Ribbons: Their Geometry and Topology

C. K. Au[1] and T. C. Woo[2]

[1]Nanynag Technological University, mckau@ntu.edu.sg
[2]Nanynag Technological University, mchwoo@ntu.edu.sg

ABSTRACT

Ribbons may be used for the modeling of DNAs and proteins. The topology of a ribbon can be described by the link *Lk*, while its geometry is represented by the writhe *Wr* and the twist *Tw*. These three quantities are numerical integrals and are related by a single formula from knot theory. This article discusses the meanings of these three quantities, offers an approach for calculating their numerical values, and provides some examples.

Keywords: Ribbon model, link, writhe, twist, Gauss Integral, supercoiling

1. INTRODUCTION

A curve has only length; it has no width or thickness. But if endowed with a width in an orthogonal direction, a curve becomes a *ribbon*. (If the width is uniform in all directions, then a *rope* results.) Ribbons serve as a convenient way to model macromolecules such as DNA and protein[1-3]. The functions of these macromolecules are determined by their form, or *geometry*, while their inter-connectedness, or *topology*, is important to many biological processes[4,5] such as protein folding, replication and transcription.

Curvature and torsion characterize how a curve *K* changes with respect to the Frenet-Serret frame on the curve itself. But suppose the frame of reference is on another curve *L*. Then, two new quantities, *writhe* and *twist*, arise. In a ribbon, let there be a central "spine" *K*. Also, let one of the two boundary curves of the ribbon be *L*. Then, the "tangling" between *K* and *L* gives an indication of how complex the ribbon is, spatially. Intuitively, as writhe and twist are analogous to curvature and torsion, they describe the geometry of a ribbon. Yet, because *K* "threads" *L*, or vice versa, there must be another parameter that characterizes the "knottiness" of the tangle – called *link*, a topological quantity. Indeed, the White formula[5,6]

$$Lk(K,L) = Wr(K) + Tw(K,L) \qquad (1)$$

gives the connection. The two geometric quantities on the right hand side are real numbers and the topological quantity on the left is an integer – in a fashion analogous to the Gauss-Bonnet formula (with angles and areas on the one side and the Euler characteristic on the other).

This paper addresses the computation of the three quantities in (1). Several algorithms are for computing the writhe of a polygonal curve[7-10] and for simple analytic curves[11]. No prior result is known for the calculation of twist. More fundamentally, it turns out that the three quantities are rooted in the evaluation of the so-called ***Gauss Integral***. This paper offers a discrete computation scheme for (1).

2. TOPOLOGY AND GEOMETRY OF A RIBBON

A ribbon is characterized by two curves: its central spine *K* and one of its two boundary curves *L*. —An "equilibrium condition" in the changes of the three quantities in (1) comes from two pieces of intuition. First, topologically, the link is an invariant. Second, algebraically, the derivative of a constant is zero. Therefore,

$$\delta Wr(K) + \delta Tw(K,L) = 0 \qquad (2)$$

In other words, when a ribbon is isotropic to a new conformation, any change in twist has to be exactly balanced by the change in its writhe.

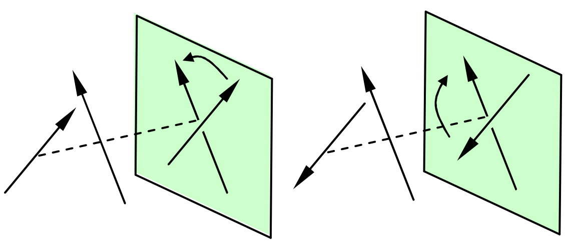
Two concepts, the *crossing* number and the *Gauss integral*, are important for calculating the link *Lk(K,L)*, writhe *Wr(K)* and twist *Tw(K,L)*.

2.1 Crossing

Let a curve be represented by a series of line segments. When the 2D projections of two segments (of the same curve or from two different curves) intersect, there is a *crossing*, suggesting that in 3D the line segments pass "over" or "under" each other. Three assumptions on projection are necessary for the computation:

i.) that the two end points of a line segment do not coincide;
ii.) that an end point from one segment will not be on another line segment; and
iii.) that no three line segments intersect at a point.

Crossings are signed when the line segments are oriented, as shown in Figure 1. A crossing is *positive* if the angle ($<\pi$) required to rotate the arrow (for the segment on top) onto the arrow at the bottom is counter-clockwise; otherwise, it is negative.



(a) positive crossing (b) negative crossing

Fig. 1. Signed crossing

Crossing number is the sum of the signed crossings occurring in a curve or between two curves. Clearly, crossing depends on the direction of projection; so does the crossing number.

2.2 Gauss Integral and its Geometric Meaning

Some preliminaries for calculating the Gaussian Integral are necessary. Suppose two oriented segments $\mathbf{p}_j\mathbf{p}_{j+1}$ and $\mathbf{q}_k\mathbf{q}_{k+1}$ cross each other. Let $\mathbf{p}$ and $\mathbf{q}$ be any two points on the segments $\mathbf{p}_j\mathbf{p}_{j+1}$ and $\mathbf{q}_k\mathbf{q}_{k+1}$ respectively. The mapping $\Psi : \mathbf{p}_j\mathbf{p}_{j+1} \times \mathbf{q}_k\mathbf{q}_{k+1} \rightarrow \mathbf{R}^3$ such that $\Psi(\mathbf{p},\mathbf{q}) = \dfrac{\mathbf{q}-\mathbf{p}}{|\mathbf{q}-\mathbf{p}|}$, produces a region on a unit (Gaussian) sphere characterized by four vertices $\Psi(\mathbf{p}_j,\mathbf{q}_k)$, $\Psi(\mathbf{p}_{j+1},\mathbf{q}_k)$, $\Psi(\mathbf{p}_{j+1},\mathbf{q}_{k+1})$ and $\Psi(\mathbf{p}_j,\mathbf{q}_{k+1})$. These vertices are arranged in the counter clockwise direction, and the area of the region denoted by $S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{q}_k\mathbf{q}_{k+1})$ is positive, as shown in Figure 2. If, on the other hand, the two oriented segments cross negatively, then the arrangement of the vertices would be Ψ_{jk}, $\Psi_{(j+1)k}$, $\Psi_{(j+1)(k+1)}$ and $\Psi_{j(k+1)}$, in the clockwise order and the area $S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{q}_k\mathbf{q}_{k+1})$ is negative. Note that the vertices on the sphere, in Figure 2, are the four pairs of normalized distances between the four end points of the two line segments.

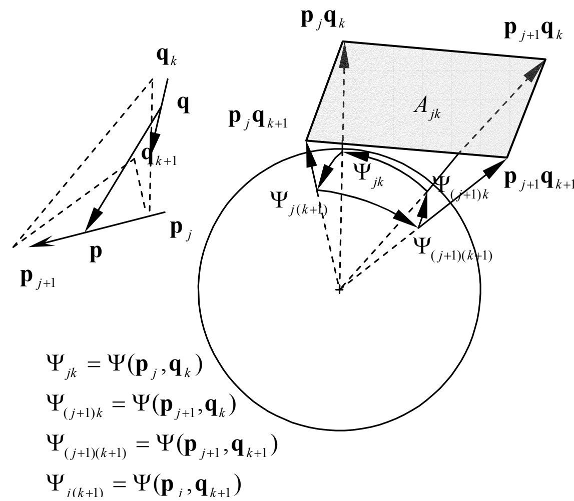


Fig. 2. Crossing and unit sphere

The shaded rectangle in Figure 2 warrants some explanations. Consider two small elements $d\mathbf{p}$ and $d\mathbf{q}$ on $\mathbf{p}_j\mathbf{p}_{j+1}$ and $\mathbf{q}_k\mathbf{q}_{k+1}$. The segments cross when the component of the area $d\mathbf{p}\times d\mathbf{q}$ is perpendicular to the projective direction $\mathbf{pq}$. Hence its area A_{jk} is given as

$$dA_{jk} = \frac{(d\mathbf{p}\times d\mathbf{q})\mathbf{pq}}{|\mathbf{pq}|} \tag{3}$$

Since both area A_{jk} and its *pull back* area $S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{q}_k\mathbf{q}_{k+1})$ on the unit sphere subtend the same solid angle, it follows that

$$\frac{dA_{jk}}{|\mathbf{pq}|^2} = dS(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{q}_k\mathbf{q}_{k+1}) \tag{4}$$

while it is understood that the radius of the sphere is unity.

Substituting (3) into (4) and integrating yields

$$S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{q}_k\mathbf{q}_{k+1}) = \int_j^{j+1}\int_k^{k+1}\frac{(d\mathbf{p}\times d\mathbf{q})\cdot\mathbf{pq}}{|\mathbf{pq}|^3} \tag{5}$$

$S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1})$ is the signed area on the unit sphere signifying all the directions from which $\mathbf{p}_j\mathbf{p}_{j+1}$ crosses $\mathbf{q}_k\mathbf{q}_{k+1}$ when projected along $\mathbf{pq}$. Hence, the Gauss Integral is given by

$$\oiint_{K\times L} \frac{(d\mathbf{p}\times d\mathbf{q})\cdot\mathbf{pq}}{|\mathbf{pq}|^3} = \sum_j \sum_k S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1}) \quad (6)$$

3. LINK, WRITHE, AND TWIST

Details on the terms in (1) are now ready.

Definition 1

The *link* between two oriented curves K and L is defined as

$$Lk(K,L) = \frac{1}{4\pi}\oiint_{K\times L} \frac{(d\mathbf{p}\times d\mathbf{q})\cdot\mathbf{pq}}{|\mathbf{pq}|^3} \quad (7)$$

where $\mathbf{p}$ and $\mathbf{q}$ are two points on the curves K and L, respectively.

Definition 2

The *writhe* of a curve K is the *average* value of the signed crossing number, over all possible projection directions:

$$Wr(K) = \frac{1}{4\pi}\int_K \frac{(d\mathbf{p}\times d\mathbf{q})\cdot\mathbf{pq}}{|\mathbf{pq}|^3} \quad (8)$$

Definition 3

The *twist* of a curve L (parameterized by arc length s) around another curve K is defined as

$$Tw(K,L) = \frac{1}{2\pi}\int_L (\mathbf{t}\times\mathbf{v})\cdot\mathbf{v}'ds \quad (9)$$

where $\mathbf{t}$ is the unit tangent vector of K at s and $\mathbf{v}$ is the unit vector perpendicular to the unit tangent vector $\mathbf{t}$ pointing from K to L.

4. DISCRETE RIBBON MODEL

A ribbon is characterized by two curves K and L as shown in Figure 3(a). Curve K represents the central spine of the ribbon while its boundary is the curve L. Any curve M on the ribbon parallel to K and L is represented by

$$M = (1-t)K + tL, \forall t \in R \quad (10)$$

A complicated conformation can be simplified into the discrete ribbon model by representing its spine and the boundaries by a series of line segments. Let $K = \mathbf{p}_1\mathbf{p}_2\cdots\mathbf{p}_n$ and $L = \mathbf{q}_1\mathbf{q}_2\cdots\mathbf{q}_n$ be two such series. An illustration is given in Figure 3(b) which relates all the points on the curve K to those on L. When the two free ends of the ribbon are connected into a closed knot, then $K = \mathbf{p}_1\mathbf{p}_2\cdots\mathbf{p}_n\mathbf{p}_1$ and $L = \mathbf{q}_1\mathbf{q}_2\cdots\mathbf{q}_n\mathbf{q}_1$.

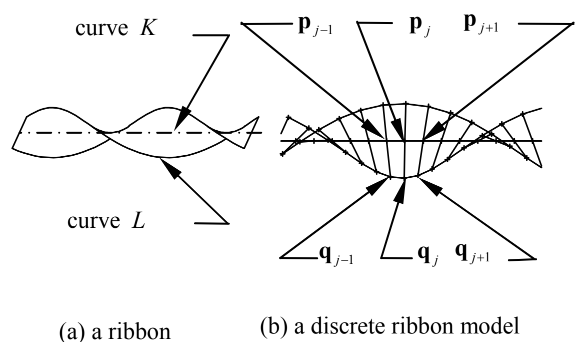


Fig. 3. A ribbon and its model

In a discrete ribbon model, the integrals expressed by (7), (8) and (9) can be computed more efficiently, and with nearly equal effectiveness, by considering their geometric meanings.

5. GEOMETRIC MEANING OF THE INTEGRALS

Let $K = \mathbf{p}_1\mathbf{p}_2\cdots\mathbf{p}_n\mathbf{p}_1$ and $L = \mathbf{q}_1\mathbf{q}_2\cdots\mathbf{q}_m\mathbf{q}_1$ be two non-intersecting closed line segments running from 1 to *n* and *m* in the space for a discrete ribbon model.

***Lemma 1*:**

The link of a ribbon conformation is

$$Lk(K,L) = \frac{1}{4\pi}\sum_{j=1}^{n}\sum_{k=1}^{m} S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1}) \quad (11)$$

Proof.

By definition, $Lk(K,L) = \frac{1}{4\pi}\oiint_{K\times L} \frac{(d\mathbf{p}\times d\mathbf{q})\cdot\mathbf{pq}}{|\mathbf{pq}|^3}$.

Discretizing it gives

$$Lk(K,L) = \frac{1}{4\pi}\sum_{j=1}^{n}\sum_{k=1}^{m} S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1})$$

Corollary 1.1

The link of two curves is the number of times that the area of the unit sphere covered by the image of the two curves under the mapping Ψ .

Proof.
Since K and L are closed, identify $n+1$ with 1 and likewise $m+1$ with 1. Hence the expression $\sum_{j=1}^{n}\sum_{k=1}^{m} S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1})$ covers the whole unit sphere. Dividing $\sum_{j=1}^{n}\sum_{k=1}^{m} S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1})$ by the unit sphere surface area (4π) gives the number of times that the unit sphere is covered.

Corollary 1.2
The link is an integer when K and L are closed curves.

Proof.
Since $Lk(K,L) = \frac{1}{4\pi}\sum_{j=1}^{n}\sum_{k=1}^{m} S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1})$ where $S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1})$ is the pull back area on the unit sphere. The link is the number of times that the unit sphere being covered by $S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{q}_k\mathbf{q}_{k+1})$ which is an integer.

***Lemma 2*:**

$$Wr(K) = \frac{1}{4\pi}\sum_{j,k} S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{p}_k\mathbf{p}_{k+1}) \text{ and } j \neq k, j \neq k \pm 1 \quad (12)$$

Proof.
By definition,
$Wr(K) = \frac{1}{4\pi}\int_K \frac{(d\mathbf{p} \times d\mathbf{q}) \cdot \mathbf{pq}}{|\mathbf{pq}|^3}$. Discretizing the integral gives

$$\frac{1}{4\pi}\int_K \frac{(d\mathbf{p} \times d\mathbf{q}) \cdot \mathbf{pq}}{|\mathbf{pq}|^3} = \sum_{j \neq k, j \neq k \pm 1} {}_j \sum_k \int_j^{j+1}\int_k^{k+1} \frac{(d\mathbf{p} \times d\mathbf{q}) \cdot \mathbf{pq}}{|\mathbf{pq}|^3} .$$

When $k = j \pm 1$, the region produced on the unit sphere is the great circle in the plane containing the two segments; the area $|S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{p}_k\mathbf{p}_{k+1})| = 0$. When $k = j$, the area degenerates to a point on the unit sphere. Figure 4 shows the degenerate area $|S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{p}_k\mathbf{p}_{k+1})|$ in both situations. Hence, $Wr(K) = \frac{1}{4\pi}\sum_{j,k} S(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{p}_k\mathbf{p}_{k+1}) \ \forall j \neq k, j \neq k \pm 1$.

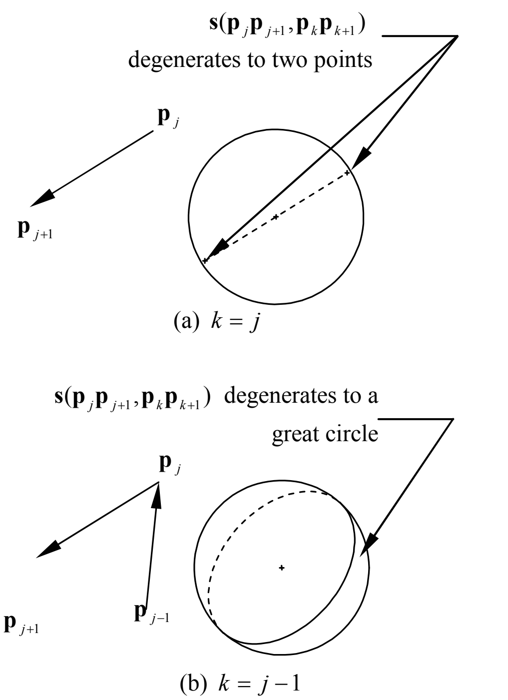


Fig. 4. The pull back area on the unit sphere, when $k = j$ or $k = j-1$

The writhe of a ribbon is

***Lemma 3*:**
The twist of a ribbon is

$$Tw(K,L) = \sum_j \frac{\alpha_j}{2\pi} \quad (13)$$

where α is the dihedral angle as shown in Figure 5.

Proof.
From equation (9), $Tw(K,L) = \frac{1}{2\pi}\int_L \tau ds + d(K,\mathbf{v})$.
Therefore,
$Tw(K,L) = \sum_j \frac{1}{2\pi}\tau_j \cdot |\mathbf{q}_j\mathbf{q}_{j+1}| + \sum_j d(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{v}_j)$ where $\mathbf{v}_j = \mathbf{p}_j\mathbf{q}_j$. Referring to Figure 5, $d(\mathbf{p}_j\mathbf{p}_{j+1}, \mathbf{v}_j) = \frac{\alpha_j}{2\pi}$.
Hence, $Tw(K,L) = \sum_j \frac{\alpha_j}{2\pi}$.

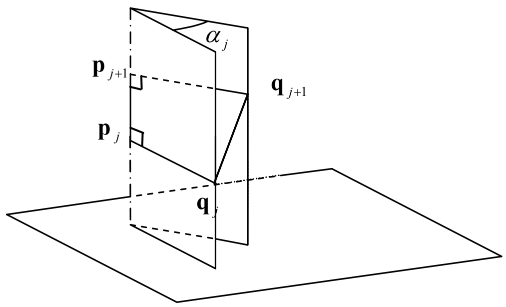


Fig. 5. The twist of segment $\mathbf{q}_j\mathbf{q}_{j+1}$ around $\mathbf{p}_j\mathbf{p}_{j+1}$

***Lemma 4*:**
Let $K = \mathbf{p}_1\mathbf{p}_2\cdots\mathbf{p}_n\mathbf{p}_1$ and $L = \mathbf{q}_1\mathbf{q}_2\cdots\mathbf{q}_m\mathbf{q}_1$ be two non-intersecting closed line segments running from 1 to *n* and *m*; then

$$Tw(K,L) = \sum_j \frac{\lim_{t\to 0} S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{r}_j\mathbf{r}_{j+1})}{4\pi} \qquad (14)$$

Proof.
Consider the j[th] segment $\mathbf{p}_j\mathbf{p}_{j+1}$ and $\mathbf{q}_j\mathbf{q}_{j+1}$ of the curves K and L, respectively. Without loss of generality, assume that $\mathbf{p}_j\mathbf{p}_{j+1}$ is vertical. The j[th] segment $\mathbf{r}_j\mathbf{r}_{j+1}$ of curve M, that lies between *K* and *L*, is shown in Figure 6(a). Figure 6(b) depicts the locations of $\Psi(\mathbf{p}_{j+1},\mathbf{r}_j)$, $\Psi(\mathbf{p}_{j+1},\mathbf{q}_{j+1})$, $\Psi(\mathbf{p}_j,\mathbf{r}_{j+1})$ and $\Psi(\mathbf{p}_j,\mathbf{q}_j)$ on the unit Guassian sphere. As the parameter $t\to 0$, $\mathbf{r}_j \to \mathbf{p}_j$ and $\mathbf{r}_{j+1} \to \mathbf{p}_{j+1}$; hence $\Psi(\mathbf{p}_{j+1},\mathbf{r}_j) \to \Psi(\mathbf{p}_{j+1},\mathbf{p}_j)$ and $\Psi(\mathbf{p}_j,\mathbf{r}_{j+1}) \to \Psi(\mathbf{p}_j,\mathbf{p}_{j+1})$ which are the south pole and north pole of the unit sphere, respectively. Therefore, $\lim_{t\to 0} S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{r}_j\mathbf{r}_{j+1})$ is the area of the shaded region on the unit sphere which is $2\alpha_j$ or $\lim_{t\to 0} S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{r}_j\mathbf{r}_{j+1}) = 2\alpha_j$. From Lemma 3, $\lim_{t\to 0} S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{r}_j\mathbf{r}_{j+1}) = 2\cdot 2\pi\cdot Tw(\mathbf{p}_j,\mathbf{q}_j) = 4\pi\cdot Tw(\mathbf{p}_j,\mathbf{q}_j)$.

Therefore, $Tw(K,L) = \sum_j \frac{\lim_{t\to 0} S(\mathbf{p}_j\mathbf{p}_{j+1},\mathbf{r}_j\mathbf{r}_{j+1})}{4\pi}$.

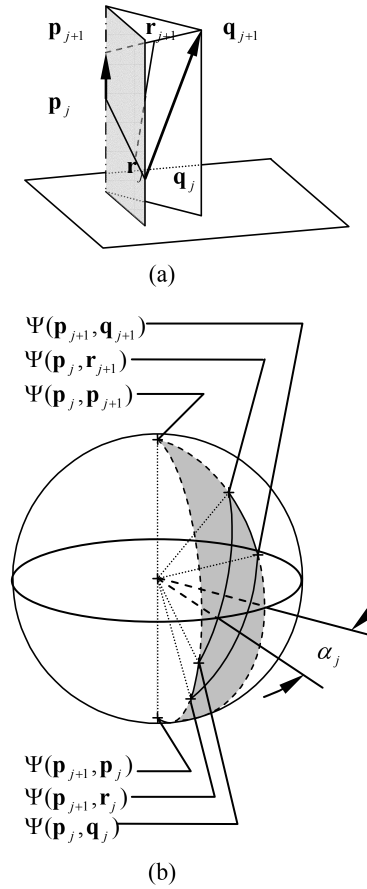


Fig. 6. Twist of $\mathbf{q}_j\mathbf{q}_{j+1}$ around $\mathbf{p}_j\mathbf{p}_{j+1}$ and its image on the Gaussian sphere.

6.CONCLUSION

The geometry and the topology of a ribbon conformation are related to each other by link, writhe and twist. Gaussian integrals are involved in these three quantities. These integrals can be very complicated and are hard to compute for a complex ribbon conformation, since no analytic expression is available for the curves. The calculation are shown simplified by considering the geometric meanings of these integrals. This paper reveals the assumptions and details the steps.

In order to understand the related biological processes, two issues deserve further exploration in the future:

i.) the reason that drives the macromolecules transforming from one conformation to another;

ii.) the process of transforming.

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