neq 0$ is handled in the next subsection.

1.1.2 Boundary conditions

The boundary condition $\nabla u \cdot \mathbf{n} = f$ can be written as

$$\nabla u \cdot \mathbf{n} = \sum_{j=1}^N u_j\,(\nabla\varphi_j \cdot \mathbf{n}) = f,$$

We discretize the flow over the boundary, f, by different ansatz functions, ψ_j, with coefficients f_j:

$$f = \sum_{j=1}^N f_j\,\psi_j$$

We get from (6)

$$
\begin{aligned}
&\sum_{j=1}^{N} \big(\theta\, u_j^{(i+1)} + (1-\theta)\, u_j^{(i)}\big) \left(-\int_\Omega \nabla\varphi_j \cdot \nabla\varphi_k \,\mathrm{d}\mathbf{x}\right) + \int_{\Gamma_f} \big(\theta\, f^{(i+1)} + (1-\theta)\, f^{(i)}\big)\, \varphi_k \,\mathrm{d}\mathbf{x} \\
&\quad = \frac{1}{dt} \sum_{j=1}^{N} \big(u_j^{(i+1)} - u_j^{(i)}\big) \int_\Omega \varphi_j\, \varphi_k \,\mathrm{d}\mathbf{x}, \quad \forall k = 1 \dots N, \\
\Leftrightarrow\quad &\sum_{j=1}^{N} \big(\theta\, u_j^{(i+1)} + (1-\theta)\, u_j^{(i)}\big) \left(-\int_\Omega \nabla\varphi_j \cdot \nabla\varphi_k \,\mathrm{d}\mathbf{x}\right) + \sum_{j=1}^{N} \big(\theta\, f_j^{(i+1)} + (1-\theta)\, f_j^{(i)}\big) \int_{\Gamma_f} \psi_j\, \varphi_k \,\mathrm{d}\mathbf{x} \\
&\quad = \frac{1}{dt} \sum_{j=1}^{N} \big(u_j^{(i+1)} - u_j^{(i)}\big) \int_\Omega \varphi_j\, \varphi_k \,\mathrm{d}\mathbf{x}, \quad \forall k = 1 \dots N,
\end{aligned}
$$

In matrix notation,

$$
\mathbf{A}\, \mathbf{u}^{(i+1)} = \mathbf{b}(\mathbf{u}^{(i)}), \tag{9}
$$

we have

$$
\begin{aligned}
\mathbf{A} &= \theta\, \mathbf{K} - \frac{1}{dt}\, \mathbf{M}, \\
\mathbf{b} &= \big((\theta - 1)\, \mathbf{K} - \frac{1}{dt}\, \mathbf{M}\big)\, \mathbf{u}^{(i)} - \mathbf{B}_{\Gamma_f} \big(\theta\, \mathbf{f}^{(i+1)} + (1-\theta)\, \mathbf{f}^{(i)}\big),
\end{aligned} \tag{10}
$$

with

$$
\begin{aligned}
\mathbf{K}_{kj} &= -\int_\Omega \nabla\varphi_j \cdot \nabla\varphi_k \,\mathrm{d}\mathbf{x} \qquad \text{(note, the minus sign is correct for } +\Delta\text{)}, \\
\mathbf{M}_{kj} &= \int_\Omega \varphi_j\, \varphi_k \,\mathrm{d}\mathbf{x}, \\
\mathbf{B}_{\Gamma_f, kj} &= \int_{\Gamma_f} \psi_j\, \varphi_k \,\mathrm{d}\mathbf{x},
\end{aligned}
$$

1.1.3 Laplace problem

We consider $\Delta u = 0, \partial u / \partial \mathbf{n} = f$. This leads to

$$
(\mathbf{K} + \mathbf{B})\, \mathbf{u} = \mathbf{0} \qquad \text{or} \qquad \mathbf{K}\, \mathbf{u} + \mathbf{B}_{\Gamma_f}\, \mathbf{f} = 0.
$$

1.1.4 First multidomain equation

Back to the first multidomain equation (2):

$$
\operatorname{div}\Big(\underbrace{(\boldsymbol{\sigma}_e + \sum_{k}^{M_{\text{mu}}} f_r^k \boldsymbol{\sigma}_i^k)}_{=:\boldsymbol{\sigma}_i} \operatorname{grad}(\phi_e)\Big) + \sum_{k=1}^{M_{\text{mu}}} f_r^k \operatorname{div}\big(\boldsymbol{\sigma}_i^k \operatorname{grad}(V_m^k)\big) = 0,
$$

The weak form can be written as

$$\sum_{j=1}^{N}\phi_{e,j}\left(-\int_\Omega(\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i)\nabla\varphi_j\cdot\nabla\varphi_\ell\,\mathrm{d}\mathbf{x}+\int_{\partial\Omega}((\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i)\nabla\varphi_j\cdot\mathbf{n})\varphi_\ell\,\mathrm{d}\mathbf{x}\right)$$
$$+\sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\left(\sum_{j=1}^{N}V_{m,j}^k\left(-\int_\Omega\boldsymbol{\sigma}_i^k\nabla\varphi_j\cdot\nabla\varphi_\ell\,\mathrm{d}\mathbf{x}+\int_{\partial\Omega}(\boldsymbol{\sigma}_i^k\nabla\varphi_j\cdot\mathbf{n})\varphi_\ell\,\mathrm{d}\mathbf{x}\right)\right)=0\quad\forall\ell=1,\dots,N,$$

which is in matrix notation,

$$\big(\mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}+\mathbf{B}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}\big)\boldsymbol{\phi}_e+\sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\big(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k}\big)\mathbf{V}_m^k=0 \tag{11}$$

1.1.5 Second multidomain equation

The diffusion part of the second multidomain equation is given by

$$\frac{V_m^{k,(i+1)}-V_m^{k,(*)}}{dt}=\frac{1}{A_m^k\,C_m^k}\,\mathrm{div}\left(\boldsymbol{\sigma}_i^k\,\mathrm{grad}\,(V_m^{k,(i+1)})\right)+\frac{1}{A_m^k\,C_m^k}\,\mathrm{div}\left(\boldsymbol{\sigma}_i^k\,\mathrm{grad}\,(\phi_e)\right).$$

The weak form is given by

$$\frac{1}{A_m^k\,C_m^k}\sum_{j=1}^{N}\left(\theta\,V_{m,j}^{(i+1)}+(1-\theta)\,V_{m,j}^{(i)}\right)\left(-\int_\Omega\boldsymbol{\sigma}_i^k\,\nabla\varphi_j\cdot\nabla\varphi_\ell\,\mathrm{d}\mathbf{x}+\int_{\partial\Omega}(\boldsymbol{\sigma}_i^k\,\nabla\varphi_j\cdot\mathbf{n})\varphi_\ell\,\mathrm{d}\mathbf{x}\right)$$
$$+\frac{1}{A_m^k\,C_m^k}\sum_{j=1}^{N}\left(\theta\,\phi_{e,j}^{(i+1)}+(1-\theta)\,\phi_{e,j}^{(i)}\right)\left(-\int_\Omega\boldsymbol{\sigma}_i^k\,\nabla\varphi_j\cdot\nabla\varphi_\ell\,\mathrm{d}\mathbf{x}+\int_{\partial\Omega}(\boldsymbol{\sigma}_i^k\,\nabla\varphi_j\cdot\mathbf{n})\varphi_\ell\,\mathrm{d}\mathbf{x}\right)$$
$$=\frac{1}{dt}\sum_{j=1}^{N}\left(V_{m,j}^{(i+1)}-V_{m,j}^{(i)}\right)\int_\Omega\varphi_j\,\varphi_\ell\,\mathrm{d}\mathbf{x},\quad\forall\ell=1\dots N$$

Analogous to (9) we get

$$\mathbf{A}\begin{pmatrix}\mathbf{V}_m^{(i+1)}\\ \boldsymbol{\phi}_e^{(i+1)}\end{pmatrix}=\mathbf{b}, \tag{12}$$

where

$$\begin{aligned}\mathbf{A}&=\begin{pmatrix}\frac{1}{A_m^k\,C_m^k}\,\theta\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})-\frac{1}{dt}\mathbf{M} & \frac{1}{A_m^k\,C_m^k}\,\theta\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})\end{pmatrix}\\ \mathbf{b}&=\Big(\frac{1}{A_m^k\,C_m^k}\,(\theta-1)\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})-\frac{1}{dt}\mathbf{M}\Big)\mathbf{V}_m^{(i)}+\frac{1}{A_m^k\,C_m^k}\,(\theta-1)\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})\,\boldsymbol{\phi}_e^{(i)}\end{aligned} \tag{13}$$

Together, (11) and (12),(13) form the following system

$$\begin{aligned}
&\begin{bmatrix} \frac{1}{A_m^k\, C_m^k}\,\theta\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})-\frac{1}{dt}\,\mathbf{M} & \frac{1}{A_m^k\, C_m^k}\,\theta\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k}) \\ f_r^k\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k}) & (\mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}+\mathbf{B}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}) \end{bmatrix} \begin{bmatrix} \mathbf{V}_m^{(i+1)} \\ \boldsymbol{\phi}_e^{(i+1)} \end{bmatrix} \\
&= \begin{bmatrix} \left((\theta-1)\,\frac{1}{A_m^k\, C_m^k}\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})-\frac{1}{dt}\,\mathbf{M}\right)\mathbf{V}_m^{(i)}+(\theta-1)\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})\,\boldsymbol{\phi}_e^{(i)} \\ \mathbf{0} \end{bmatrix}
\end{aligned} \tag{14}$$

By multiplying the first row with $-dt\,\mathbf{M}^{-1}$ we get

$$\begin{aligned}
&\begin{bmatrix} \frac{-dt\,\theta}{A_m^k\, C_m^k}\,\mathbf{M}^{-1}(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})+\mathbf{I} & \frac{-dt\,\theta}{A_m^k\, C_m^k}\,\mathbf{M}^{-1}(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k}) \\ f_r^k\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k}) & (\mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}+\mathbf{B}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}) \end{bmatrix} \begin{bmatrix} \mathbf{V}_m^{(i+1)} \\ \boldsymbol{\phi}_e^{(i+1)} \end{bmatrix} \\
&= \begin{bmatrix} \left(\frac{(1-\theta)\,dt}{A_m^k\, C_m^k}\,\mathbf{M}^{-1}(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})+\mathbf{I}\right)\mathbf{V}_m^{(i)}+(1-\theta)\,dt\,\mathbf{M}^{-1}\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{B}_{\boldsymbol{\sigma}_i^k})\,\boldsymbol{\phi}_e^{(i)} \\ \mathbf{0} \end{bmatrix}
\end{aligned} \tag{15}$$

For a forward Euler scheme ($\theta = 1$) and homogeneous Dirichlet boundary conditions ($\mathbf{B} = \mathbf{0}$) the equation simplifies to

$$\begin{bmatrix} \frac{1}{A_m^k\, C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k}-\frac{1}{dt}\,\mathbf{M} & \frac{1}{A_m^k\, C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} \\ f_r^k\mathbf{K}_{\boldsymbol{\sigma}_i^k} & \mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i} \end{bmatrix} \begin{bmatrix} \mathbf{V}_m^{(i+1)} \\ \boldsymbol{\phi}_e^{(i+1)} \end{bmatrix} = \begin{bmatrix} -\frac{1}{dt}\,\mathbf{M}\,\mathbf{V}_m^{(i)} \\ \mathbf{0} \end{bmatrix}$$

or equivalently,

$$\begin{bmatrix} \frac{-dt}{A_m^k\, C_m^k}\,\mathbf{M}^{-1}\mathbf{K}_{\boldsymbol{\sigma}_i^k}+\mathbf{I} & \frac{-dt}{A_m^k\, C_m^k}\,\mathbf{M}^{-1}\mathbf{K}_{\boldsymbol{\sigma}_i^k} \\ f_r^k\mathbf{K}_{\boldsymbol{\sigma}_i^k} & \mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i} \end{bmatrix} \begin{bmatrix} \mathbf{V}_m^{(i+1)} \\ \boldsymbol{\phi}_e^{(i+1)} \end{bmatrix} = \begin{bmatrix} \mathbf{V}_m^{(i)} \\ \mathbf{0} \end{bmatrix}$$

1.2 Boundary conditions

The boundary conditions to the multidomain equations are given by

$$(\boldsymbol{\sigma}_i^k\,\nabla\phi_i^k)\cdot\mathbf{n}_m = 0 \qquad \text{on } \Gamma_M$$

With $\phi_i = V_m + \phi_e$ this translates to

$$(\boldsymbol{\sigma}_i^k\,\nabla V_m^k)\cdot\mathbf{n}_m = -(\boldsymbol{\sigma}_i^k\,\nabla\phi_e)\cdot\mathbf{n}_m =: p^k \qquad \text{on } \Gamma_M \tag{16}$$

For now, we assume $\partial\phi_e/\partial\mathbf{n} = 0$ on Γ_M.

1.2.1 Multidomain example

Starting from (14) with $\mathbf{B} = \mathbf{0}$ we have

$$\begin{bmatrix} \frac{1}{A_m^k\, C_m^k}\,\theta\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} - \frac{1}{dt}\,\mathbf{M} & \frac{1}{A_m^k\, C_m^k}\,\theta\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} \\ f_r^k\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} & \mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i} \end{bmatrix} \begin{bmatrix} \mathbf{V}_m^{(i+1)} \\ \boldsymbol{\phi}_e^{(i+1)} \end{bmatrix}$$
$$= \begin{bmatrix} \Big((\theta-1)\,\frac{1}{A_m^k\, C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} - \frac{1}{dt}\,\mathbf{M}\Big)\mathbf{V}_m^{(i)} + (\theta-1)\,\frac{1}{A_m^k\, C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k}\,\boldsymbol{\phi}_e^{(i)} \\ \mathbf{0} \end{bmatrix}. \tag{17}$$

For boundary integrals and a Neumann boundary condition $(\boldsymbol{\sigma}\nabla u\cdot\mathbf{n}) = f$ on $\partial\Omega = \Gamma$, we have:

$$\begin{aligned}
&\boldsymbol{\sigma}\nabla u\cdot\mathbf{n} = \sum_{j=1}^{N} u_j\,(\boldsymbol{\sigma}\nabla\varphi_j\cdot\mathbf{n}) = \sum_{j=1}^{N} f_j\,\psi_j \\
\Leftrightarrow\quad &\sum_{j=1}^{N} u_j\int_{\partial\Omega}(\boldsymbol{\sigma}\nabla\varphi_j\cdot\mathbf{n})\,\varphi_\ell\,\mathrm{d}\mathbf{x} = \sum_{j=1}^{N} f_j\int_{\partial\Omega}\psi_j\,\varphi_\ell\,\mathrm{d}\mathbf{x} \\
\Leftrightarrow\quad &\mathbf{B}_{\boldsymbol{\sigma}}\mathbf{u} = \mathbf{B}_\Gamma\mathbf{f}
\end{aligned}$$

Now, we know how to incorporate the boundary condition (16) by replacing $\mathbf{B}_{\boldsymbol{\sigma}}\mathbf{u}$ by $\mathbf{B}_\Gamma\mathbf{f}$ and put the terms on the right hand side. We get eq. (17) with a different right hand side $\mathbf{b}$:

$$\begin{aligned}
\mathbf{b} = &\Big(\frac{1}{A_m^k\, C_m^k}\,(\theta-1)\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} - \frac{1}{dt}\,\mathbf{M}\Big)\mathbf{V}_m^{(i)} + \frac{1}{A_m^k\, C_m^k}\,(\theta-1)\,\mathbf{K}_{\boldsymbol{\sigma}_i^k}\,\boldsymbol{\phi}_e^{(i)} \\
&\underbrace{+\frac{1}{A_m^k\, C_m^k}\,(\theta-1)\,\mathbf{B}_{\Gamma_M}\mathbf{p}^{k,(i)} - \frac{1}{A_m^k\, C_m^k}\,(\theta-1)\,\mathbf{B}_{\Gamma_M}\mathbf{p}^{k,(i)}}_{=\mathbf{0}} \\
&\underbrace{-\frac{1}{A_m^k\, C_m^k}\,\theta\,\mathbf{B}_{\Gamma_M}\mathbf{p}^{k,(i+1)} + \frac{1}{A_m^k\, C_m^k}\,\theta\,\mathbf{B}_{\Gamma_M}\mathbf{p}^{k,(i+1)}}_{=\mathbf{0}}
\end{aligned} \tag{18}$$

Analogously for the first monodomain equation in matrix notation, eq. (11), with $\mathbf{B}_{\boldsymbol{\sigma}}\mathbf{u} = \mathbf{B}_\Gamma\mathbf{f}$ and $q := (\boldsymbol{\sigma}_e\nabla\phi_e)\cdot\mathbf{n}_m$:

$$\begin{aligned}
&(\mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i} + \mathbf{B}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i})\boldsymbol{\phi}_e + \sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k} + \mathbf{B}_{\boldsymbol{\sigma}_i^k})\mathbf{V}_m^k = 0 \\
\Leftrightarrow\quad &\mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}\boldsymbol{\phi}_e + \mathbf{B}_{\boldsymbol{\sigma}_e}\boldsymbol{\phi}_e + \underbrace{\mathbf{B}_{\boldsymbol{\sigma}_i}\boldsymbol{\phi}_e}_{=\sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\,\mathbf{B}_{\boldsymbol{\sigma}_i^k}\,\boldsymbol{\phi}_e} + \sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}\mathbf{V}_m^k + \mathbf{B}_{\boldsymbol{\sigma}_i^k}\mathbf{V}_m^k) = 0 \\
\Leftrightarrow\quad &\mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}\boldsymbol{\phi}_e + \mathbf{B}_{\boldsymbol{\sigma}_e}\boldsymbol{\phi}_e - \mathbf{B}_{\Gamma_M}\sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\mathbf{p}^k + \sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\,(\mathbf{K}_{\boldsymbol{\sigma}_i^k}\mathbf{V}_m^k + \mathbf{B}_{\Gamma_M}\mathbf{p}^k) = 0 \\
\Leftrightarrow\quad &\mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}\boldsymbol{\phi}_e + \mathbf{B}_{\Gamma_M}\mathbf{q} + \sum_{k=1}^{M_{\mathrm{mu}}} f_r^k\mathbf{K}_{\boldsymbol{\sigma}_i^k}\mathbf{V}_m^k = 0
\end{aligned} \tag{19}$$

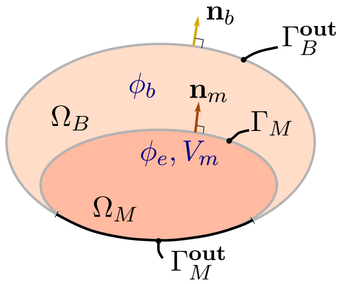

Abbildung 1: Computational domains

The same operations can also be done by adding the flux terms to the vector of unknowns:

$$\begin{bmatrix} \dfrac{\theta}{A_m^k\,C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} - \dfrac{1}{dt}\,\mathbf{M} & \dfrac{\theta}{A_m^k\,C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} & \underbrace{\dfrac{(1-\theta)}{A_m^k\,C_m^k}\,\mathbf{B}_{\Gamma_M} - \dfrac{(1-\theta)}{A_m^k\,C_m^k}\,\mathbf{B}_{\Gamma_M}}_{=\mathbf{0}} & \underbrace{\dfrac{\theta}{A_m^k\,C_m^k}\,\mathbf{B}_{\Gamma_M} - \dfrac{\theta}{A_m^k\,C_m^k}\,\mathbf{B}_{\Gamma_M}}_{=\mathbf{0}} & \\ f_r^k\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} & \mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i} & & 0 & \mathbf{B}_{\Gamma_M} \end{bmatrix} \begin{bmatrix} \mathbf{V}_m^{(i+1)} \\ \boldsymbol{\phi}_e^{(i+1)} \\ \mathbf{p}^{k,(i)} \\ \mathbf{p}^{k,(i+1)} \\ \mathbf{q}^{(i+1)} \end{bmatrix} = \begin{bmatrix} \big((\theta-1)\,\dfrac{1}{A_m^k\,C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} - \dfrac{1}{dt}\,\mathbf{M}\big)\,\mathbf{V}_m^{(i)} + (\theta-1)\,\mathbf{K}_{\boldsymbol{\sigma}_i^k}\,\boldsymbol{\phi}_e^{(i)} \\ \mathbf{0} \end{bmatrix}, \tag{20}$$

where

$$p^{k,(i)} \quad = (\boldsymbol{\sigma}_i^k\,\nabla V_m^{k,(i)})\cdot\mathbf{n}_m \quad = -(\boldsymbol{\sigma}_i^k\,\nabla \phi_e^{(i)})\cdot\mathbf{n}_m$$

So far we haven't specified a boundary condition for the second row.

1.3 Additional body region

To simulate surface-electromyography we add a domain Ω_B which represents fat tissue. The setting is visualized by Fig. 1.

On the muscle domain Ω_M, we have the 1st and 2nd Multidomain equation,

$$\begin{aligned} &\operatorname{div}\big((\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i)\,\operatorname{grad}(\phi_e)\big) + \sum_{k=1}^{M_{\text{mu}}} f_r^k\,\operatorname{div}\big(\boldsymbol{\sigma}_i^k\,\operatorname{grad}(V_m^k)\big) = 0,\\ &\operatorname{div}\big(\boldsymbol{\sigma}_i^k\,\operatorname{grad}(\phi_i^k)\big) = A_m^k\,\big(C_m^k\,\frac{\partial V_m^k}{\partial t} + I_{\text{ion}}(V_m^k)\big), \qquad \forall\,k\in 1\ldots M_{\text{mu}}. \end{aligned}$$

The 2nd Multidomain equation is solved using an operator splitting approach, which yields the following diffusion equation to be solved as one part of the splitting (4):

$$\frac{\partial V_m^k}{\partial t} \;=\frac{1}{A_m^k\,C_m^k}\,\operatorname{div}\big(\boldsymbol{\sigma}_i^k\,\operatorname{grad}(V_m^k+\phi_e)\big)$$

We assume a harmonic electric potential on Ω_B:

$$\operatorname{div}\big(\boldsymbol{\sigma}_b \operatorname{grad}(\phi_b)\big) = 0 \qquad \text{on } \Omega_B.$$

The boundary conditions on Γ_M are given by (16):

$$\begin{aligned} &(\boldsymbol{\sigma}_i^k \nabla\phi_i^k)\cdot\mathbf{n}_m = 0 && \text{on } \Gamma_M \\ \Rightarrow\quad &(\boldsymbol{\sigma}_i^k \nabla V_m^k)\cdot\mathbf{n}_m = -(\boldsymbol{\sigma}_i^k \nabla\phi_e)\cdot\mathbf{n}_m =: p^k && \text{on } \Gamma_M. \end{aligned} \tag{21}$$

For the diffusion part of the 2nd Multidomain equation, boundary condition (21) is satisfied automatically when all flux terms are neglected (cf. (20)).

The connection between muscle and body domain is given by the following conditions:

$$\begin{aligned} &\phi_e = \phi_b && \text{on } \Gamma_M, \\ &(\boldsymbol{\sigma}_e\nabla\phi_e)\cdot\mathbf{n}_m = -(\boldsymbol{\sigma}_b\nabla\phi_b)\cdot\mathbf{n}_m =: q && \text{on } \Gamma_M. \end{aligned}$$

Furthermore we have with $\phi_e = \phi_i^k - V_m^k$:

$$\begin{aligned} &\big((\boldsymbol{\sigma}_e + \boldsymbol{\sigma}_i)\nabla\phi_e\big)\cdot\mathbf{n}_m \\ &= (\boldsymbol{\sigma}_e\nabla\phi_e)\cdot\mathbf{n}_m + (\boldsymbol{\sigma}_i\nabla\phi_e)\cdot\mathbf{n}_m \\ &= q + \sum_{k=1}^{M_{\text{mu}}} f_r^k\Big(-\underbrace{(\boldsymbol{\sigma}_i^k \nabla V_m^k)\cdot\mathbf{n}_m}_{=p^k} + \underbrace{(\boldsymbol{\sigma}_i^k \nabla\phi_i^k)\cdot\mathbf{n}_m}_{=0,\,(21)}\Big) \\ &= q - \sum_{k=1}^{M_{\text{mu}}} f_r^k\, p^k \end{aligned}$$

The boundary conditions on the outer boundary of $\partial\Omega_B$ are given by

$$(\boldsymbol{\sigma}_b\nabla\phi_b)\cdot\mathbf{n}_b = 0 \quad \text{on } \Gamma_B^{\text{out}} \cup \Gamma_M^{\text{out}}.$$

1.4 System of linear equations

With the body potential, $\boldsymbol{\phi}_b$, and for $M_{\text{mu}} = 1$ motor unit, we get the following system:

$$\left[\begin{array}{c|c|c|ccc}
\mathbf{A}_{V_m,V_m} & \mathbf{B}_{V_m,\phi_e} & & & & \\
\mathbf{B}_{\phi_e,V_m} & \mathbf{B}_{\phi_e,\phi_e} & & f_r^k\,\mathbf{B}_{\Gamma_M} & -\,f_r^k\,\mathbf{B}_{\Gamma_M} & \mathbf{B}_{\Gamma_M} \\ \hline
 & & \mathbf{C}_{\phi_b,\phi_b} & & & -\mathbf{B}_{\Gamma_M} \\ \hline
 & \mathbf{I}_{\Gamma_M} & -\mathbf{I}_{\Gamma_M} & & &
\end{array}\right]
\left[\begin{array}{c}
V_m^{(i+1)} \\ \hline \boldsymbol{\phi}_e^{(i+1)} \\ \hline \boldsymbol{\phi}_b^{(i+1)} \\ \hline \mathbf{p}^{k,(i+1)} \\ \mathbf{q}^{(i+1)}
\end{array}\right]
=
\left[\begin{array}{c}
\mathbf{b}_{V_m}^{(i+1)} \\ \mathbf{0} \\ \hline \mathbf{0} \\ \hline \mathbf{0}
\end{array}\right],$$

$$\Leftrightarrow \quad
\left[\begin{array}{c|c|c|c}
\mathbf{A}_{V_m,V_m} & \mathbf{B}_{V_m,\phi_e} & & \\
\mathbf{B}_{\phi_e,V_m} & \mathbf{B}_{\phi_e,\phi_e} & & \mathbf{B}_{\Gamma_M} \\ \hline
 & & \mathbf{C}_{\phi_b,\phi_b} & -\mathbf{B}_{\Gamma_M} \\ \hline
 & \mathbf{I}_{\Gamma_M} & -\mathbf{I}_{\Gamma_M} &
\end{array}\right]
\left[\begin{array}{c}
V_m^{(i+1)} \\ \hline \boldsymbol{\phi}_e^{(i+1)} \\ \hline \boldsymbol{\phi}_b^{(i+1)} \\ \hline \mathbf{q}^{(i+1)}
\end{array}\right]
=
\left[\begin{array}{c}
\mathbf{b}_{V_m}^{(i+1)} \\ \mathbf{0} \\ \hline \mathbf{0} \\ \hline \mathbf{0}
\end{array}\right]$$

where

$$\begin{aligned}
\mathbf{A}_{V_m,V_m} &= \frac{1}{A_m^k\,C_m^k}\,\theta\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} - \frac{1}{dt}\,\mathbf{M}, \\
\mathbf{B}_{V_m,\phi_e} &= \frac{1}{A_m^k\,C_m^k}\,\theta\,\mathbf{K}_{\boldsymbol{\sigma}_i^k}, \\
\mathbf{B}_{\phi_e,V_m} &= f_r^k\,\mathbf{K}_{\boldsymbol{\sigma}_i^k}, \\
\mathbf{B}_{\phi_e,\phi_e} &= \mathbf{K}_{\boldsymbol{\sigma}_e+\boldsymbol{\sigma}_i}, \\
\mathbf{B}_{\Gamma_B,kj} &= \int_{\Gamma_M} \psi_j\,\varphi_k\,\mathrm{d}\mathbf{x}, \\
\mathbf{C}_{\phi_b,\phi_b} &= \mathbf{K}_{\boldsymbol{\sigma}_b},
\end{aligned}$$

$\mathbf{I}_{\Gamma_M}$ containing 1 entries for boundary dofs,

$$\mathbf{b}_{V_m}^{(i+1)} = \big((\theta-1)\,\frac{1}{A_m^k\,C_m^k}\,\mathbf{K}_{\boldsymbol{\sigma}_i^k} - \frac{1}{dt}\,\mathbf{M}\big)\mathbf{V}_m^{(i)} + (\theta-1)\,\mathbf{K}_{\boldsymbol{\sigma}_i^k}\,\boldsymbol{\phi}_e^{(i)}$$

This matrix can be condensed and takes the form

$$\Leftrightarrow \quad
\left[\begin{array}{c|c|c}
\mathbf{A}_{V_m,V_m} & \mathbf{B}_{V_m,\phi_e} & \\
\mathbf{B}_{\phi_e,V_m} & \mathbf{B}_{\phi_e,\phi_e} & \mathbf{D} \\ \hline
 & \mathbf{E} & \mathbf{C}_{\phi_b,\phi_b}
\end{array}\right]
\left[\begin{array}{c}
V_m^{(i+1)} \\ \hline \boldsymbol{\phi}_e^{(i+1)} \\ \hline \hat{\boldsymbol{\phi}}_b^{(i+1)}
\end{array}\right]
=
\left[\begin{array}{c}
\mathbf{b}_{V_m}^{(i+1)} \\ \mathbf{0} \\ \hline \mathbf{0}
\end{array}\right].$$

Here, $\mathbf{D}$ and $\mathbf{E}$ contain entries for the dofs in the elements that are adajacent to the border dofs. The size of the last row and column of the system matrix is the number of dofs in the fat domain, without the border dofs, as they are already included in the second column and row.

$\hat{\boldsymbol{\phi}}_b^{(i+1)}$ is the vector of body potential without dofs on the border.

1.5 Summary

$$\left[\begin{array}{cccc|c}
\mathbf{A}^1_{V_m,V_m} & & & \mathbf{B}^1_{V_m,\phi_e} & \\
& \mathbf{A}^2_{V_m,V_m} & & \mathbf{B}^2_{V_m,\phi_e} & \\
& & \mathbf{A}^k_{V_m,V_m} & \mathbf{B}^k_{V_m,\phi_e} & \\
\mathbf{B}^1_{\phi_e,V_m} & \mathbf{B}^2_{\phi_e,V_m} & \mathbf{B}^k_{\phi_e,V_m} & \mathbf{B}_{\phi_e,\phi_e} & \mathbf{D} \\
\hline
& & & \mathbf{E} & \mathbf{C}_{\phi_b,\phi_b}
\end{array}\right]
\left[\begin{array}{c}
V_m^{1,(i+1)} \\
V_m^{2,(i+1)} \\
V_m^{k,(i+1)} \\
\hline
\boldsymbol{\phi}_e^{(i+1)} \\
\hline
\hat{\boldsymbol{\phi}}_b^{(i+1)}
\end{array}\right]
=
\left[\begin{array}{c}
\mathbf{b}_{V_m}^{1,(i+1)} \\
\mathbf{b}_{V_m}^{2,(i+1)} \\
\mathbf{b}_{V_m}^{k,(i+1)} \\
\mathbf{0} \\
\hline
\mathbf{0}
\end{array}\right] .$$

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