Simulating Cardiac Electromechanics using Abaqus UEL

Introduction

From a finite elements point of view, modeling the complex beating of heart tissues involves solving strongly coupled electromechanical equations. The field variables that govern the overall evolution of cardiac electromechanics are the transmembrane potential $\phi(x_i, t)$ (difference between intracellular and extracellular electrical potential), extracellular potential $\phi^e(x_i, t)$ and the deformation $u_i(x_i, t)$. The electromechanical coupling occurs as the cardiac tissue responds mechanically to induced electrical excitations and the flow of ions through the heart membranes is partially influenced by the current state of tissue deformation.

The process involved in implementing the fully coupled electromechanical equations can be segregated into steps as follows:

1. **Monodomain (Electrical only):**
   Field variable: $\phi(x_i, t)$
   The only solution variable is the intracellular electrical potential ϕ. The general evolution of the potential is governed by higher order ODEs and is generally recast into two first order ODEs with an equation for a recovery variable that needs to be solved internally at every integration point.
   Field Equations:
$$\dot{\phi} + \vec{\nabla} \cdot \vec{q} = F^{\phi}, where\ \vec{q} = -\widetilde{D}(\vec{u})\vec{\nabla}\phi$$
$$\dot{r} = f^r(\phi, r)$$

2. **Bidomain (Electrical only):**
   Field variables: $\phi(x_i, t), \phi^e(x_i, t)$
   The equations now account for an additional transmembrane potential.
   Field Equations:
$$\dot{\phi} + \vec{\nabla} \cdot \vec{q}_i + \vec{\nabla} \cdot \vec{q}_{ie} = F^{\phi}$$
$$\vec{\nabla} \cdot \vec{q}_i + \vec{\nabla} \cdot \vec{q}_e = 0$$
$$where$$
$$\vec{q}_i = -\widetilde{D}_i(\vec{u})\vec{\nabla}\phi, \vec{q}_{ie} = -\widetilde{D}_i(\vec{u})\vec{\nabla}\phi_e, and\ \vec{q}_e = -\widetilde{D}(\vec{u})\vec{\nabla}\phi_e$$
$$\dot{r} = f^r(\phi, r)$$

3. **Monodomain and Bidomain Electromechanical Coupling:**
   Field variables: $\phi(x_i, t), \phi^e(x_i, t), u_i(x_i, t)$
   For these cases, the RHS of mono and bidomain electrical equations are extended to include contributions from mechanical deformation and the mechanical deformation itself is solved separately. This represents the fully coupled behavior.
   Field Equations:

$$Mechanical\ PDE\colon\ \ \vec{\nabla} \cdot \tilde{\tau} + \vec{b} = \vec{0} \quad (in\ B) \quad with\colon \begin{cases} \tilde{\tau} = \tilde{\tau}_{pas}(\vec{u}) + \tilde{\tau}_{act}(\vec{u}, \gamma) \\ \dot{\gamma} = f^{\gamma}(\phi, \gamma)\ (fiber\ tension\ ODE) \end{cases}$$

$$BC's\colon \begin{cases} \vec{u} = \bar{u} & (on\ \partial B_u) \\ \tilde{\tau} \cdot \hat{n} = \bar{t} & (on\ \partial B_t) \end{cases}$$

$$Electrical\ (monodomain)\ PDE:\ \dot{\phi} + \vec{\nabla}\cdot\vec{q} = F^{\phi} \quad (in\ B) \quad with: \begin{cases} \vec{q} = -\widetilde{D}(\vec{u})\vec{\nabla}\phi \\ F^{\phi} = F^{\phi}_{elec}(\phi, r) + F^{\phi}_{mech}(\vec{u}, \phi) \\ \dot{r} = f^{r}(\phi, r)\ \ (recovery\ variable\ ODE) \end{cases}$$

$$Electrical\ (bidomain) PDE's: \begin{cases} \dot{\phi} + \vec{\nabla}\cdot\vec{q}_i + \vec{\nabla}\cdot\vec{q}_{ie} = F^{\phi} \\ \vec{\nabla}\cdot\vec{q}_i + \vec{\nabla}\cdot\vec{q}_e = 0 \end{cases} \quad (in\ B) \quad with: \begin{cases} \begin{cases} \vec{q}_i = -\widetilde{D}_i(\vec{u})\vec{\nabla}\phi \\ \vec{q}_{ie} = -\widetilde{D}_i(\vec{u})\vec{\nabla}\phi_e \\ \vec{q}_e = -\widetilde{D}(\vec{u})\vec{\nabla}\phi_e \end{cases} \\ F^{\phi} = F^{\phi}_{elec}(\phi, r) + F^{\phi}_{mech}(\vec{u}, \phi) \\ \dot{r} = f^{r}(\phi, r)\ \ (recovery\ variable\ ODE) \end{cases}$$

Project Scope

Though the final objective of this work is to implement the fully coupled electromechanical equations through an Abaqus UEL, due to limited time available, the scope of the project was restricted to implementing only the first step of the process (monodomain electrical equations only). concentrating on modeling the FitzHugh-Nagumo type pacemaker cells responsible for generating and transmitting the electrical signals leading to heart beat and the Aliev-Panfilov type muscular cells that are both excitable and contractile.

Finite Element Implementation of Monodomain electrical equations

The governing monodomain electrical equations are

$$\frac{\partial \phi}{\partial t} = \frac{\partial q_i}{\partial x_i} + f^{\phi}\ , q_i = D_{ij}\frac{\partial \phi_i}{\partial x_j}$$
$$\frac{\partial r}{\partial t} = f^{r}$$
$$\phi \rightarrow action\ potential$$
$$r \rightarrow local\ recovery\ variable$$
$$D_{ij} \rightarrow conduction\ tensor$$
$$f^{\phi} \rightarrow f^{\phi}(\phi, r) \rightarrow flux\ term\ for\ \phi$$
$$f^{r} \rightarrow f^{r}(\phi, r) \rightarrow flux\ term\ for\ r$$

Applying the principle of virtual work to the above set of equations and following the usual procedure of integrating over volume, multiplying by $\delta\phi$, applying divergence theorem, assuming $\delta\phi = N^a\delta\phi^a$ and $\phi = N^a\phi^a$, and approximating $\frac{\partial\phi}{\partial t} = \frac{\phi - \phi^n}{\Delta t}$, the final expressions for the residual vector and stiffness matrix using consistent linearization are as follows (with the absence of any flux terms for simplicity):

$$R^a = \int N^d\left(\frac{\phi^d - \phi^{d(n)}}{\Delta t}\right)N^a dV + \int D_{ij}\frac{\partial N^a}{\partial x_i}\frac{\partial N^d}{\partial x_j}\phi^d dV - \int f^{\phi}\, N^a dV$$

$$K_{ab} = \frac{\partial R^a}{\partial \phi^b} = \int \left(\frac{N^a N^b}{\Delta t}\right) dV + \int D_{ij} \frac{\partial N^a}{\partial x_i} \frac{\partial N^b}{\partial x_j} dV - \int \frac{\partial f^\phi}{\partial \phi^b} N^a dV$$

FitzHugh-Nagumo Pacemaker Cells

These cells are self-excited, do not contract and are primarily responsible for generating and transmitting the electrical signals responsible for heart beat. The flux terms for the primary and the recovery variables along with its derivative and the update formula for the recover variable are as follows:

$$f^\phi = c(\phi(\phi - \alpha)(1 - \phi) - r)$$

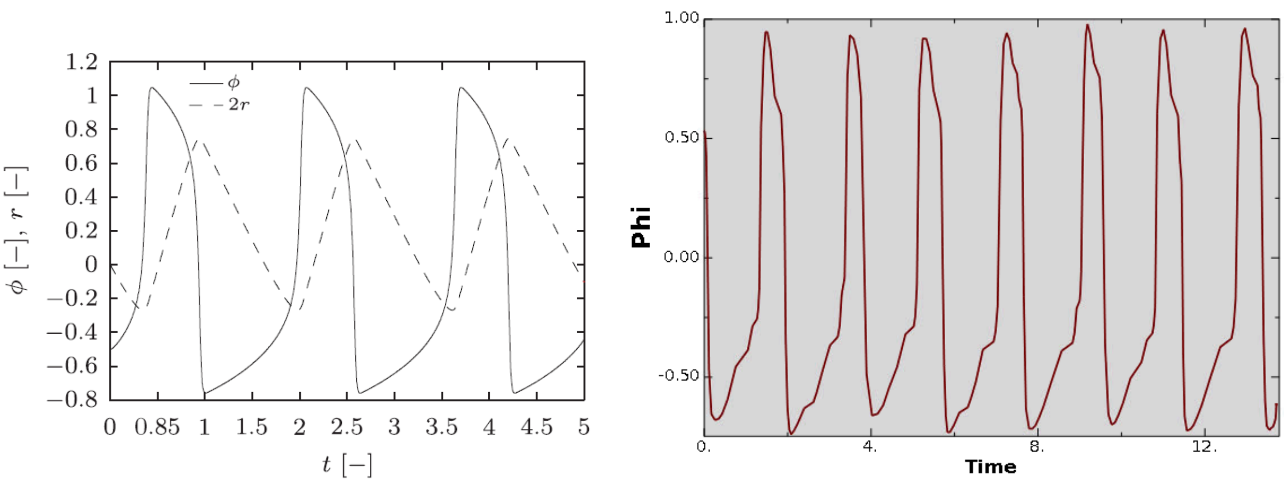
$$f^r = \phi - br + a$$

$$r = \frac{r_n + (\phi + \alpha)\Delta t}{1 + b\Delta t}$$

$$\frac{df^\phi}{d\phi} = \frac{\partial f^\phi}{\partial \phi} + \frac{\partial f^\phi}{\partial r}\frac{\partial r}{\partial \phi}$$

$$\frac{df^\phi}{d\phi} = c(-3\phi^2 + 2(1 - \alpha)\phi - \alpha) - \frac{c\Delta t}{1 + \mathrm{b}\Delta t}$$

A 2D Abaqus UEL was developed to model the pacemaker cells implementing the stiffness matrix and force vectors after incorporating the flux term and its derivative. The UEL implementation was validated by leaving a square grid of these cell elements with an initial potential condition and left to see if the self-oscillatory response could be predicted. The figures below compare the oscillatory response of these cells discussed in [1] and what the Abaqus UEL predicted. Note that in the referred paper [1], the plot was of a normalized entity but for the UEL implementation this normalization was not performed and hence the difference in the scales.



Aliev-Panfilov Muscular Cells

Contrary to the pacemaker cells, the Aliev-Panfilov musclular cells make up the cardiac musculature and are responsible for causing the heart beat through muscle contraction. The potential inputs for these cells are given from the pacemaker cells and the electric charge flowing through them causes these muscles to contract. In actuality, solving equations for these muscles entail incorporating a loading term to the electrical equation that is influenced by tissue deformation and on the mechanical side, the muscle contracts due to the current electrical potential. However, for this project only the electrical response of these cells is considered. The flux terms for the primary and the recovery variables along with its derivative and the update formula for the recover variable are as follows:

$$f^{\phi} = c\big(\phi(\phi-\alpha)(1-\phi)\big) - r\phi$$

$$f^{r} = \left[\gamma + \frac{\mu_1 r}{\mu_2+\phi}\right]\big(-r - c\phi(\phi-b-1)\big)$$

Since the choice of flux term for the recovery variable makes the governing equation non-linear, a Newton-Raphson scheme is implemented at each iteration for the global variable to solve for the update for recovery variable. The residual and tangent terms for solving the recovery variable update are as follows:

$$\frac{\partial R^r}{\partial r} dr = -R^r$$

$$R^r = r - r_n - \left[\left[\gamma + \frac{\mu_1 r}{\mu_2+\phi}\right]\big(-r - c\phi(\phi-b-1)\big)\right]\Delta t$$

$$\frac{\partial R^r}{\partial r} = 1 + \left[\gamma + \left[\frac{\mu_1}{\mu_2+\phi}\right]\big(2r + c\phi(\phi-b-1)\big)\right]\Delta t$$

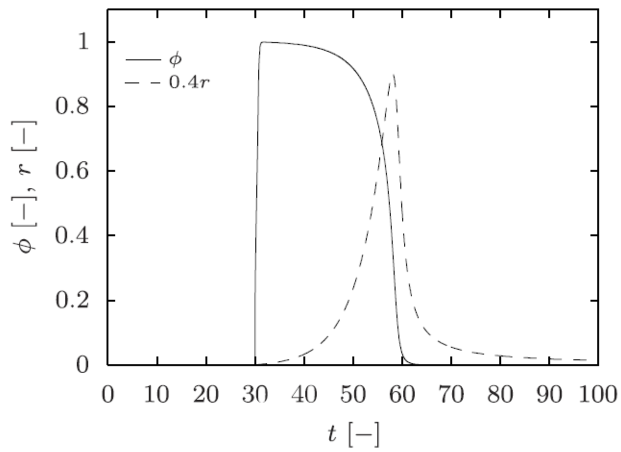
And the derivative of the flux term appearing in the stiffness matrix is given as

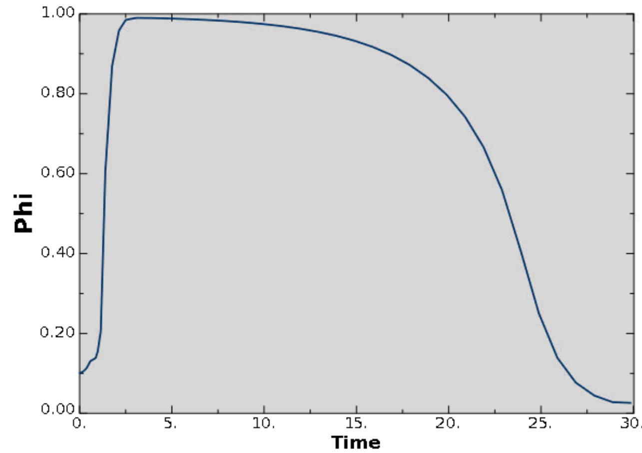
$$\frac{df^{\phi}}{d\phi} = c(-3\phi^2 + 2(1-\alpha)\phi + \alpha) - r - \phi\frac{\partial r}{\partial \phi}$$

$$\frac{dR^r}{d\phi} = \frac{\partial R^r}{\partial \phi} + \frac{\partial R^r}{\partial r}\frac{\partial r}{\partial \phi} = 0$$

$$\frac{\partial R^r}{\partial \phi} = \left[\left[\gamma + \frac{\mu_1 r}{\mu_2+\phi}\right]c(2\phi-b-1) - \frac{\mu_1 r}{(\mu_2+\phi)^2}\big(r + c\phi(\phi-b-1)\big)\right]\Delta t$$

As opposed to the oscillatory nature of the pacemaker cells, the muscular cells show a steady decline to original potential state when subject to excitation. The Abaqus UEL developed prior was enhanced to include the modified flux terms and the Newton-Raphson iteration items for the recovery variable. The implementation was validated using a 2D grid of these muscular cells subject to initial excitation against the results discussed in [1]. The results from the reference paper and from Abaqus UEL are compared below. As mentioned earlier, the plot from the reference paper was normalized for potential and time but this was not done for the Abaqus implementation and hence the difference in scales.





Future Work

The topics covered for this project is a part of ongoing work to implement the fully coupled electromechanical equations through Abaqus UEL. The next steps in accomplishing that would be to implement the electrical bidomain equations followed by adding the coupling terms on both mechanical and structural sides.

References

1. S. Göktepe, E. Kuhl *"Computational modeling of cardiac electrophysiology: A novel finite element approach"*, International Journal for Numerical methods in Engineering.

2. S. Göktepe, E. Kuhl *"Electromechanics of the heart: a unified approach to the strongly coupled excitation-contraction problem"*, Comput. Mech. 2010.

3. H. Dal, S. Göktepe, M. Kaliske, E. Kuhl *"A fully implicit finite element method for bidomain models of cardiac electromechanics"*, Comput. Methods. Appl. Mech. Eng. 2013.