Hyper-elastic constitutive equation for cardiomyocytes

Humphrey's hyper-elastic constitutive equation for the cardiac muscle

$$W = c_{p1}(\alpha - 1)^2 + c_{p2}(\alpha - 1)^3 + c_{p3}(I_1 - 3) + c_{p4}(I_1 - 3)(\alpha - 1) + c_{p5}(I_1 - 3)^2$$

, where X_i is original coordinates, x_i is current coordinates, u_i is displacement $(x_i - X_i)$, $F_{ij} = \frac{\partial x_i}{\partial X_j}$ is deformation tensor, $C_{ij} = F_{ki}F_{kj}$ is right Cauchy-Green tensor, N is fiber direction normal vector, and $I_1 = \frac{tr(C)}{\det(C)}$, $I_3 = \det(C)$, $I_4 = N^T CN$, $\alpha = \sqrt{I_4}$ are invariants. Parameters are in Table 1.

Table 1. Humphrey model parameters

Param	c_{p1}	c_{p2}	c_{p3}	c_{p4}	c_{p5}
Value [kPa]	3.080	3.240	0.359	-1.940	1.660

Assume 1 directional elongation (stretch = α), incompressible condition leads following deformation gradient tensor F and right Cauchy-Green tensor can be expressed as:

$$F = \begin{bmatrix} \alpha & & \\ & \frac{1}{\sqrt{\alpha}} & \\ & & \frac{1}{\sqrt{\alpha}} \end{bmatrix}, \quad C = \begin{bmatrix} \alpha^2 & & \\ & \frac{1}{\alpha} & \\ & & \frac{1}{\alpha} \end{bmatrix}, \quad C^{-1} = \begin{bmatrix} \frac{1}{\alpha^2} & & \\ & \alpha & \\ & & \alpha \end{bmatrix}$$

Therefore,

$$I_1 = \alpha^2 + \frac{2}{\alpha}, \qquad I_2 = 2\alpha + \frac{1}{\alpha^2}, \qquad I_3 = 1, \qquad I_4 = \alpha^2$$

The second Piola-Kirchhoff stress can be expressed as:

$$S_{ij} = 2\frac{\partial W}{\partial C_{ij}} = 2\frac{\partial W}{\partial I_1}\frac{\partial I_1}{\partial C_{ij}} + 2\frac{\partial W}{\partial I_4}\frac{\partial I_4}{\partial C_{ij}}$$

$$= 2\frac{\partial W}{\partial I_1}\left(I_3^{-\frac{1}{3}}\delta_{ij} - \frac{1}{3}I_3^{-\frac{1}{3}}I_1 C_{ij}^{-1}\right) + 2\frac{\partial W}{\partial I_4}N_i N_j$$

$$S_{11} = 2\left\{\frac{\partial W}{\partial I_1}\frac{2}{3}\left(1 - \frac{1}{\alpha^2}\right) + \frac{\partial W}{\partial I_4}\right\}$$

Boundary value problem of partial differential equation

Potential energy of the hyperelastic material under certain boundary conditions

$$\Phi = \int_\Omega W d\Omega - \int_{\partial\Omega} \boldsymbol{t} \cdot \boldsymbol{u}\, dS$$

Principle of stationary potential energy leads equilibrium of internal force $\boldsymbol{Q}$ and external force $\boldsymbol{F}$.

$$
\begin{aligned}
0 = \delta\Phi &= \int_\Omega \frac{\partial W}{\partial C_{ij}} \delta C_{ij} d\Omega - \int_{\partial\Omega} \boldsymbol{t} \cdot \delta\boldsymbol{u}\, dS \\
&= \int_\Omega 2\frac{\partial W}{\partial C_{ij}} \delta E_{ij} d\Omega - \int_{\partial\Omega} \boldsymbol{t} \cdot \delta\boldsymbol{u}\, dS \\
&= \int_\Omega 2\frac{\partial W}{\partial C_{ij}} B_j \delta u_i d\Omega - \int_{\partial\Omega} t_i \delta u_i\, dS \\
&= \int_\Omega S_{ij} B_j \delta u_i d\Omega - \int_{\partial\Omega} t_i \delta u_i\, dS \\
&= \delta\boldsymbol{u}\{\boldsymbol{Q} - \boldsymbol{F}\}
\end{aligned}
$$

To obtain tangential stiffness, linearize the internal force variational work to the strain:

$$
\begin{aligned}
\Delta(\boldsymbol{Q}\delta\boldsymbol{u}) &= \Delta\left\{\int_\Omega S_{ij}\delta E_{ij} d\Omega\right\} \\
&= \int_\Omega \{\Delta S_{ij}\delta E_{ij} + S_{ij}\Delta(\delta E_{ij})\} d\Omega \\
&= \int_\Omega \left\{2\frac{\partial \Delta \mathrm{W}}{\partial \mathrm{C_{ij}}}\delta E_{ij} + S_{ij}\Delta\left(\frac{1}{2}\delta F_{ki}F_{kj} + \frac{1}{2}F_{ki}\delta F_{kj}\right)\right\} d\Omega \\
&= \int_\Omega \left\{2\frac{\partial^2 \mathrm{W}}{\partial \mathrm{C_{ij}}\,\partial \mathrm{C_{kl}}}\Delta C_{kl}\delta E_{ij} + \frac{1}{2}S_{ij}\left(\delta F_{ki}\Delta F_{kj} + \Delta F_{ki}\delta F_{kj}\right)\right\} d\Omega \\
&= \int_\Omega \left\{4\frac{\partial^2 \mathrm{W}}{\partial \mathrm{C_{ij}}\,\partial \mathrm{C_{kl}}}\Delta E_{kl}\delta E_{ij} + S_{ij}\delta F_{ki}\Delta F_{kj}\right\} d\Omega \\
&= \int_\Omega \left\{4\frac{\partial^2 \mathrm{W}}{\partial \mathrm{C_{ij}}\,\partial \mathrm{C_{kl}}}[\mathrm{B_{kl}}]\{\Delta u^e\}[B_{ij}]\{\delta u^e\} + S_{ij}[Z_{ki}]\{\delta u^e\}[Z_{kj}]\{\Delta u^e\}\right\} d\Omega \\
&= \{\delta u^n\}\int_\Omega \{[\mathrm{B}]^T[D][B] + S_{ij}[Z_{ki}][Z_{kj}]\} d\Omega\ \{\Delta u^n\}
\end{aligned}
$$

$\{u^e\}$ is element's node displacement vector, $\{\delta u^e\}$ is element's node variational displacement vector, $\{u^n\}$ is node displacement vector and $\{\delta u^n\}$ is node variational displacement vector.

$$
[D] = D_{ijkl} = 4\frac{\partial^2 W}{\partial C_{ij}\partial C_{kl}} = 2\frac{\partial}{\partial C_{kl}}\left(\frac{\partial W}{\partial I_1}\frac{\partial I_1}{\partial C_{ij}} + 2\frac{\partial W}{\partial I_4}\frac{\partial I_4}{\partial C_{ij}}\right)
$$

To obtain [B], note that variational Cauchy-Green strain tensor is expressed as follows:

$$
\delta E_{ij} = \frac{1}{2}\left(\frac{\partial \delta u_i}{\partial X_j} + \frac{\partial \delta u_j}{\partial X_i} + \frac{\partial \delta u_k}{\partial X_i}\frac{\partial u_k}{\partial X_j} + \frac{\partial \delta u_k}{\partial X_j}\frac{\partial u_k}{\partial X_i}\right), \qquad \delta F_{ij} = \frac{\partial \delta x_i}{\partial X_j} = \frac{\partial \delta u_i}{\partial X_j}
$$

$$\delta E_{11} = \frac{1}{2}\left(\frac{\partial \delta u_1}{\partial X_1} + \frac{\partial \delta u_1}{\partial X_1} + \frac{\partial \delta u_k}{\partial X_1}\frac{\partial u_k}{\partial X_1} + \frac{\partial \delta u_k}{\partial X_1}\frac{\partial u_k}{\partial X_1}\right) = \left(1 + \frac{\partial u_1}{\partial X_1}\right)\frac{\partial \delta u_1}{\partial X_1} = \alpha\frac{\partial \delta u_1}{\partial X_1}$$

Element shape function $[N^e]$ for the finite element discretization of 1-dimensional truss of length L between node k and l can be expressed as follows:

$$u_1(r) = \left[1 - \frac{r}{L}, \quad \frac{r}{L}\right]\begin{Bmatrix} u_1^k \\ u_1^l \end{Bmatrix} = [N^e]\{u^e\}, \;\; \delta u_1(r) = [N^e]\{\delta u^e\}$$

Where r is parametric coordinate 0<r<L.

$$\frac{\partial \delta u_1}{\partial X_1} = \frac{\partial [N^e]\{\delta u^e\}}{\partial X_1} = \left[\frac{\partial}{\partial r}\left(1 - \frac{r}{L}\right), \quad \frac{\partial}{\partial r}\left(\frac{r}{L}\right)\right]\{\delta u^e\} = \frac{1}{L}[-1, \quad 1]\{\delta u^e\} = [Z]\{\delta u^e\}$$

$$\delta E_{11} = \alpha\frac{\partial \delta u_1}{\partial X_1} = \frac{\alpha}{L}[-1, \quad 1]\{\delta u^e\} = [B]\{\delta u^e\}$$

$$\{\delta u^n\}\int_\Omega \{[\mathrm{B}]^T[D][B] + S_{ij}[Z]^T[Z]\}d\Omega \;\{\Delta u^n\}$$

$$= \{\delta u^n\}\sum^{elem}\{[\mathrm{B}]^T[D][B] + S_{ij}[Z]^T[Z]\}V_{elem}\;\{\Delta u^n\}$$

$\{[\mathrm{B}]^T[D][B] + S_{ij}[Z]^T[Z]\}V_{elem}$ is the element stiffness matrix. For this 1-dimensional case,

$$[\mathrm{B}]^T[D][B] = \frac{\alpha}{L}\begin{bmatrix} -1 \\ 1 \end{bmatrix} D_{1111}\frac{\alpha}{L}[-1, \quad 1] = D_{1111}\frac{\alpha^2}{L^2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$S_{11}[Z]^T[Z] = S_{11}\frac{1}{L^2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$V_{elem} = L \cdot Area$$

$$\{[\mathrm{B}]^T[D][B] + S_{ij}[Z]^T[Z]\}V_{elem} = \frac{Area}{L}(D_{1111}\alpha^2 + S_{11})\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

Generalized Maxwell model for viscoelasticity (N elements)

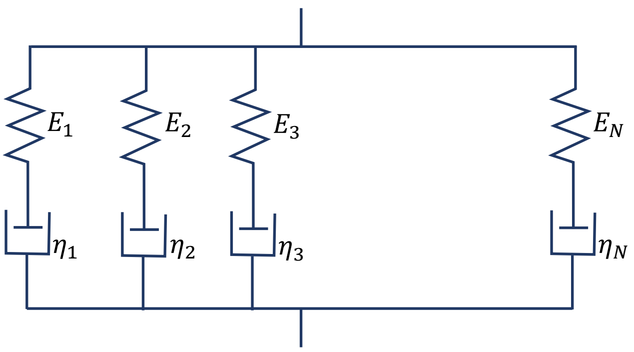


Figure 1. Generalized Maxwell model (N elements)

E_i: elastic modulus of i[th] element

η_i: material coefficient of viscosity of i[th] element

σ_i: stress of of i[th] element

σ: stress of the total unit

ε_i: strain of i[th] element

ε: strain of the total unit

The relationship of the material parameters for viscoelastic Maxwell units (E_i and η_i) and parameters in relaxation function is as follows:

$$\tau_i = \frac{\eta_i}{E_i}, \quad 3(G_0 - G_\infty)\xi_i = E_i, \quad E_0 = 3G_\infty$$

Strain in each element is the same.

$$\varepsilon = \varepsilon_1 = \varepsilon_2 = \cdots = \varepsilon_N$$

Total unit's stress is sum of all elements.

$$\sigma = \sum_{i=1}^{N} \sigma_i$$

Governing equation of a single element:

$$\dot{\varepsilon_i} = \frac{1}{E_i}\dot{\sigma_i} + \frac{1}{\eta_i}\sigma_i$$

Take Laplace Transformation.

$$s\bar{\varepsilon_i} = \frac{s}{E_i}\bar{\sigma_i} + \frac{1}{\eta_i}\bar{\sigma_i}$$

$$\bar{\sigma_i} = \frac{s\bar{\varepsilon_i}}{\frac{s}{E_i} + \frac{1}{\eta_i}}$$

Take Laplace Transformation of equations of the strain and stress.

$$\bar{\varepsilon} = \bar{\varepsilon}_i, \qquad \bar{\sigma} = \sum_{i=1}^{N} \bar{\sigma}_i$$

Using above three equations, obtain the following governing equation for the model (LT form).

$$\bar{\sigma} = s\bar{\varepsilon}\sum_{i=1}^{N} \frac{1}{\frac{s}{E_i} + \frac{1}{\eta_i}}$$

Adding 0[th] element with only spring E_0 ($\because \eta_0 \to \infty$) then, governing equation becomes:

$$\bar{\sigma} = \sum_{i=0}^{N} \frac{1}{\frac{s}{E_i} + \frac{1}{\eta_i}} = \frac{E_0}{s} + \sum_{i=1}^{N} E_i \frac{1}{s + \frac{E_i}{\eta_i}}$$

Taking the inverse Laplace transformation of the above:

$$\sigma(t) = E_0 + \sum_{i=1}^{N} E_i e^{-\frac{E_i}{\eta_i}t}$$

Assuming the material is linear and incompressible ($\nu = 0.5$), $E = 2(1+\nu)G = 3G$. Comparing the above equation with the relaxation function in Kazemi-Lari's paper below,

$$G(t) = G_\infty + (G_0 - G_\infty) \sum_{j=1}^{N_\tau} \xi_j e^{\frac{-t}{\tau_j}}$$

$$\tau_i = \frac{\eta_i}{E_i}, \quad 3(G_0 - G_\infty)\xi_i = E_i, \quad E_0 = 3G_\infty$$

The number of the generalized Maxwell unit N is set to 13, and $\tau_i = \{2^{-10}, 2^{-9}, \cdots, 2^{2}\}$ were used for the calculation in accordance with Kazemi-Lari et al.

Discretization of viscoelastic model

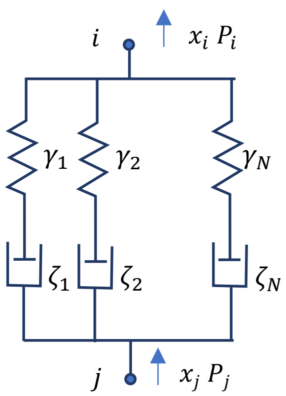


Figure 2. An element of Generalized Maxwell model for 1D finite element method

Consider the viscoelastic unit (generalized maxwell model) composed of N elements between node i and j. In the following, right superscript denotes time step index, right subscript denotes Maxwell element number, left subscript denotes node index.

Q_k : force exerted by the maxwell element k

P : force exerted by the whole unit $(= \sum_{k=1}^{N} Q_k)$

${}_iP$: force exerted by the whole unit on node i $(P = {}_iP = -{}_jP)$

$\zeta_k = \frac{S}{d}\eta_k$: dashpot coefficient of the Maxwell element k for length d and cut area S finite element between node i and j.

$\gamma_k = \frac{S}{d}E_k$: spring constant (elastic modulus) of the Maxwell element k for length d and cut area S finite element between node i and j.

$x = {}_ix - {}_ix$: displacement is common in all Maxwell parallel elements.

Consider deriving values for time step n+1 using the values of time step n. $\Delta t = t^{n+1} - t^n$

Displacement is expressed as the sum of dashpot and spring. For all k,

$$\dot{x}^n = \frac{Q^n}{\zeta_k} + \frac{\dot{Q}^n}{\gamma_k}$$

$$\dot{x}^{n+1} = \frac{Q^{n+1}}{\zeta_k} + \frac{\dot{Q}^{n+1}}{\gamma_k}$$

Assume linear increase of P and Q during Δt

$$Q_k^{n+1} = Q_k^n + \frac{\Delta t}{2}(\dot{Q}_k^{n+1} + \dot{Q}_k^n)$$

Using the above three equations, remove the $\dot{Q}$ term.

$$\dot{x}^{n+1} + \dot{x}^n = \frac{Q_k^{n+1} + Q_k^n}{\zeta_k} + \frac{2(Q_k^{n+1} - Q_k^n)}{\gamma_k \Delta t}$$

Solving the above for Q^{n+1} then

$$Q_k^{n+1} = \frac{1}{\frac{2}{\gamma_k \Delta t} + \frac{1}{\zeta_k}} \left\{ \dot{x}^{n+1} + \dot{x}^n + \left(\frac{2}{\gamma_k \Delta t} - \frac{1}{\zeta_k} \right) Q_k^n \right\}$$

The total force exerted by the Maxwell model P is the sum of force by each element:

$$P^{n+1} = \sum_{k=1}^{N} Q_k^{n+1} = \frac{1}{\frac{2}{\gamma_k \Delta t} + \frac{1}{\zeta_k}} \left\{ \dot{x}^{n+1} + \dot{x}^n + \left(\frac{2}{\gamma_k \Delta t} - \frac{1}{\zeta_k} \right) Q_k^n \right\}$$

$$= \sum_{k=1}^{N} \left\{ \frac{1}{\frac{2}{\gamma_k \Delta t} + \frac{1}{\zeta_k}} \right\} (\dot{x}^{n+1} + \dot{x}^n) + \sum_{k=1}^{N} \left\{ \frac{\frac{2}{\gamma_k \Delta t} - \frac{1}{\zeta_k}}{\frac{2}{\gamma_k \Delta t} + \frac{1}{\zeta_k}} Q_k^n \right\}$$

$$= B\dot{x}^{n+1} + B\dot{x}^n + \Sigma_{k=1}^{N} \beta_k Q_k^n$$

Denote the above equation in matrix notation with node values.

$$\begin{Bmatrix} {}_iP^{n+1} \\ {}_jP^{n+1} \end{Bmatrix} = \begin{bmatrix} B & -B \\ -B & B \end{bmatrix} \begin{Bmatrix} {}_i\dot{x}^{n+1} \\ {}_j\dot{x}^{n+1} \end{Bmatrix} + (B\dot{x}^n + \Sigma_{k=1}^{N} \beta_k Q_k^n) \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}$$

In incremental notation of P and $\dot{x}$ are following:

$$\begin{Bmatrix} {}_iP^{n+1} \\ {}_jP^{n+1} \end{Bmatrix} = \begin{Bmatrix} {}_i\Delta P^{n+1} \\ {}_j\Delta P^{n+1} \end{Bmatrix} + P^n \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}$$

$$\begin{bmatrix} B & -B \\ -B & B \end{bmatrix} \begin{Bmatrix} {}_i\dot{x}^{n+1} \\ {}_j\dot{x}^{n+1} \end{Bmatrix} = \begin{bmatrix} B & -B \\ -B & B \end{bmatrix} \begin{Bmatrix} {}_i\Delta\dot{x}^{n+1} \\ {}_j\Delta\dot{x}^{n+1} \end{Bmatrix} + B\dot{x}^n \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}$$

Incremental matrix notation of the equilibrium obtained:

$$\begin{Bmatrix} {}_i\Delta P^{n+1} \\ {}_j\Delta P^{n+1} \end{Bmatrix} = \begin{bmatrix} B & -B \\ -B & B \end{bmatrix} \begin{Bmatrix} {}_i\Delta\dot{x}^{n+1} \\ {}_j\Delta\dot{x}^{n+1} \end{Bmatrix} + (\Sigma_{k=1}^{N} \beta_k Q_k^n - P^n) \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}$$

Note that $B = \sum_{k=1}^{N} \left\{ \frac{1}{\frac{2}{\gamma_k \Delta t} + \frac{1}{\zeta_k}} \right\}$, $\beta_k = \frac{\frac{2}{\gamma_k \Delta t} - \frac{1}{\zeta_k}}{\frac{2}{\gamma_k \Delta t} + \frac{1}{\zeta_k}}$

Constant velocity method for dynamic simulation

Consistently solve the viscosity equation depending on the node velocity and hyperelastic equation depending on the node displacement, define the relationship between velocity and displacement. Assume displacement linearly changes during Δt at the velocity ${}^{t+\gamma\Delta t}\dot{u}$, the velocity at the time dividing t and $t + \Delta t$ by the ratio of γ.

$${}^{t+\gamma\Delta t}\dot{u} = (1-\gamma)\ {}^{t}\dot{u} + \gamma\, {}^{t+\Delta t}\dot{u} = {}^{t}\dot{u} + \gamma({}^{t+\Delta t}\dot{u} - {}^{t}\dot{u})$$

$${}^{t+\Delta t}u = {}^{t}u + \Delta t\ {}^{t+\gamma\Delta t}\dot{u} = {}^{t}u + \Delta \mathrm{t}\{ {}^{t}\dot{u} + \gamma\left({}^{t+\Delta t}\dot{u} - {}^{t}\dot{u}\right)\}$$

Subtracting ${}^{t+\Delta t}u$ with ${}^{t+\Delta t}\dot{u}$ to the governing equation will derive nonlinear equation depending only on ${}^{t+\gamma\Delta t}\dot{u}$. Applying Newton-Raphson method to obtain ${}^{t+\gamma\Delta t}\dot{u}$ that equivalates the equation. During the iteration process of obtaining $t + \Delta t$ variables from t variables, right prefix i denotes the value at i^th iteration.

$$u^i = {}^{t}u + \Delta \mathrm{t}\ {}^{t}\dot{u} + \gamma\Delta \mathrm{t}\left(\dot{u}^i - {}^{t}\dot{u}\right)\}$$

$$u^{i-1} = {}^{t}u + \Delta \mathrm{t}\ {}^{t}\dot{u} + \gamma\Delta \mathrm{t}\left(\dot{u}^{i-1} - {}^{t}\dot{u}\right)\}$$

$$\Delta u^i = \qquad \gamma\Delta \mathrm{t}\Delta\dot{u}^i$$

In starting the equation (i=0), set $\dot{u}^0 = {}^{t}\dot{u}$. Then u^0 is,

$$u^0 = {}^{t}u + \Delta \mathrm{t}\ {}^{t}\dot{u} + \gamma\Delta \mathrm{t}\left(\dot{u}^0 - {}^{t}\dot{u}\right)\} = {}^{t}u + \Delta \mathrm{t}\, \dot{u}^0$$

Therefore, upon the initial update (i=0),

$$\dot{u}^0 = {}^{t}\dot{u}$$

$$u^0 = {}^{t}u + \Delta \mathrm{t}\, \dot{u}^0$$

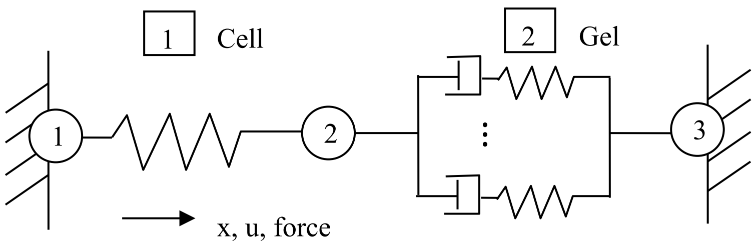
Afterword, i>=1,

$$\dot{u}^i = \dot{u}^{i-1} + \Delta\dot{u}^i$$

$$u^i = u^{i-1} + \gamma\Delta \mathrm{t}\, \Delta\dot{u}^i$$

Implementation

Consider the situation in the following figure, having only one degree of freedom (node 2, direction 1) and cell contractile force applied on the node.



○ Node number, □ Element number

Figure 3. Simplified mechanical model of cell and gel.

Combining the velocity-based governing equations, its linearization and nonlinear iteration explained above,

For the ith time step $t + \Delta t$:

Iteration 0: Initial solution estimation

$$\dot{u}^0 = {}^t\dot{u}$$

$$u^0 = {}^tu + \Delta\mathrm{t}\,\dot{u}^0,\ \alpha^0 = 1 + u^0/L_{cell}$$

$$\begin{Bmatrix} Q^0 \\ -Q^0 \end{Bmatrix} = Q(\alpha^0) \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} \begin{matrix} \text{node 1} \\ \text{node 2} \end{matrix}$$

$$\begin{Bmatrix} P^0 \\ -P^0 \end{Bmatrix} = 2B\{{}^t\dot{u}\} + \left(\Sigma_{k=1}^N \beta_k\, {}^tQ_k\right) \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} \begin{matrix} \text{node 2} \\ \text{node 3} \end{matrix}$$

Iteration $i \geq 1$:

$$\{Resid\} = \{F\} - \{P^{i-1}\} - \{Q^{i-1}\}$$

If $|\mathrm{Resid}|^2 <$ threshold, break and go to next time step.

Else, Merge total equation for viscosity and hyper-elasticity (linearized)

$$\left\{B\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \underset{\text{MERGE}}{+} K\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\right\}\{\Delta\dot{u}^i\} = \{Resid\}$$

For node 2,

$$(B + K)\Delta\dot{u}^i = F - \left(-Q^{i-1}\right) - P^{i-1}$$

Obtain $\{\Delta\dot{u}^i\}$,

$\{\Delta\dot{u}^i\} = [\mathrm{MERGED}]^{-1}\{Resid\}$, in this case $\Delta\dot{u}^i = \{F - \left(-Q^{i-1}\right) - P^{-1}\}/(B + K)$

update u and $\dot{u}$, and updated viscoelastic force P^i, Q^i.

$$\dot{u}^i = \dot{u}^{i-1} + \Delta\dot{u}^i$$

$$u^i = u^{i-1} + \gamma\Delta\mathrm{t}\,\dot{u}^i, \qquad \alpha^i = 1 + u^i/L_{cell}$$

$P^i = B\left(\dot{u}^i + \dot{u}^0\right) + \sum_{\mathrm{k}} \beta_k\, {}^tQ_k$, note that $\dot{u}^0 = {}^t\dot{u}$

$$Q^i = \alpha^i\, Area\, S_{11}(\alpha^i)$$

End Iteration loop

Update the variables with converged value and derive each Maxwell elements internal force ${}^{t+\Delta t}Q_k$ for history record.

${}^{t+\Delta t}\dot{u} = \dot{u}^i$, ${}^{t+\Delta t}u = u^i$, ${}^{t+\Delta t}Q_k = B_k\left({}^{t+\Delta t}\dot{u} + {}^{t}\dot{u}\right) + \beta_k\, {}^{t}Q_k$

End time step

Code verification

Test the implementation of the Maxwell Model by applying step strain input to the model and compare the obtained temporal changes in output stress and relaxation function G(t) which should be equivalent in theory. Because the model principal variable is velocity, apply delta function on the input velocity, and for numerical approximation for the delta function, here we used the following and used $n = 1000$.

$$\dot{u} = \delta(t) \cong \lim_{n\to\infty} \frac{n\exp(-nt)}{2} \qquad *1$$

Regarding other parameters, we used the following values: dt = 0.0001 [s], the gel length of 10 [μm], the gel cut area of 100 [μm^2].

From Figure4, the simulated relaxation function, which is stress response to the step strain input, well agreed with theoretical solution, except for the peak value of the initial impact. This cannot be avoided with finite expression of delta function. Delta function cannot be rigorously expressed numerically. The values of dt and gamma for Newmark beta were insensitive to the stress maximum value.

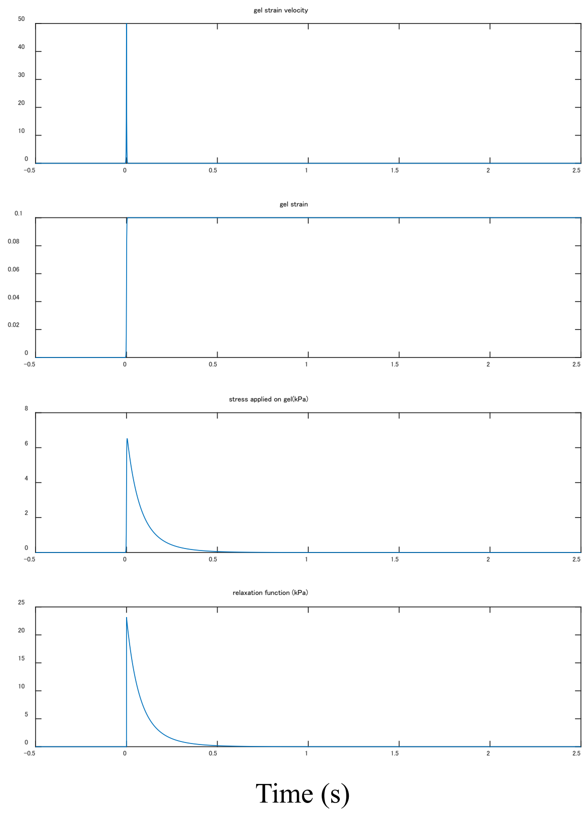


Figure 4. Calculated stress in response to step input of gel strain compared to the theoretical solution, Case1 with equation *1. The top panel shows the input in this calculation, the delta function shown in equation *1, which corresponds to the gel velocity. Second and third panels are calculated gel strain and stress. The bottom panel is analytical solution for step strain input with the same parameters.

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