Numerical issues regarding distributed constraint implementation

Physics of the Problem:

A 3D block of hydrogel is undergoing a continuous contraction and subsequent recovery processes due to molecular motor activities inside the gel. Hydrogel is an agglomeration of cross-linked polymer network and water. Assuming incompressibility for both polymer and water, the contraction of the hydrogel happens due to water outflow, while recovery is due to water inflow. Molecular motor activities shorten the polymer chains and increases the cross-link density. These activities modify the chemical potential of water (relative to equilibrium) and drive the water to flow out/in - corresponding to contraction/recovery of the gel.

Modeling of the problem:

Model PDE/ODEs are in Lagrangian format, where hydrogel with no water (dry polymer network) is considered as the reference state. Three different processes are modelled: (1) Shortening/recovery of polymer chains, (2) Increment/recovery of polymer cross-link density, and (3) Contraction/recovery of hydrogel.

1.0 Shortening/recovery of polymer chains

We consider a domain ODE to model the shortening/recovery of polymer chains, as follows:

$$\frac{\partial w}{\partial t} = -\frac{P\tau}{NkT}\frac{w^3}{\sum_i u_i^2 - 3w^2} \qquad [1.1]$$

Here, w $(0 < w \leq 1)$ represents shortening/recovery of the polymer chains that depends on the input power density P.

u_i $(i = 1, 2, 3)$ represent the contraction/recovery of the gel in three principal directions.

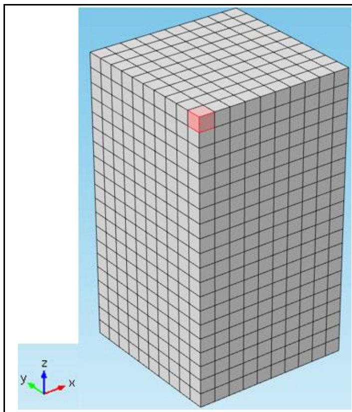
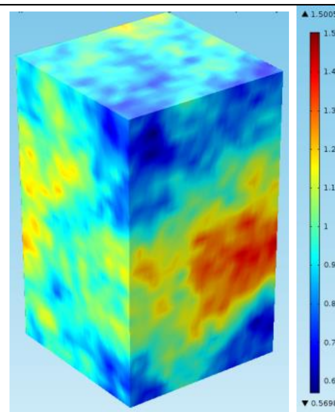
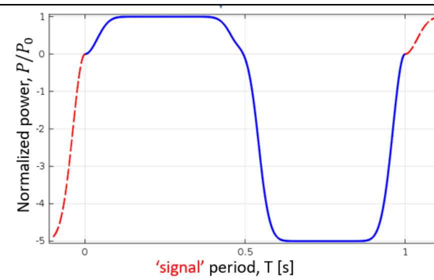
NkT is the polymer stiffness, $\tau(= L^2/\mathcal{D}\,)$ is the time scale, L being the length scale, $\mathcal{D}$ being the diffusion constant of water.

1.1 Modeling of Power density, $P(x, y, z, t)$

We model the following aspects:

a) We model power density as spatially inhomogeneous, $P(x, y, z)$, with a 3D random distribution function (Fig.1b).
b) We consider an analytic periodic function to model our power cycle, $P(t)$, (Fig.1c).
c) Positive P cycle (Fig.1c): polymer chain shortening $(0 < w < 1)$ for 0.5s as per Eq. (1.1).
d) Negative P cycle (Fig.1c): polymer chain recovery $(w = 1)$ as per Eq. (1.1);
e) Recovery intended to be instantaneous (different than 0.5s as depicted in Fig.1c); controlled via introducing “Events” interface into the model.
f) When $P = 0$, no shortening of polymer chains as per Eq. (1.1).

g) We model power cycles as spatially non-synchronous by subdividing the domain block into sub-domains (i.e. cubes) (Fig. 1a) and by assigning different phase values, δ, to different sub-domains.

		 $P = P_0\,'\mathbf{signal}'\left(\frac{2\pi}{T}t - \delta\right)$
Fig. 1a: Sub-divided gel block.	Fig. 1b: 3D random function.	Fig. 1c: Power density cycle ($\delta = 0$).

1.2 "Events" interface: Enforcing distributed inequality constraint, $w \leq 1$

a) We define "Events" for each sub-domain to control the power density, as follows:
   (i) When $(\max(w) \leq 1 \,\&\&\, P > 0)\ ||\ (\max(w) < 1 \,\&\&\, P < 0)\ ||\ (\max(w) \geq 1 \,\&\&\, P > 0)$: Power density is non-zero ($P \neq 0$).
   (ii) When $(\max(w) \geq 1 \,\&\&\, P < 0)$: Power density is zero ($P = 0$).

b) Drawbacks with "Events" interface: for each sub-domain, pointwise recovery ($w = 1$) is incomplete, as we use "$\max()$" operator.

c) "Events" interface can be eliminated from the model if the distributed inequality constraint is enforced via Lagrange multiplier based method as described in a COMSOL blog: https://www.comsol.com/blogs/methods-for-enforcing-inequality-constraints/. We have been trying to adopt this method in our model but failed. Any help in this regard would be highly appreciated.

2.0 Increment/recovery of polymer cross-link density

We consider a domain algebraic equation to model the increment/recovery of cross-link density, as follows:

$$n_1 = n_0 + n_m[1 - \exp(-k_m t)] \qquad [2.1]$$

Here, $n_1 (= N\Omega/N_A)$ represents the increment/recovery of the cross-link density. N being cross-link density (dimensional), Ω being the molar volume of water and N_A being the Avogadro's number.

n_0 is the initial cross-link density, n_m being the molecular motor density, and k_m being the molecular motor attachment rate.

(i) We model n_m as spatially inhomogeneous using the same 3D random distribution function as shown in Fig. 1b.

(ii) For each sub-domain, n_1 evolves from n_0, when $P = 0$; n_1 recovers to n_0, when $P \neq 0$.

3.0 Contraction/recovery of hydrogel

We model this process by linking fluid flow to the contraction/recovery of the gel. We consider the species conservation equation for water flow, as follows:

$$\frac{\partial C}{\partial t} = -\frac{\partial H_i}{\partial X_i} \qquad (3.1)$$

Where, C is molar concentration of water; The water flux, H_i, is given by the Fick's law, as follows:

$$H_i = -\frac{\mathcal{D}}{\Omega}\frac{(J-1)}{u_i^2}\frac{\partial}{\partial X_i}\left(\frac{\mu}{RT}\right) \qquad (3.2)$$

Here, $\frac{\mu}{RT}$ is chemical potential of water. The swelling ratio, J, is defined as follows:

$$J = \prod_i u_i = 1 + \Omega C \quad ==\gg \quad \frac{\partial}{\partial t}\left(\prod_i u_i\right) = \Omega\frac{\partial C}{\partial t} \qquad (3.3)$$

Combining Eq. (3.1) - (3.3) and non-dimensionalization yields,

$$\frac{\partial}{\partial t}\left(\prod_i u_i\right) = \left(\frac{\tau\mathcal{D}}{L^2}\right)\frac{\partial}{\partial X_i}\left\{\frac{(J-1)}{u_i^2}\frac{\partial}{\partial X_i}\left(\frac{\mu}{RT}\right)\right\}$$

$$==\gg \quad u_2u_3\frac{\partial u_1}{\partial t} + u_3u_1\frac{\partial u_2}{\partial t} + u_1u_2\frac{\partial u_3}{\partial t} = \left(\frac{\tau\mathcal{D}}{L^2}\right)\left[\frac{\partial}{\partial X_1}\left\{\frac{(J-1)}{u_1^2}\frac{\partial}{\partial X_1}\left(\frac{\mu}{RT}\right)\right\} + \frac{\partial}{\partial X_2}\left\{\frac{(J-1)}{u_2^2}\frac{\partial}{\partial X_2}\left(\frac{\mu}{RT}\right)\right\} + \frac{\partial}{\partial X_3}\left\{\frac{(J-1)}{u_3^2}\frac{\partial}{\partial X_3}\left(\frac{\mu}{RT}\right)\right\}\right]$$

Simplifying further into components yields another set of model equations to be solved, as follows:

$$u_2u_3\frac{\partial u_1}{\partial t} = \left(\frac{\tau\mathcal{D}}{L^2}\right)\left[\frac{\partial}{\partial X_1}\left\{\frac{(J-1)}{u_1^2}\frac{\partial}{\partial X_1}\left(\frac{\mu}{RT}\right)\right\}\right] \qquad (3.4a)$$

$$u_3u_1\frac{\partial u_2}{\partial t} = \left(\frac{\tau\mathcal{D}}{L^2}\right)\left[\frac{\partial}{\partial X_2}\left\{\frac{(J-1)}{u_2^2}\frac{\partial}{\partial X_2}\left(\frac{\mu}{RT}\right)\right\}\right] \qquad (3.4b)$$

$$u_1u_2\frac{\partial u_3}{\partial t} = \left(\frac{\tau\mathcal{D}}{L^2}\right)\left[\frac{\partial}{\partial X_3}\left\{\frac{(J-1)}{u_3^2}\frac{\partial}{\partial X_3}\left(\frac{\mu}{RT}\right)\right\}\right] \qquad (3.4c)$$

The chemical potential of water, $\frac{\mu}{RT}$, is linked to the molecular motor activities, as follows:

$$\frac{\mu}{RT} = \ln\left(\frac{J-1}{J}\right) + \frac{\chi+J}{J^2} + \frac{n_1}{J}\left(\frac{u_3^2}{w^2} - 1\right) + \frac{2n_1}{3}\frac{\tau_v}{\tau}\left(\frac{J-1}{J}\right)\left(\frac{2}{u_3}\frac{\partial u_3}{\partial t} - \frac{1}{u_1}\frac{\partial u_1}{\partial t} - \frac{1}{u_2}\frac{\partial u_2}{\partial t}\right) \qquad (3.5)$$

Here, $\tau_v\left(=\frac{\eta}{NkT}\right)$ is the viscous time scale; η being the water viscosity.

Problem setup:

Eqns. (1.1), (2.1), (3.4) and (3.5) are the model equations to be solved. Five equations for five unknowns: u_1, u_2, u_3, w and n_1. For our problem, we solve them for a 3d block of gel (see Fig.1a) subject to the following boundary/initial conditions:

(i) Top boundary surface is subjected to the constraint, which has a term with time derivative (red marked), as follows:

$$\ln\left(\frac{J-1}{J}\right)+\frac{\chi+J}{J^2}+\frac{n_1}{J}\left(\frac{u_3^2}{w^2}-1\right)+\frac{2n_1}{3}\frac{\tau_v}{\tau}\left(\frac{J-1}{J}\right)\left(\frac{2}{u_3}\frac{\partial u_3}{\partial t}-\frac{1}{u_1}\frac{\partial u_1}{\partial t}-\frac{1}{u_2}\frac{\partial u_2}{\partial t}\right)=\mu_{ext} \qquad (3.6)$$

(ii) Bottom boundary surface is fixed:
$u_1 = u_2 = u_3 = u_0$; $\frac{\partial u_1}{\partial X_1} = \frac{\partial u_2}{\partial X_2} = \frac{\partial u_3}{\partial X_3} = 0$.

(iii) Left-right and front-rear boundary surfaces are subject to periodic conditions.

(iv) Initial conditions: $u_1 = u_2 = u_3 = u_0$; $w = 1$; $n_1 = n_0$.

Issues:

(i) We cannot solve the model due to the inclusion of time-derivative term in the boundary constraint [Eq. (3.6)]. We were able to solve without this term. Could you please help us to solve the problem with the time-derivative term?

(ii) We want to omit the "Events" interface from our model. To do that we need to enforce the distributed inequality constraint, $w \leq 1$, using Lagrange multiplier based method or any other method as suggested by the COMSOL blog: https://www.comsol.com/blogs/methods-for-enforcing-inequality-constraints/. Could you please help us to implement the domain inequality constraint using this Lagrange multiplier-based method?

Your Kind help would be highly appreciated!!