Coding the Hessian

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1 Derivation of the Hessian

For a given configuration of the system, the total energy U is a combination of the strain energy of the microgels, the mixing energy, plus the contacts "artificial" energy. The latter should have a minimal contribution to the total deformation energy (in other words, the penalty stiffness should be large relative to the gels stiffness but not too large as to cause numerical instabilities) which is a numerical trick to avoid the costly ideal requirement of zero overlap (hence, zero energy) between particles, where here we allow for some interpenetration with some penalty. In these notes I am assuming I already have a system that is discretized in space.

$$U = \sum_I V_{oI}[W_e(\boldsymbol{F}_I) + W_m(J_I)] + \sum_k W_c(d_k) \tag{1}$$

Where I is the I'th element, V_{oI} is the reference (dry) volume, W_e is the stretching free energy per unit reference volume, $\boldsymbol{F}_I$ is the deformation gradient tensor that maps vectors in the reference configuration to vectors in the deformed configuration, W_m is the free energy of mixing per unit reference volume, $J_I = det[\mathbf{F}_I]$ is the volumetric ratio, W_c is the contact energy associated with the d_k interference. For node-to-segment contact method, d_k is the closest approach between the "slave" surface node and its "master" mesh. The contact energy is that for a harmoic repulsion.

$$W_c = \frac{1}{2}\epsilon d^2 \tag{2}$$

Where ϵ is the penalty stiffness, and d is the interference as defined previously.
The first term on the right hand side of equation 1 is Flory-Rehner free energy, where:

$$W_e = \frac{NkT}{2}(F_{\alpha\beta}F_{\alpha\beta} - D - 2\log(J)) \tag{3}$$

$$W_m = \frac{kT}{\Omega}(J-1)\left(\log\left[\frac{(J-1)}{J}\right] + \frac{\chi}{J}\right) \tag{4}$$

Where D is the dimension. N is the total number of polymer networks per unit volume of the dry, undeformed reference state. kT is the temperature in energy units. Ω is the volume per solvent particle. χ is a dimensionless parameter representing the quality of mixing.

The forces are then given by:

$$\begin{aligned} f_{i\alpha} &= -\frac{\partial U}{\partial r_{i\alpha}} = -\sum_{I\mu\nu}\left[V_{oI}\frac{\partial(W_s+W_m)}{\partial F_{I\mu\nu}}\frac{\partial F_{I\mu\nu}}{\partial r_{i_\alpha}}\right] - \sum_k \frac{\partial W_c}{\partial d_k}\frac{\partial d_k}{\partial r_{i\alpha}} \\ &= -\sum_{I\mu\nu} V_{oI} P_{I\mu\nu} M_{I\mu\nu i\alpha} - \epsilon \sum_k d_k S_{ki\alpha} \end{aligned} \tag{5}$$

Where

$$P_{I\mu\nu} := \frac{\partial(W_s+W_m)}{\partial F_{I\mu\nu}} \tag{6}$$

$$M_{I\mu\nu i\alpha} := \frac{\partial F_{I\mu\nu}}{\partial r_{i_\alpha}} \tag{7}$$

$$S_{ki\alpha} := \frac{\partial d_k}{\partial r_{i\alpha}} \tag{8}$$

Where $P_{\mu\nu}$ is the first Piola-Kirchhof stress. Notice that $M_{I\mu\nu i\alpha}$ and $S_{ki\alpha}$ are very sparse matrices. $M_{I\mu\nu i\alpha}$ is only nonzero if the i'th node is one of the nodes of the I'th element, and similarly, $S_{ki\alpha}$ is only nonzero if the i'th node is one of the three nodes defining the interference distance d (either i is the slave node or one of the two end nodes of the master segment).

$$\begin{aligned} P_{\alpha\beta} &= \frac{\partial}{\partial F_{\alpha\beta}}(W_s+W_m) = NkT(F_{\alpha\beta} - \frac{1}{J}\frac{dJ}{dF_{\alpha\beta}}) + \frac{\partial W_m}{\partial J}\frac{dJ}{dF_{\alpha\beta}} \\ &= (NkT)F_{\alpha\beta} + (W'_m J - NkT)F^{-1}_{\beta\alpha} \end{aligned} \tag{9}$$

$$W'_m = \frac{kT}{\Omega}\left(\log\left[\frac{(J-1)}{J}\right] + \frac{\chi+J}{J^2}\right) \tag{10}$$

We need to take one more derivative of U with respect to position to find the Hessian $H_{i\alpha j\beta}$ which gives you the increment of the α component of the force on the i'th node as a result of moving the the β component of the poistion vector of the j'th node. From now on we are going to drop the summation symbol and assume implicit summation over repeated indices.

$$\begin{aligned} H_{i\alpha j\beta} &= \frac{\partial f_{i\alpha}}{\partial r_{j\beta}} = -\frac{\partial U^2}{\partial r_{i\alpha} r_{j\beta}} = -V_{oI}\frac{\partial P_{I\mu\nu}}{\partial F_{I\rho\sigma}} M_{I\rho\sigma j\beta} M_{I\mu\nu i\alpha} - \epsilon\left(S_{kj\beta}S_{ki\alpha} + d_k\frac{S_{ki\alpha}}{\partial r_{j\beta}}\right) \\ &= -V_{oI} M_{I\mu\nu i\alpha} K_{I\mu\nu\rho\sigma} M_{I\rho\sigma j\beta} - \epsilon\left(S_{kj\beta}S_{ki\alpha} + d_k\frac{S_{ki\alpha}}{\partial r_{j\beta}}\right) \end{aligned} \tag{11}$$

Where

$$K_{I\mu\nu\rho\sigma} := \frac{\partial P_{I\mu\nu}}{\partial F_{I\rho\sigma}} \tag{12}$$

Where we used the fact that $\frac{\partial M_{I\mu\nu\rho\sigma}}{\partial r_{j\beta}} = 0$, since $\mathbf{M}$ is constant for the three nodes triangle element as we will see later. So, equation 11 is **only** valid for CST triangle element and should be adjusted if other types of elements are considered. $K_{I\mu\nu\rho\sigma}$ is the the stiffnes matrix for the gel material.

For a Flory material, we obtain:

$$K_{\mu\nu\rho\sigma} = NkT\delta_{\mu\rho}\delta_{\nu\sigma} + (NkT - W'_m J)F^{-1}_{\sigma\mu}F^{-1}_{\nu\rho} + (W''_m J^2 + W'_m J)F^{-1}_{\sigma\rho}F^{-1}_{\nu\mu} \tag{13}$$

Where the relations $\frac{\partial F^{-1}_{\nu\mu}}{\partial F_{\rho\sigma}} = -F^{-1}_{\sigma\mu}F^{-1}_{\nu\rho}$ and $\frac{\partial J}{\partial F_{\rho\sigma}} = JF^{-1}_{\sigma\rho}$ where used .

2 Checking the Hessian code for bugs

As a check for the correct implemintation of the Hessian in the code I compared the incremental forces on select nodes as obtained from using the Hessian expression (that is $\boldsymbol{H}\cdot\Delta\boldsymbol{r}$) with that obtained from running the simulation for the same small random diplacement of the tested nodes. Note I included boundary nodes for a configuration with contact (which is important to include the conatct part of the Hessian). Figure 1 shows machine precision agreement between the two. Notice that the Hessian implemintation accunts for periodic boundary conditions too.

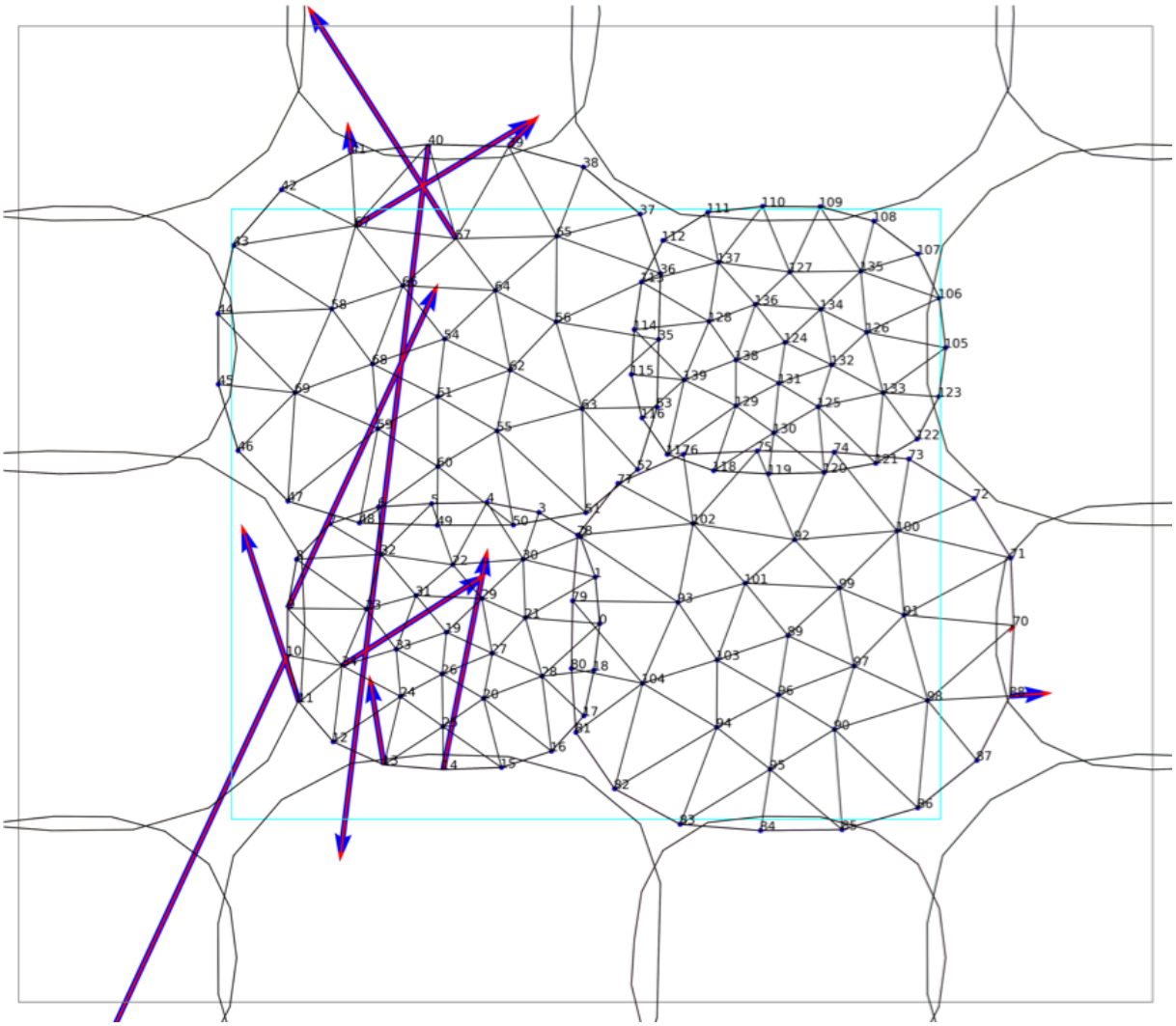

Figure 1: Incremental force field. It is a comparsion between the Hessian forces (red) and the gradient dynamics forces (blue) resulting from small, O(10^{-5}), random displacements on nodes 10 and 40.

3 Conclusion

The Hessian matrix was implemented successfully.