

## Application to DNA Topology



Motivation from Biology: Molecular interactions involving DNA can be modeled using knot theory.

Figure 1: Protein DNA complex (AFM).

Vetcher, Alexandre A., et al. "DNA topology and geometry in Flp and Cre recombination." Journal of molecular biology 357.4 (2006).

### Solution from Mathematics:

These interactions describe a system of tangle equations modeling entwined strings of DNA.





Figure 2: Example of a system of tangle equations with solution.

A **tangle** consists of multiple entwined strings embedded inside of a ball. They are best interpreted as the building blocks of knots.

### **Database of 2-String Tangles**

Prototype database of tangles is accessible at http://www.nick-connolly.com/tangles.



Figure 3: Table of 5 crossing tangles, excluding mirror images. Blue denotes integer, red for rational, and green for generalized Montesinos.

# A Database of Tangles: Knot Theoretic Models for DNA Topology

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**Figure 4:** Operations of tangle sum (horizontal join) and tangle product (vertical join). Rational tangles are built using sums and products of integer tangles, described by a twist vector  $(n_1, \cdots, n_k)$ .

Simple tangles can be stacked together like blocks to build more complicated diagrams (Figure 4). Rational tangles, described by a twist vector  $(n_1, \dots, n_k)$ , are in bijection with  $\mathbb{Q} \cup \{\infty\}$  via the continued fraction

$$n_k + \frac{1}{n_{k-1} + \dots + \frac{1}{n_1}} = \frac{p}{q}$$

Tangles are divided into families based on their structure.

### **Special Types of Tangles**



**Figure 5:** Examples of tangle families by increasing generalizability.

- An **integer** tangle is a horizontal sequence of twists.
- A **rational** tangle is constructed from a sequence of alternately horizontal and vertical twists  $(n_1, \cdots, n_k)$ .
- A **Montesinos** tangle is a sum of rational tangles.
- An **algebraic** tangle is constructed from any combination of sums and products of rational tangles.

 $\{\text{Integer}\} \subseteq \{\text{Rational}\} \subseteq \{\text{Montesinos}\} \subseteq \{\text{Algebraic}\}$ 

• Otherwise, a tangle is **non-algebraic**.

Rational tangle (5, 4, 3, 2, 1)



## Subtangle Decompositions

Subtangle Planar Diagram Code Non-Algebraic Diagram Decomposition W 4 SE (P:0')W 5 NE (P:0)2 SE (P:0)V 5 SW (P:1')E 4 SW (P:1)Constellation Notation  $, \left(\frac{1}{3}\right), \left(\frac{3}{7}\right)$ 

(2/3)	0	NW	2	NW	5	N
(3/2) * (2/1)	1	NE	0	NE	3	SV
(4/1)	0	SE	4	NW	5	SE
(1/3)	3	NE	0	SW	1	SV
(3/7)	1	SE	2	SW	3	SE

$$C_{5+1}\left(\left(\frac{2}{3}\right),\left(\frac{3}{2}*\frac{2}{1}\right),\left(\frac{4}{1}\right)\right)$$

Figure 6: Example of a subtangle decomposition for a non-algebraic diagram and corresponding notations. This configuration of subtangles matches the first constellation graph of Figure 7.

### Constellations

A k+1 constellation (C, p) consists of a graph C with k vertices and a special marked  $k + 1^{st}$  vertex such that C is <u>connected</u>, planar, <u>4-valent</u>, and contains no bigons.







Non-algebraic tangles can be decomposed into algebraic subtangles (Figure 6). This decomposition is described by a subtangle planar diagram notation encoding the adjacency list of a graph. Non-algebraic subtangle graphs have special properties and are known as constellations.

Figure 7: The first 10 constellation graphs for constructing nonalgebraic diagrams. With sums and products, these can be used to describe all non-algebraic tangle diagrams with at most 9 crossings.