Negative Gaussian curvature from induced metric changes

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Nature has long been a primary source of inspiration for engineering, and the recent development of shape-programmable materials is no different. Similar to the differential growth rates in plant leaves or flowers giving rise to ruffled, intricate three dimensional shapes from originally flat specimens, thin flat sheets of nematic elastica can be induced to adopt new natural in-material lengths by different amounts in different directions relative to the nematic director. Here we consider the case of producing asters, “e-cones,” or “anti-cones,” and analyze the deformation map from the point of view of both the local, differential distortions and the known global properties of the target shape.

An extraordinary zoo of complex shapes may be seen to result from pure growth processes over time, and indeed one need look no further than a very literal zoo for evidence of this as much of macroscopic biological diversity arises from this source [1]. It has recently been understood that some striking instances of botanical growth can be explained by differentials in radial and azimuthal growth rates, resulting in changes of Gaussian curvature from an initially flat specimen [2, 3] to give cones, ruffles, or asters. These shapes are also known as “e-cones” or “anti-cones,” the latter of which we will use here. Changed topography obviates any stretch, but at the cost of some bend, the energy cost of which one can ignore for sufficiently thin systems [2, 3]. Such shape change complexity may be encountered beyond nature in the manmade as well: nematic elastica – liquid crystal elastomers or glasses – can respond to heat [4] or light [5–8] by contracting their natural lengths along their director $n$ and elongating in the two directions perpendicular to $n$ — a form of (reversible) growth that may be thought to mimic the differential growth rates of flora but on vastly shorter time scales. The material deformation gradients can be huge ($\times 4$) for elastomers and less so ($\times 1.04$) for glasses, and the reciprocal of these when reversing by cooling or in the dark. Shape change effects are spectacular but straightforward if $n$ is uniform, but nearly any non-uniform patterns $n(r)$ in the plane give an in-plane incompatibility of deformation that can only be resolved by a change of topography. This shape change necessarily involves a change of the natural Gaussian curvature of the surface, or, lacking the ability to achieve its new natural intrinsic geometry, by the development of large stretches relative to the new stress-free state. We consider only 2-D director patterns in the plane of an initially flat sheet.

Effectively, a heated or illuminated sheet of such a nematic solid suffers a change of metric. Analysis of the metric change for illuminated $n(r)$ fields of topological charge $m \neq 1$ [9], and of circular/radial patterns ($m = 1$) on initially spherical shells [10] yields changes in Gaussian curvature and thus new shapes. This metric change approach also has recently been exploited in these sorts of problems, and also those of $n(r)$ patterns on sheets without defects, in an ambitious work also concerned with general shape determination [11]. A synthetic equivalent of the botanically-inspired [2, 3] aster shapes is that of azimuthal or radial $n$ patterns (2-D $m = 1$ defects, see Fig. 1) in nematic elastica. For glasses, on cooling azimuthals or heating radials (or darkness/light respectively) a circular perimeter elongates and the radius contracts so that their ratio is $> 2\pi$ and a topographical change to an “anti-cone” (Fig. 1) was predicted [12, 13] and observed [14].

Anti-cones are entirely generated by straight director rays emanating from the “tip,” where the disclination defect core gives rise to a singular point in the Gaussian curvature, which is zero elsewhere as a consequence of the ruled, ray-generated nature of the surface. In the event that there has been escape into the third dimension of the reference director field near the disclination defect, the resultant geometry local to the defect may vary, with the curvature singular point smeared out over a small neighborhood; farther from this region the surface will

![FIG. 1: Azimuthal and radial 2D. +1 disclinations, an $n = 2$ “anti-cone”, and an initially flat disc of radius $R$ deformed into an anti-cone with an in-material radius $r$.](image-url)
again agree with the idealized version. We examine anti-cones in light of some recent work [15] that revisits the problem with a metric method, but which obtains anti-cones of a character differing from that of [12, 13].

Consider concentric circles of \( n \) in a flat sheet of nematic glass. (We discuss at the end nematic elastomers and also radial systems – there are subtle questions of director rotation.) Let the elongation along \( n(r) \) be by a factor of \( \lambda > 1 \) (on cooling or return to the dark). There is a corresponding contraction by \( \lambda^{-v} \) in the two perpendicular directions. Volume changes locally by a factor of \( \text{Det} \left( \lambda \right) = \lambda^{1-2v} \) where \( \lambda, \lambda^{-v}, \lambda^{-v} \) are the elements of the deformation gradient tensor \( \lambda \) in its principal frame (based upon \( n \)). The opto-thermal Poisson ratio \( v \) takes values typically in the range \((1/2, 2)\) in nematic glasses [7], and \( v = \frac{1}{2} \) in nematic elastomers where volume is conserved. Note that area would be conserved for \( v = 1 \), but this value is of no physical significance. If elastic stretches are to be avoided on cooling/darkness, then one simply requires that, in deformation to a different topography, the deformation gradients take principal values \( \lambda \) and \( \lambda^{-v} \) corresponding to the natural opto-thermal value under those conditions. We restrict ourselves to avoidance of stretch, and we ignore bend energy.

In cylindrical coordinates, a reference state point is \((R, \Phi, z = 0)\) in the initially flat disc, see Fig. 1. On cooling, its image in the target state is \((p, \phi, z = h(\phi))\), where \( h \) is the elevation from the initial plane (note the use of lower and upper case variables). The target state curve is on a sphere of radius \( r \), see the trajectory in the last panel of Fig. 1, and the in-material radius is now

\[
r^2 = \rho^2 + z^2 \rightarrow r = \rho \sqrt{1 + (h/\rho)^2}.
\]

We take an ansatz for distortion:

\[
h = pA \sin(n \phi),
\]

with integer \( n \) for closure and discuss the motivation shortly. The amplitude \( A \), after scaling by the cylindrical radius \( \rho \), is \( A = \tan\alpha \). The angle \( \alpha \) is made between an anticone generator at a displacement antinode and the equatorial plane initially taken by the flat disc; see Fig. 1. The amplitude needed to take up the extra length of the perimeter with respect to the radius is a global requirement, not local, [12], that we also return to.

An element \( dp \) of length in the target space image of the element \( Rd\Phi \) is

\[
dp = d\Phi \left( \frac{\partial p}{\partial \Phi} \right)^2 + \rho^2 + \left( \frac{\partial h}{\partial \phi} \right)^2.
\]

We now require the sheet deforms locally according to \( \lambda \):

\[
r = \lambda^{-v} R \quad \text{and} \quad dp = \lambda(R \ d\Phi) \rightarrow \frac{dp}{R \ d\Phi} = \lambda.
\]

From eqn. (1) we have

\[
\rho(\phi) = \lambda^{-v}R / (1 + A^2 \sin^2 n\phi)^{\frac{1}{2}}
\]

\[
h(\phi) = \lambda^{-v}RA \sin(n\phi) / (1 + A^2 \sin^2 n\phi)^{\frac{1}{2}}.
\]

We restrict ourselves to avoidance of stretch, and we ignore bend energy.

Pismen [15] restricts all distortions in his model of anti-cones to be meridional and radial as in the more straightforward case of simple cones, whereas these distortions to anti-cones described above have an extra degree of freedom. The differential method employed above is in effect equivalent to the metric method of Pismen, eqns. (12)–(14), but with differing assumptions (about \( \Phi \) and \( \phi \)) with the result that these anti-cones do not have creases. It is interesting to integrate relation (2) to give \( \phi(\Phi) \), see Fig. 2, to see for instance the azimuthal variation in this model for an \( n = 2 \) anticone which repeats at \( \Phi = \phi = \pi \). It has its first node at \( \Phi = \phi = \pi/2 \), and its first antinode at \( \Phi = \phi = \pi/4 \). At both points it is clear, for symmetry reasons, that \( \Phi = \phi \).

The case \( n = 1 \) is simply a uniform body rotation by an \( \alpha \) about a diameter, whereas for \( n \geq 2 \) the rotation by \( \alpha \) such that \( A = \tan\alpha \) is identifiable only at the antinodal lines. Though trivial, the \( n = 1 \) case is instructive: simple geometry applied to the \( n = 1 \) transformation gives the mapping of the azimuthal angle:

\[
\tan \phi = \cos \alpha \tan \Phi.
\]
Alternatively, explicit integration of eqn. (8) is trivial and yields (9) if \( \lambda = 1 \) and if one uses \( \sqrt{1 + A^2} = \sec \alpha \). This analysis of simple rotation is a motivation for adopting \( h = p \lambda \sin(\phi \lambda) \) for the axial distortions into an anticone, and underscores a need to have a \( \Phi(\lambda) \) for non trivial cases when it already arises for \( n = 1 \).

The method of [12, 13] for anti-cones was to take a global version of eqn. (8) by integrating \( dp \) to give the whole new perimeter \( p \) which must, since the perimeter is along \( n \), be \( p = 2\pi \lambda R \), that is \( \lambda \) times the original perimeter. The integral of the right hand side of eqn. (8) over \( \phi = (0, 2\pi) \) yields \( \lambda^{-\nu} 2\pi \nu (A,n) \) where the integral \( I \) is eqn (6) and the form of \( I(A,n) \) given below it in [12]. One sees from the current analysis that a stretch-free state is guaranteed globally since it is built-in locally. However one cannot fully specify this problem locally. From the above, the amplitude \( A \) and the distortion \( \lambda \) are connected through \( I(A,n) = \lambda^{1+\nu} \). As \( \lambda \) changes, so too must the amplitude \( A \) of the ruffles in order that all surplus length around a perimeter is accommodated. The negative Gaussian curvature localized at the apex of the anticone is \( 2\pi(1 - I) \). Eventual re-entrance and the transition to higher \( n \) anticones are discussed in [12, 13].

Indeed, many of these matters may be better understood in light of this differential treatment or the metric treatment of Pismen. If, instead of making the simple ansatz of eqn. (2) we had instead posited the following entirely general form corresponding to any surface generated by rays emanating from a single point: the target shape is defined by a closed, non-self-intersecting curve on the sphere whose center coincides with the defect, and this curve is the same (up to scaling) regardless of the size of the sphere. That is, parametrically:

\[
\begin{align*}
\hat{\phi}(t), \phi(t); & \quad t \in [0, 1) \\
\hat{\phi}(0) = \phi(0) & = \phi(1) \\
(\hat{\phi}(t_1), \phi(t_1)) & \neq (\hat{\phi}(t_2), \phi(t_2)); \quad t_1, t_2 \in (0, 1)
\end{align*}
\]

where \( \phi, \hat{\phi} \) are the spherical coordinates on the defect-centered sphere of the surface-defining curve. Any such pair of parametric functions that satisfy these constraints give rise to a surface that is, in its intrinsic geometry, a cone or an anticone, as the ray-generated nature of the surface guarantees Gaussian flatness everywhere but at the center. In order to restrict this large, general family of shapes to one that satisfies the imposed local spontaneous distortion we must simply impose one further global constraint on the curve, the analogue in this generalized setting of eqn. (3):

\[
2\pi \lambda^{1+\nu} = \int_0^1 dt \left( \left( \frac{\partial \phi}{\partial t} \right)^2 + \sin^2 \hat{\phi} \left( \frac{\partial \phi}{\partial t} \right)^2 \right)^{\frac{1}{2}}.
\]

Hence the determination of actually achieved, stretch-free shapes may be restricted to those surfaces from the family of isometries satisfying these constraints. Note that \( \lambda \) less than, greater than, and equal to 1 correspond to cones, anti-cones, and developable surfaces, respectively, and in this light the available shapes associated to isolated curvature defects can be seen as a generalization of the origami problem, at least with respect to an isolated fold intersection. Specific cases may result in different shapes as the effect of boundary conditions, bend energy, external load, or other complications may preference varying aspects of the surfaces. As it happens, the original, specific ansatz of eqn. (2) is a very good approximation for small distortions if the stretch-free shape is only subject to bend energy minimization.

Elastomers were not discussed in [12, 13] – they are more subtle than glasses since they can sometimes alleviate stress by director rotation. For instance in the azimuthal example considered above and by Pismen, if an elastomer disc were held flat on cooling so that extensible radial stress developed because of the deficit of natural length in the radial direction, then director rotation from the azimuthal towards the radial direction would re-attribute length from the azimuthal to radial direction, i.e. from a direction of surplus to one of deficit. Little or no energy cost for such a distortion is required – so-called soft elasticity [16] – and the need for anticones obviated. Thus general analyses of nematic elastica mentioning nematic elastomers require caution.

An elastomer example that would produce anti-cones would be a radial, 2-D, +1 defect being heated, that is \( \lambda < 1 \); see the second panel of Fig. 1. Now a circular path obtains surplus length (by a factor of \( \lambda^{-\nu} \) and a radius is in deficit by a factor of \( \lambda \). The radius cannot become longer by rotation of the director towards it – it is already radial, and the glass and elastomer responses are identical in character. The difference is that elastomer contractions can be huge, for instance \( \lambda \rightarrow 0.25 \) on heating (\( \rightarrow 4 \) on cooling) is possible and the topography changes could be accordingly larger than in glasses.

We have explored and contrasted the differing assumptions one can make about deformations involved in anticone formation, principally the role of azimuthal displacements of material points. We also point to possible experiments on elastomers rather than glasses where effects could be very large.

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