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## Shape optimization of self-avoiding curves



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## ABSTRACT

This paper presents a softened notion of proximity (or self-avoidance) for curves. We then derive a sensitivity result, based on shape differential calculus, for the proximity. This is combined with a gradient-based optimization approach to compute three-dimensional, parameterized curves that minimize the sum of an elastic (bending) energy and a proximity energy that maintains self-avoidance by a penalization technique. Minimizers are computed by a sequential-quadratic-programming (SQP) method where the bending energy and proximity energy are approximated by a finite element method.

We then apply this method to two problems. First, we simulate adsorbed polymer strands that are constrained to be bound to a surface and be (locally) inextensible. This is a basic model of semi-flexible polymers adsorbed onto a surface (a current topic in material science). Several examples of minimizing curve shapes on a variety of surfaces are shown. An advantage of the method is that it can be much faster than using molecular dynamics for simulating polymer strands on surfaces. Second, we apply our proximity penalization to the computation of ideal knots. We present a heuristic scheme, utilizing the SQP method above, for minimizing rope-length and apply it in the case of the trefoil knot. Applications of this method could be for generating good initial guesses to a more accurate (but expensive) knot-tightening algorithm.

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## 1. Introduction

Self-assembly of micro structures is a growing research area with applications in basic science and material design [22, 37,32]. In particular, polymers confined to curved surfaces have great scientific interest. The packing of strands of DNA onto a protein complex, as well as packaging DNA into a small volume to fit inside a cell, is of fundamental importance in biology [35,41,52]. In the design of materials, micro-scale patterned surfaces can be used to create material components with novel optical, electronic and magnetic properties [43]. Moreover, elastic polymer chains can be forced into regular patterns when they are energetically bound to a deformable membrane [33,61,62,53]. Therefore, modeling and simulating the equilibrium configurations of semi-flexible polymer strands on surfaces is important for basic physics understanding and developing technological applications [12,1,46].

A crucial driving force of these patterns is self-contact [19,20], i.e. an object's matter cannot overlap itself. A long polymer chain that is forced to reside on a closed, bounded surface must interact with *itself* when obtaining its equilibrium configuration. Hence, the presence of self-contact (or self-avoidance) in these systems plays a fundamental role in their equilibrium states and dynamic evolutions [50], so we must account for it when modeling these systems. Multiple characterizations of self-contact have been developed in the literature [29,30,19] (all in the context of knots).

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This paper presents a smoothed notion of self-avoidance for curves that is suitable for gradient-based optimization methods. Our method is based on a modified version of the *global radius of curvature* [19,20,31,42,47]. This concept possesses some very nice analytical properties [42,47] and was used to prove the existence of optimal shapes of “thick” knots [19,20,24]. But it is certainly not limited to this one application. We demonstrate our method by applying it to two problems.

The first problem is on the adsorption of semi-flexible polymers onto surfaces, which has been done in several research works [35,41,52,59,61,62,53] mostly using molecular dynamics and Lennard-Jones potentials. We propose to simulate the equilibrium configuration of inextensible elastic curves that are bound to a surface and satisfy the no-penetration condition (i.e. the elastic curve is self-avoiding). By no-penetration, we assume the curve is surrounded by a *tubular neighborhood* that does not self-intersect (see Section 2.1.5), which is completely inline with modeling “thick” polymer strands.

We use an energetic continuum approach, i.e. the curves are parameterized 1-D manifolds (not beads on a string) that minimize the sum of an elastic energy and a “proximity” (penalized) energy that enforces the no-penetration condition. The proximity functional (see Section 2.3) softens the effect of self-contact, and as far as we know is new. Gradient information is computed via shape differentiation. We then discretize the problem and give a discrete sequential-quadratic-programming (SQP) method for finding local minimizers of the energy. To the best of our knowledge, this is a novel scheme, but we point out another constrained gradient scheme in [3]. As for efficiency, our method takes a few hundred to about a thousand iteration steps. A molecular dynamics simulation typically takes on the order of a few million steps. Hence, our method should be faster than a direct molecular dynamics simulation.

The second problem is on computing ideal knots. We present a heuristic algorithm for minimizing rope-length of closed curves (i.e. for approximating ideal knots), that utilizes the SQP method above, and apply it in the case of the trefoil knot. One application of the method could be for generating good initial guesses to a more accurate (but expensive) knot-tightening algorithm. Furthermore, it may be useful for probing optimal configurations of more complicated knots.

The paper is organized as follows. Section 2 reviews the concept of global radius of curvature, then we present our penalized approach for preventing self-contact. Section 3 shows how we model the equilibrium shape of semi-flexible curves as minimizers of an energy functional which includes a term to penalize self-intersection; Section 4 describes a finite element method and optimization algorithm for computing minimizers, including a heuristic method for minimizing rope-length (Section 4.7). Several numerical results are shown in Section 5, followed with some concluding remarks.

## 2. Measuring proximity

In order to model and simulate curves that do not self-intersect, we must quantify self-contact for “thick” curves (see Definition 1). We start by reviewing the concept of global radius of curvature [19,20,31]. Then, we present a softened version of the global radius of curvature (i.e. the “proximity”) that is useful for numerics and optimization. Throughout the paper, we make the following assumption.

**Assumption 1.** Let  $\Sigma \subset \mathbb{R}^3$  be a smooth (open or closed) curve in  $\mathbb{R}^3$ , with length  $L$ , and parameterized by  $\alpha : [0, 1] \rightarrow \mathbb{R}^3$  (unless otherwise stated). Moreover, assume that  $\Sigma$  is *simple*, i.e. it has no self-intersections.

### 2.1. Global radius of curvature

#### 2.1.1. Circumradius

Let  $\mathcal{R}$  be the circumradius of three non-collinear points  $\mathbf{x}, \mathbf{y}, \mathbf{z}$  in  $\mathbb{R}^3$ :

$$\mathcal{R}(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \frac{|\mathbf{x} - \mathbf{y}||\mathbf{y} - \mathbf{z}||\mathbf{z} - \mathbf{x}|}{4\mathcal{A}(\mathbf{x}, \mathbf{y}, \mathbf{z})}, \quad (1)$$

where  $|\cdot|$  is the Euclidean norm and  $\mathcal{A}(\mathbf{x}, \mathbf{y}, \mathbf{z})$  is the area of a triangle with vertices  $\mathbf{x}, \mathbf{y}, \mathbf{z}$ . Thus,  $\mathcal{R}(\mathbf{x}, \mathbf{y}, \mathbf{z}) \geq 0$  and  $\mathcal{R}(\mathbf{x}, \mathbf{y}, \mathbf{z}) := \infty$  if  $\mathbf{x}, \mathbf{y}, \mathbf{z}$  are collinear. Any three non-collinear points define a unique circumcircle and a unique circumsphere that contains the circumcircle as a great circle.

If  $\Sigma$  is a simple smooth curve, then the domain of  $\mathcal{R}$  can be extended to any triple of points on  $\Sigma$  by continuous limits. Suppose that  $\mathbf{x} = \alpha(s)$ ,  $\mathbf{y} = \alpha(t)$ ,  $\mathbf{z} = \alpha(u)$  are three distinct points on  $\Sigma$ . Then one can show that [19]

$$\mathcal{R}(\mathbf{x}, \mathbf{y}, \mathbf{y}) := \lim_{u \rightarrow t} \mathcal{R}(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \frac{|\mathbf{x} - \mathbf{y}|}{2|\sin \theta_{\mathbf{xy}}|}, \quad (2)$$

where  $\theta_{\mathbf{xy}}$  is the angle between the vector  $\mathbf{x} - \mathbf{y} \neq \mathbf{0}$  and the tangent vector  $\boldsymbol{\tau}(\mathbf{y})$  to  $\Sigma$  at  $\mathbf{y}$ . Thus, the limit circumcircle is tangent to  $\Sigma$  at  $\mathbf{y}$  and passes through  $\mathbf{x}$ . We also have that

$$\mathcal{R}(\mathbf{x}, \mathbf{x}, \mathbf{x}) := \lim_{t, u \rightarrow s} \mathcal{R}(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \rho(\mathbf{x}), \quad (3)$$

where  $\rho(\mathbf{x})$  is the standard local radius of curvature of  $\Sigma$  at  $\mathbf{x}$ , i.e. the limit circumcircle is the *osculating* circle of  $\Sigma$  at  $\mathbf{x}$ .

For any curve  $\Sigma$ , we define the *global radius of curvature*  $\rho_G(\mathbf{x})$  at each point  $\mathbf{x}$  in  $\Sigma$  by [19,20]

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