The study of semiflexible networks has direct applications to cellular mechanics. In particular, the cytoskeleton of a cell is a prime example of a nematically ordered semiflexible networks. Using computer simulations, we were able to generate a directionally ordered network and model its responses to shear. In doing so, we observed interesting nonlinear behaviour and a breakdown of rotational symmetry. Previous work had attributed this behavior due to buckling within the system, which caused filaments compressed by shear to buckle. This paper attempts to explore an interesting feature noticed within the network, namely, that as shear increased, the buckling seemed to propagate outward from a point of origin. To measure this, Matlab code was used to generate a correlation function from the buckling data, and it was found that the observed buckling did propagate outward. Currently more work is being done to model the mechanism behind this buckling propagation.

I. INTRODUCTION

Semiflexible networks play instrumental roles in the structure and function of cells. The most prevalent of these is the cytoskeleton of the cell. The cytoskeleton, a network of actin filaments, plays an important role in many cellular processes including cell division and transport. Compared to flexible networks, semiflexible networks possess a much larger persistence length, $\ell_p$. In fact, actin filaments have a persistence length on the order of microns. This in turn allows for the connecting polymer between two crosslinks to be treated as a flexible rod. Thus energy can be stored within the bending and stretching of the filament, as opposed to flexible networks where energy can only be stored within stretching. Using this, the Hamiltonian for any individual filament within the network under a tension $\tau$ can be written as

$$H = \frac{1}{2} \kappa (\nabla^2 u)^2 + \frac{1}{2} (\nabla u)^2$$

where $\kappa$ is a bending modulus and $u(x)$ is a function that represents the filament’s displacement from a straight line[1].

It was found in cells that the networks generally possess some level of directional order. This orientational order causes the network to demonstrate anisotropic properties. Traditionally for small deformations, the stress and strain of a system are linearly proportional to one another, demonstrating a "Hookian" behavior. In previous works, however it was found in the case of anisotropic networks that the linear response regime was extremely small and decreased as the system became more ordered. In addition to this, the network behaved differently depending on the direction of shear and the nematic orientation angle. This breakdown of rotational symmetry and disappearance of the linear response regime suggested that classical linear elasticity theory no longer applied. Instead these findings suggested the application of novel nonlinear elastic properties within the network[2].

A nematic order parameter,

$$S = \int_{-\pi}^{\pi} d\theta P(\theta) \cos(2\theta)$$

was used to measure the degree of anisotropy within the system. In the equation, $P(\theta)$ was the distribution of filament orientation with respect to the nematic director. $S = 0$ corresponded to a completely isotropic system whereas $S = 1$ represented a completely ordered system in which all the filaments were directed along the nematic direction angle[2].

The nonlinear behaviors of the system were hypothesized to be due to buckling within the network [2]. Buckling is a first order phase transition in which a fil-
FIG. 2: The top left picture depicts a nematically ordered network with a nematic director angle \( \hat{n} \). The network is sheared with respect to the shear angle \( \phi \). The bottom right picture depicts the distribution function \( P(\theta) \) of filament angles relative to the nematic director angle. The center depicts a close up on the network itself, with the shearing direction indicated by the black arrow. The red indicates filaments with stretching energy and the blue indicates filaments with bending energy. It can be noted here the majority of filaments in compression are in fact perpendicular to the filaments being bent.[2]

ament, under a large compressive load will bend in on itself to achieve a lower energy conformation. In doing this, energy in converted from compression into bending energy[4]. To test this hypothesis, a buckling order parameter, first defined by Conti and Macintosh, was defined as

\[
B = \frac{\Delta E_c}{\Delta E_{\text{tot}}}
\]

where \( E_c \) is the energy stored in compression, \( E_{\text{total}} \) is the total energy stored within system, and the \( \Delta \) represented discretized steps of shear within the system. Because the energy in compression is only a proportion of the total energy \( B \) should always be less than 1.[3] The buckling order parameter was measured as a function of strain for various nematic director angles of \( \pi/4 \), 0, and \( -\pi/4 \). (See Fig. 1 ) From this it can be seen that the buckling order parameter decreased significantly with strain for networks with nematic direction angles of 0 and \( -\pi/4 \), while staying relatively constant for systems with a nematic director angle of \( \pi/4 \). When applied to the network of semiflexible filaments, it was found depending on the direction of shear, a filament could be placed under compression or tension as shown in figure 3. In the case of networks where the nematic angle director was \( \pi/4 \), filaments oriented along the nematic director were placed under tension. Those filaments oriented perpendicular to the nematic director would be placed under compression, however they would possess many more crosslinks so as to resist buckling. On the other hand, when the network is rotated to angles of \( -\pi/4 \) and 0, the filaments on the

FIG. 3: As shown in this figure, depending on the direction of shear, a filament can be compressed or extended. In the case it is compressed, at large enough shears the filament will begin to buckle.
nematic director are placed under compression. As shear increases, these filaments will begin to buckle, such that the energy is converted from compression into bending, resulting in the observed decrease.

II. SIMULATION

To simulate a two dimensional anisotropic semiflexible network under shear, code written by Dr. Klug was used. The code distributed a series of N filaments randomly throughout a square box with dimensions W by W. Each filament was assigned an orientation about the nematic direction angle determined from the distribution function $P(\theta)$. Intersections between filaments were treated as crosslinks and nodes were dispersed along the filaments to allow for bending. An example of such a gel can be found by viewing Figure 2. Energy in the network was stored in the cross links as bending and stretching energy such that the energy was

$$H = \frac{\mu}{2} \sum_{\text{segments}} (s - s_0)^2 + \kappa \sum_{\text{angles}} \frac{1 - \cos(\beta)}{\ell_0}$$

where $s$ is the length of the filament, $s_0$ is the length of the filament at rest, $\beta$ is the angle between adjacent segments of a filament and $\ell_0$ is the average distance between segments of a filament at rest[2]. The system was then sheared using periodic boundary conditions and the energy equation was minimized to find the equilibrium conformations for the network at each shear step. For each network, the system was partitioned into a series of smaller mesh grids. Within each grid, the buckling order parameter was then calculated and stored along with the corresponding position values for the grid. [2]

III. RESULTS

When measuring the buckling order parameter for buckled networks, it appears that the buckling appears to propagate outwards and grow along the nematic director. To observe this directly, a spatial correlation function,

$$C(\Delta x, \Delta y) = <B(x+\Delta x, y+\Delta y)B(x, y) > - < B(x, y) >^2$$

was used, where $\Delta x$ and $\Delta y$ were steps along the $x$ and $y$ axes of the network. The correlation function allowed the comparison of one point on the buckling order parameter maps with neighboring points. Large values for the correlation function indicated a strong link between points $\Delta x$ and $\Delta y$ units away on the buckling order parameter map.

To test the accuracy of the code, the correlation function for randomly generated data was generated. As expected, the plots showed no correlation. However, a diffusive smoothing technique was used on the random data. In doing this, it was hypothesized that smoothing the data would generate a correlation function proportional to $e^{(-\Delta x)^2/C}$, where $C$ is a constant dependent upon the number of times the smoothing function was run. A cross sectional plot was then made on the smoothed data as seen in Figure 4. Being a log plot, the expected behaviour was that of an inverted parabola. The log plots indicated just that, confirming that the correlation function generator performed correctly.

After the accuracy of the code had been determined, it was then used to measure the correlation function of a variety of gels under numerous run parameters. As can be observed, for isotropic cases (S=0), the correlation showed no growth outward from the center as a function of strain. (See Figure 5) However, in the case of anisotropic cases (S=7), when the nematic director was oriented along the $-\frac{\pi}{4}$ direction, the correlation function showed a clear propagation outwards as the shearing of the system increased. (See Figure 6) When the correlation function is generated for an isotropic network, it can clearly be seen that there is no correlation in the buckling parameter between different points along the network. On the other hand, when the network was anisotropically ordered, the correlation function demonstrated a clear correlation in the buckling order parameter between two separate points along the network of the cell. As shear increased, this correlation increased and grew outwards suggesting some sort of nucleation behavior in which the buckling will propagate outwards from a site of origin.
FIG. 5: Spatial Correlation Functions for an Isotropic System with S=0 and the corresponding Buckling Map. As can be seen here, even as shear increases, the buckling map shows little to no change in the buckling order parameter which is clearly seen by the absence of noticeable correlations in the correlation plot.

IV. CONCLUSIONS AND FUTURE WORK

During this summer, we were able to simulate a variety of gels under various parameters, and for each case measured their responses to shear stresses. In doing so, we found that the networks themselves, when directionally ordered, exhibited interesting nonlinear mechanics. Upon studying these mechanics, we hypothesized that a key factor in the nonlinear mechanics of the system was buckling within the network, which caused filaments under a large enough compression to store energy into bending instead of compression to achieve a lower energy state. To test this, we measured a buckling order parameter, which was the fraction of energy stored as compression, as a function of shear for various nematic directions. Doing this it was found that depending on the nematic direction of the system. Thus when the nematic direction of the system allowed for compression of the filaments, the network was able to buckle resulting in the fraction of energy being stored in compression to decrease as shear increased. On the other hand, when the filaments in the nematic direction were stretched, the system would not be able to buckle and thus the fraction of energy stored in compression was relatively constant. It was noticed that in anisotropic systems where buckling was possible, filaments would appear to buckle along the nematic direction and grow outwards. To observe this, Matlab was used to write code that generated a spatial correlation function of the buckling order parameter. This revealed clearly that for anisotropic systems, the buckling propagated outwards from points of origin as shear increased.

The next step would be to develop a mathematical model in order to determine the mechanism by which the buckling order parameter decays. Currently, mathematical models have been developed for two rods under identical compressive loads connected by a spring. However, it was found that the buckling propagated uniformly through the system without any decay. Currently, work is being done on the model of a series of rods connected by springs with external moments on a couple randomly distributed rods. In doing this, we hope develop some sort of exponential decay in buckling to replicate the results we are finding from the simulation.

In addition, there are occasionally minor discrepancies within the data itself. Theoretically, any value of the buckling order parameter should be between 0 and 1, as the energy stored in compression of a filament is only a fraction of the total energy within the system[3]. However, it was found that in fact there are values greater than 1 and less than 0. In these cases, the code bounded these values between -1 and 1. Bounding this system in
FIG. 6: Spatial Correlation Function for an Anisotropic System with S=0.7 and the corresponding buckling map. In this case it can easily be seen that when the shear increased, the buckling order parameter seemed to propagate along the nematic director. This is seen in the corresponding spatial correlation which shows a clear growth outwards at larger shear.

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