Supplementary Information

Network Model of Active Elastic Shells Swollen by Hydrostatic Pressure

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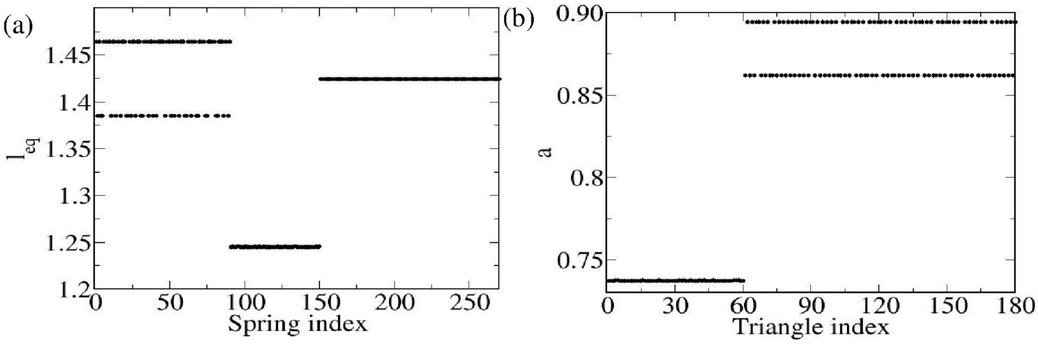
Distribution of spring lengths and triangle areas:

The equilibrium lengths of the 270 springs in the network are taken to be the lengths of the sides of the triangles in the triangulated fullerene and, therefore, are not same. The springs can be divided into four groups, each having a different value of equilibrium length l_{eq} (Fig.1). Similarly, since the equilibrium lengths of all springs are not the same, the areas of all triangles are also not identical and can be divided into three groups, each having a different value of area a_{eq}.



Supplementary Fig. 1: (a) Distribution of equilibrium lengths of different springs. (b) Distribution of area of each of the triangles.

Integration algorithm

$$\frac{d}{dt}(e^{\zeta t}\,\vec{v}_k) = e^{\zeta t}\vec{F}_k$$

Integrating both sides of this equation,

$$\int_{-\Delta/2}^{t} dt'\,\frac{d}{dt'}(e^{\zeta t'}\,\vec{v}_k) = \int_{-\Delta/2}^{t} dt'\,\vec{F}_k\,e^{\zeta t'} \tag{1}$$

where Δ is the MD time step which we take to be much shorter than the viscous damping time (mass/(friction coefficient)).

Solving equation 1, we get the following expressions for updating the velocity and position of vertex K:

$$\vec{v}_k((n+\frac{1}{2})\Delta) = \vec{v}_k((n-\frac{1}{2})\Delta)e^{-\zeta\Delta} + e^{-\zeta\frac{\Delta}{2}}\,\Delta\,\vec{F}_k(\vec{r}_k(n\Delta)) \tag{2}$$

$$\vec{v}_k(t) = \vec{v}_k(-\frac{\Delta}{2})e^{-\zeta(t+\Delta/2)} + e^{-\zeta\, t}\int_{-\Delta/2}^{t} dt'\vec{F}_k(t')e^{\zeta t'}$$

$$\implies \vec{v}_k(\tfrac{\Delta}{2}) = \vec{v}_k(-\tfrac{\Delta}{2})e^{-\zeta\Delta} + \Delta\vec{F}_k(\vec{r}_k(t=0))e^{-\zeta\frac{\Delta}{2}}$$

In general,

$$\vec{v}_k((n+\frac{1}{2})\Delta) = \vec{v}_k((n-\frac{1}{2})\Delta)e^{-\zeta\Delta} + e^{-\zeta\frac{\Delta}{2}}\ \Delta\ \vec{F}_k(\vec{r}_k(n\Delta)) \quad (3)$$

where n is the number of MD time steps.
The equation for the position can be written as,

$$\vec{r}_k(t) = \vec{r}_k(0) + \int_0^t \vec{v}_k(t')dt'$$

At $t = \Delta$,

$$\vec{r}_k(\Delta) = \vec{r}_k(0) + \Delta\ \vec{v}_k(\Delta/2)$$

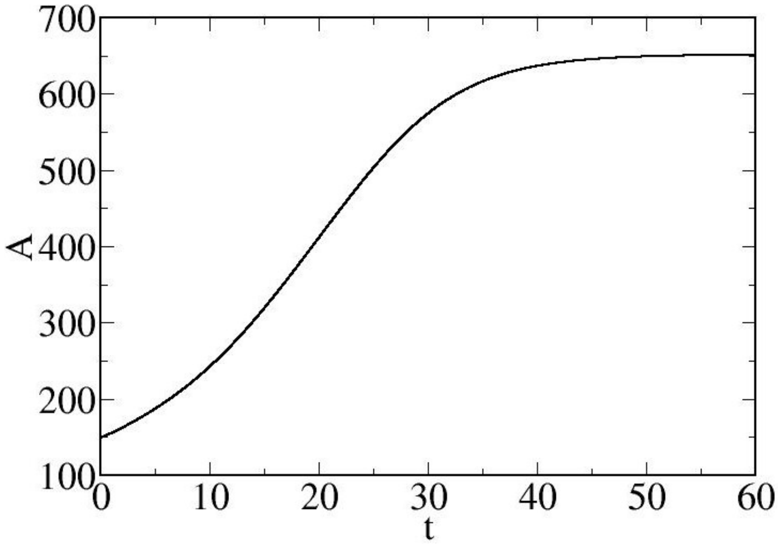
In other words,

$$\vec{r}_k((n+1)\Delta) = \vec{r}_k(n\Delta) + \Delta\ \vec{v}_k\ ((n+\frac{1}{2})\Delta) \quad (4)$$

We are using equation 3 and 4 for updating velocities and positions of the vertices

Relaxation to steady state:

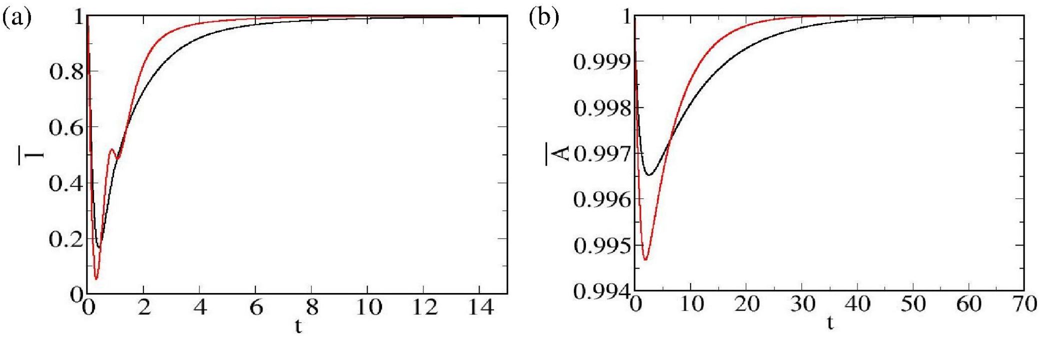
Beginning with a network in equilibrium in the absence of hydrostatic pressure, at time, $t = 0$, we suddenly switch on hydrostatic pressure by changing p_0 from 0 to 0.1. With the simulation parameters used in this paper, it takes about $40 - 50$ time units to reach a steady state characterized by a new pleatea value of the total surface area A (Fig. 2). Increasing p_0 from 0 to a higher value of pressure, increases the steady state value of the surface area but decreases the relaxation time compared to the values of shown in Fig. 2.



Supplementary Fig. 2: (a) The total surface area $A(t)$ of the network plotted as a function of time following a step-like increase of hydrostatic pressure from $p_0 = 0$ to 0.1.

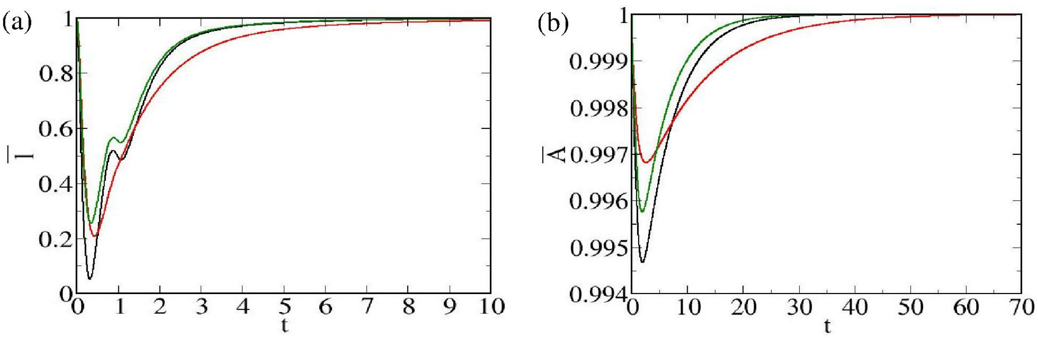
Single excitation dynamics: effect of hydrostatic pressure:

The effect of hydrostatic pressure on excitation and relaxation dynamics of a single spring and total surface area of the system can be observed by comparing the steady state results for $p_0 = 0.05$ and 0.1. Since in steady state with $p_0 = 0.1$ the network is more inflated than for $p_0 = 0.05$, the elastic energy stored in the springs is higher as well in case of $p_0 = 0.1$. Once a single spring is excited, $\bar{l}$ reaches its minimum value faster and the maximal contraction of the spring is higher in the $p_0 = 0.1$ than in the $p_0 = 0.05$ case. Since the deformation of the spring is opposed by network forces that increase with the inflation of the network, the excited spring relaxes faster to its steady state value in the $p_0 = 0.1$ than in the $p_0 = 0.05$ case (Fig. 3(a)). (b) Faster excitation and relaxation dynamics at higher hydrostatic pressure can also be observed in the normalized total surface area $\bar{A}$ versus time plot (Fig. 3(b)).



Supplementary Fig. 3: (a) The normalized length $\bar{l}$ of an excited spring and (b) the normalized total area $\bar{A}$ of the network, are plotted as a function of time following the excitation, for $p_0 = 0.05$ (black curve) and 0.1 (red curve). The relaxation time of the spring is $t_r = 1$.

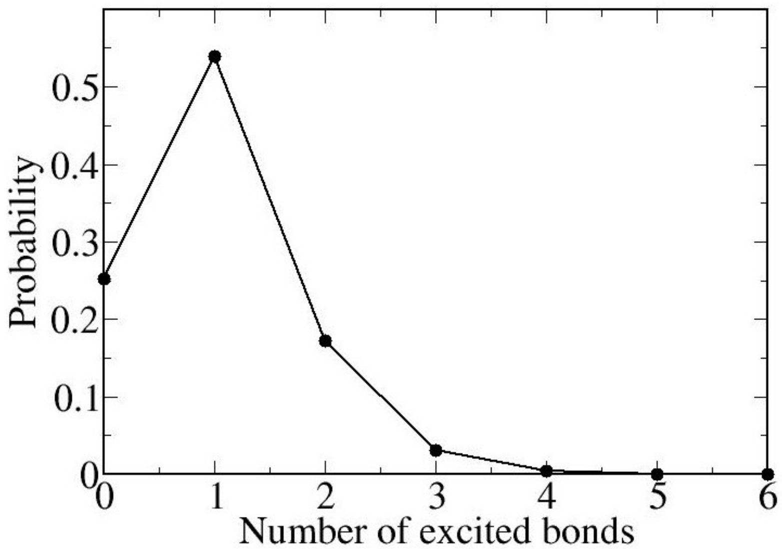
Single excitation dynamics: Effect of spring constant K and mass m



Supplementary Fig. 4: (a) The normalized length $\bar{l}$ of an excited spring and (b) the normalized total area ($\bar{A}$) as a function of time for different combinations of spring constants K and mass m: $K = 1, m = 1$ (black); $K = 1, m = 2$ (red) and K=2, m=1 (green).

Distribution of number of excited bonds during non-periodic excitations:

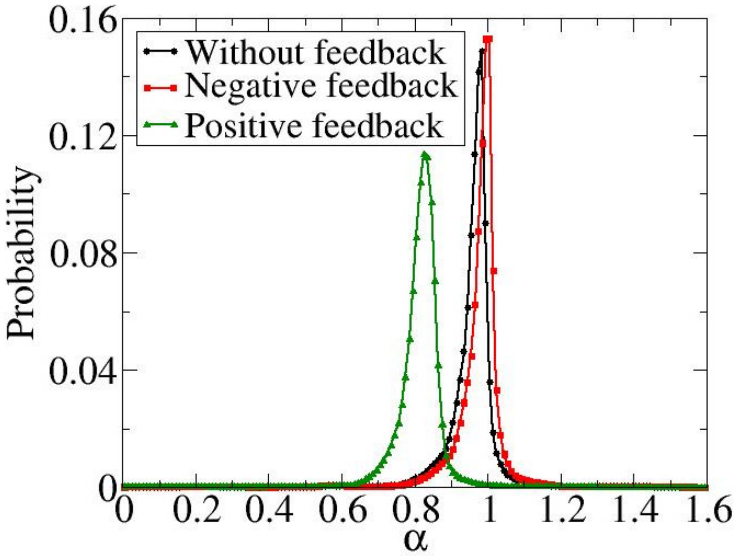
During non-periodic excitations, the time interval between two consecutive excitations is chosen from an uniform distribution with a mean of 1 time unit. In this case the number of excitations simultaneously present in the network, fluctuates in time. In Fig. 4 we plot the probability distribution of the number of simultaneous excitations (events were accumulated during the measurement time). Both the peak and the mean of the distribution occur at 1, corresponding to a single excitation).



Supplementary Fig. 5: Distribution of number of excited springs present in the system at a particular instant of time during non-periodic excitations without A-p feedback.

Distribution of normalized areas of triangles:

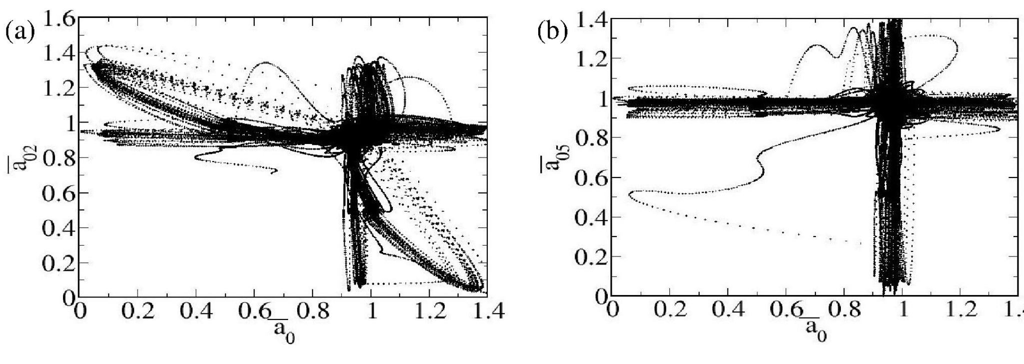
In Supplementary Fig. 6 we plot the PDFs of normalized area of triangles ($\bar{a}$) for the case of non-periodic excitations, with no total area-pressure feedback and with negative and positive feedback. The three distributions have similar widths and tails towards lower values of $\bar{a}$. The peak of the positive feedback distribution is shifted to lower area compared to the other two.



Supplementary Fig. 6: Distribution of normalized area of triangles ($\bar{a}$) in case of without feedback (black), negative feedback (red) and positive feedback (green).

Scatter plots of areas of triangles:

In Fig. 7 we present scatter plots of the instantaneous values of areas of two (a) neighboring and (b) distant triangles. While there are nearly no correlation between distant triangles (see Fig. 7(b)), negative correlations are observed between triangles that share a common vertex, in Fig. 7(a)



Supplementary Fig. 7: Scatter plots of areas of two neighboring (a) and distant (b) triangles.

Supplementary movie 1

The movie shows the active excitations in the network when the excitations are introduced non-periodically in the network.