Algebraic Systems for DNA Origami Motivated From Temperley-Lieb Algebras

UNIVERSITY OF SOUTH FLORIDA

James Garrett, Nataša Jonoska, Hwee Kim, Masahico Saito

4202 E. Fowler Ave Tampa, Fl 33620, USA

Introduction

The technique of DNA origami, pioneered by Rothemund in 2006, efficiently creates complex shapes and structures at nanolevel [3]. DNA origami uses a long, folded single-strand DNA, called a *scaffold* strand, and hundreds of short *staple* strands that connect to the scaffold, allowing it to fold into desired shapes. One way to systematically characterize DNA origami structures is to describe them abstractly, in particular, algebraically.

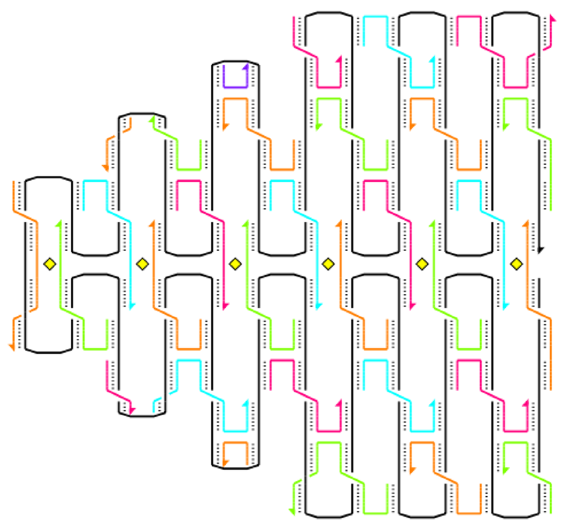


Figure 1: The original DNA diagram. Scaffold in black and staples in color [3].

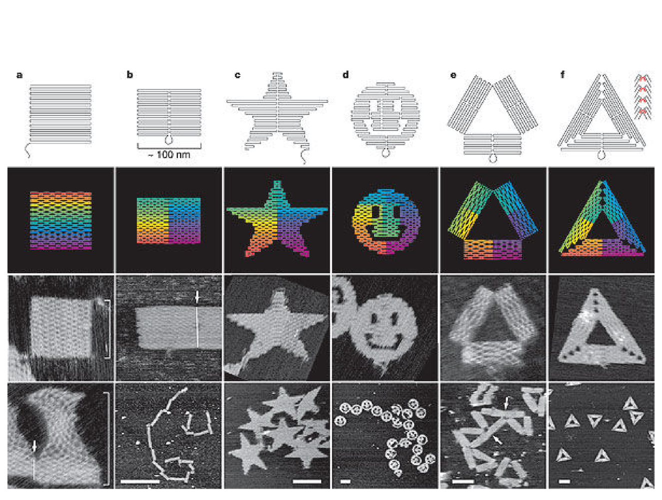


Figure 2: Examples of complex nanostructures by DNA origami [3].

Generators for an Origami Monoid

We identify two basic building blocks from the DNA origami in Figure 1, which we call α and β, pictured below. These simplest patterns are used as generators for a monoid associated to DNA origami.

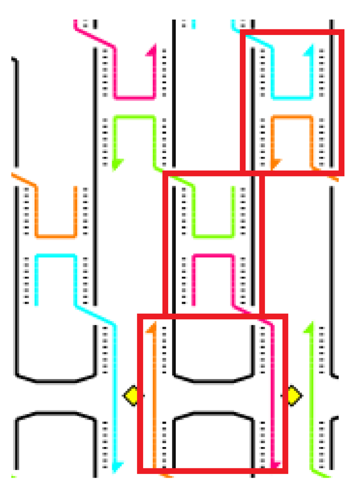
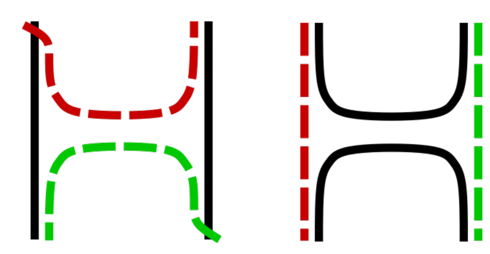


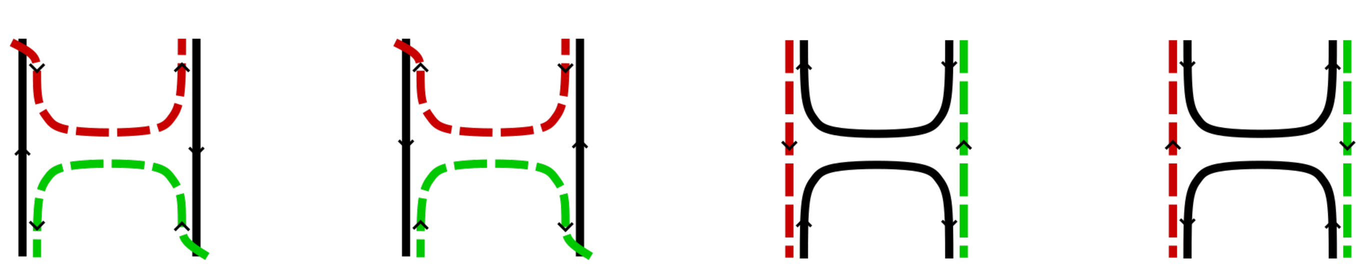
Figure 3: Two instances of α and one of β identified in the original diagram



(a) α (b) β

Figure 4: The two identified building blocks

Let n be the number of parallel scaffold strands. Define generators α_i and β_i, for $i = 1, \ldots, n-1$, where i represents the position of the left scaffold. For each generator, scaffold strands to the left of i and to the right of $i+1$ are empty, as shown in Figure 6. For brevity, these excess strands are omitted in other diagrams. The direction of the scaffold and staples are as in Figure 5.



(a) α_i, i odd (b) α_i, i even (c) β_i, i odd (d) β_i, i even

Figure 5: The generators with direction included

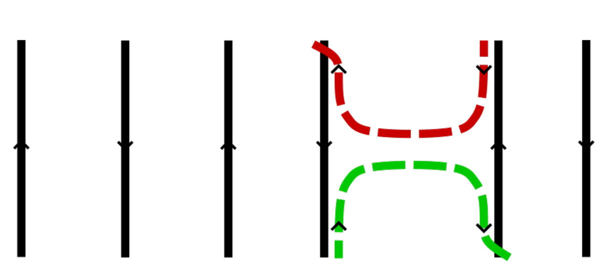


Figure 6: An example of α_4 in the monoid when $n = 6$

Temperley-Lieb Algebra

We observe that our identified generators are similar in structure to generators of the Temperley-Lieb algebra, reviewed below [1]. We borrow concepts from its rewriting rules and apply them to the origami monoid.
The generators of Temperley-Lieb algebra are represented in Figure 7.

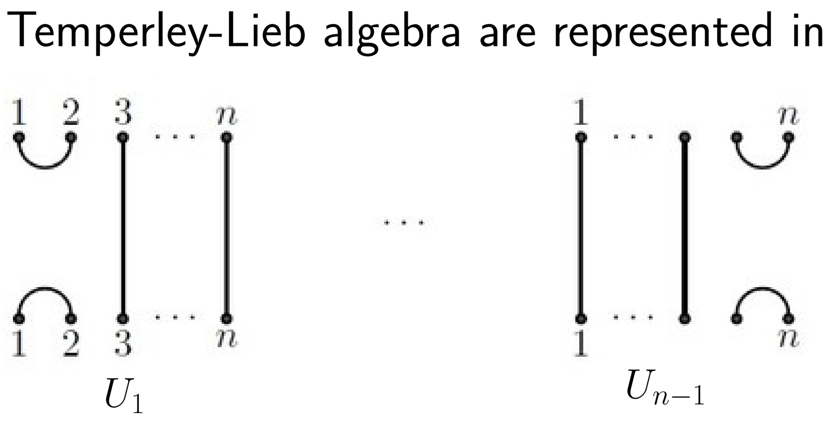
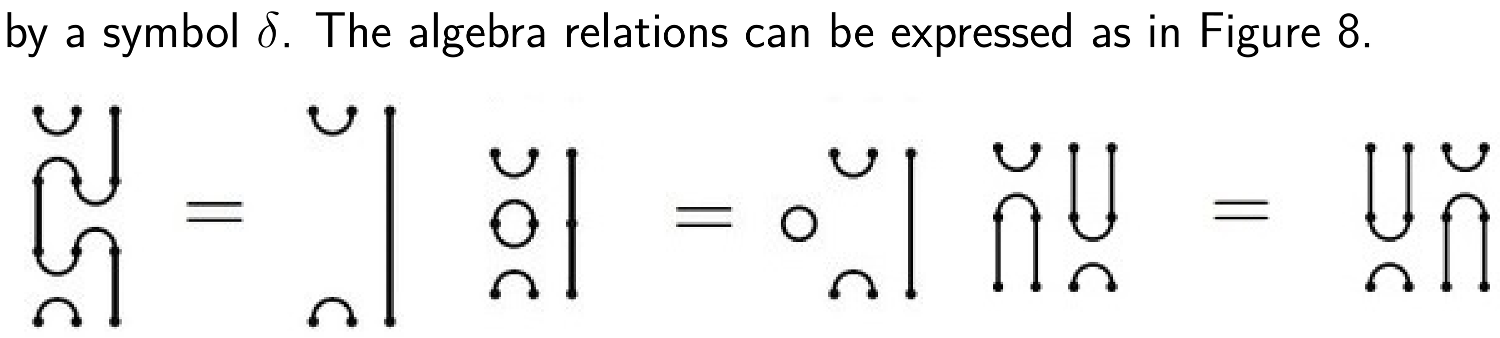


Figure 7: The generators of Temperley-Lieb algebra [1]

Multiplication is defined by vertical concatenation, and replacing closed loops by a symbol δ. The algebra relations can be expressed as in Figure 8.

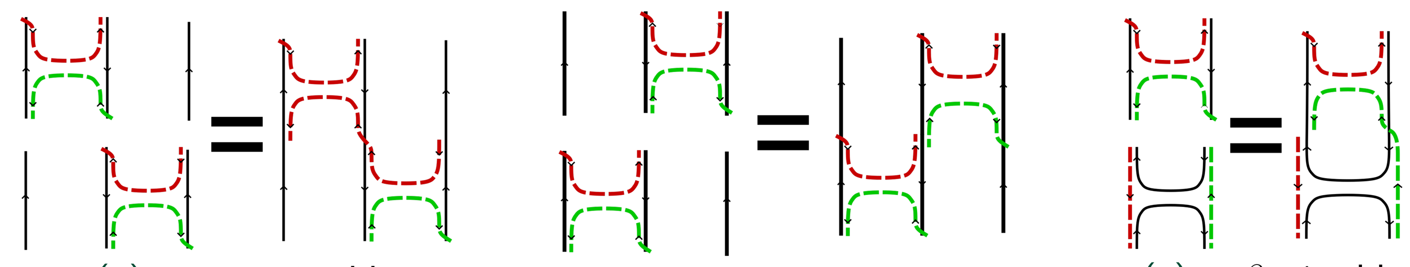


$U_1U_2U_1 = U_1$ $U_1^2 = \delta U_1$ $U_1U_3 = U_3U_1$

Figure 8: The relations of Temperley-Lieb algebra

Building Larger Structures

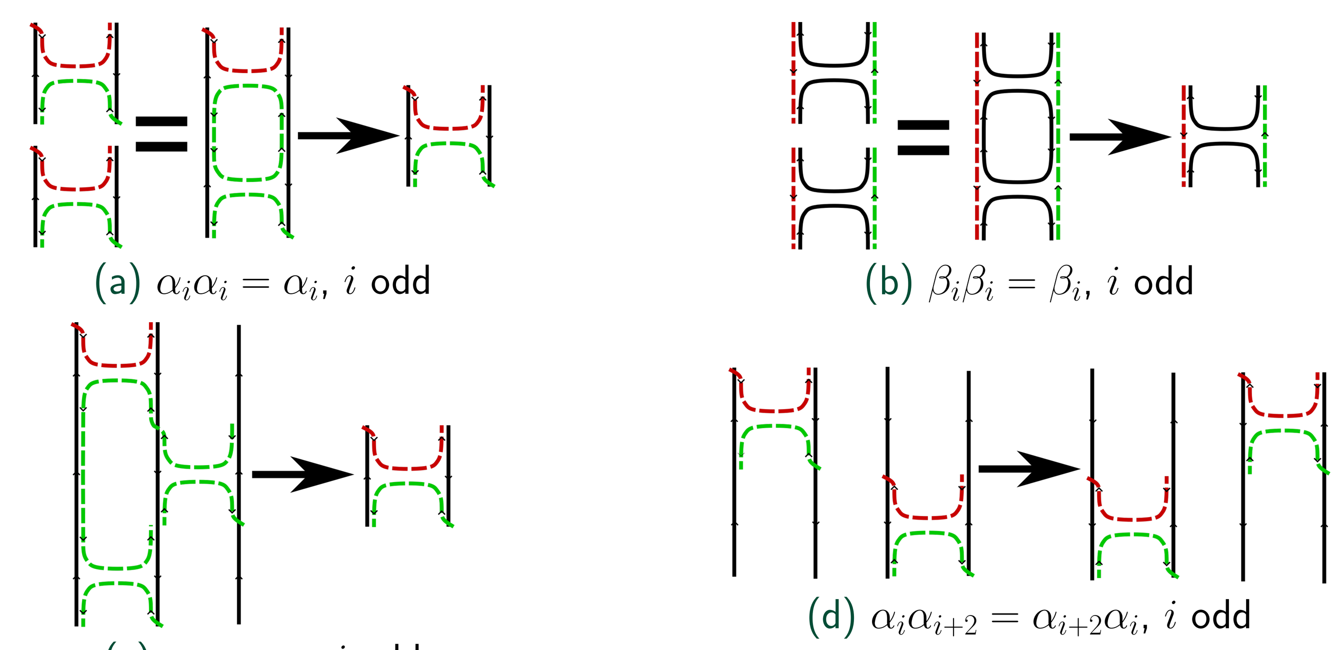
We define the product of two origami monoid generators by vertical concatenation, connecting respective scaffold strings of each generator. We also connect the staples of adjacent generators according to rules defined in Figure 9, which are based on the connection of staples observed in Figure 1.



(a) $\alpha_i\alpha_{i+1}$, i odd (b) $\alpha_i\alpha_{i-1}$, i odd (c) $\alpha_i\beta_i$, i odd

Figure 9: The staple-ends connect in (a) but not (b), and only one side in (c)

Rewriting Rules Arising From Monoid Structures



(a) $\alpha_i\alpha_i = \alpha_i$, i odd (b) $\beta_i\beta_i = \beta_i$, i odd (c) $\alpha_i\alpha_{i+1}\alpha_i$, i odd (d) $\alpha_i\alpha_{i+2} = \alpha_{i+2}\alpha_i$, i odd

Figure 10: Diagrams for some rewriting rules

For each n, the origami monoid, $\mathcal{O}_n$, is defined to be generated by α_i's and β_i's for i from 1 to $n-1$, satisfying the following set of rewriting relations. Let $\gamma \in \{\alpha, \beta\}$ and $i = 1, \ldots, n-1$. Define bar by $\overline{\alpha_i} = \beta_i$ and $\overline{\beta_i} = \alpha_i$. Then we have:

(1) $\gamma_i\gamma_i \to \gamma_i$
(2) $\gamma_i\gamma_{i+1}\gamma_i \to \gamma_i$
(3) $\gamma_i\gamma_{i-1}\gamma_i \to \gamma_i$
(4) $\gamma_i\overline{\gamma_j} \to \overline{\gamma_j}\gamma_i$, for $|i-j| \geq 1$
(5) $\gamma_i\gamma_j \to \gamma_j\gamma_i$, for $|i-j| \geq 2$

We also consider the rewriting rules obtained by substituting words of a singular index for γ in rewriting rules (1), (2), and (3).
For example, we have $\alpha_i\beta_i\alpha_i\beta_i \to \alpha_i\beta_i$ and $\beta_i\alpha_i\beta_{i+1}\alpha_{i+1}\beta_i\alpha_i \to \beta_i\alpha_i$.
Some examples of rewriting rules are shown in Figure 10, 11 and 12.

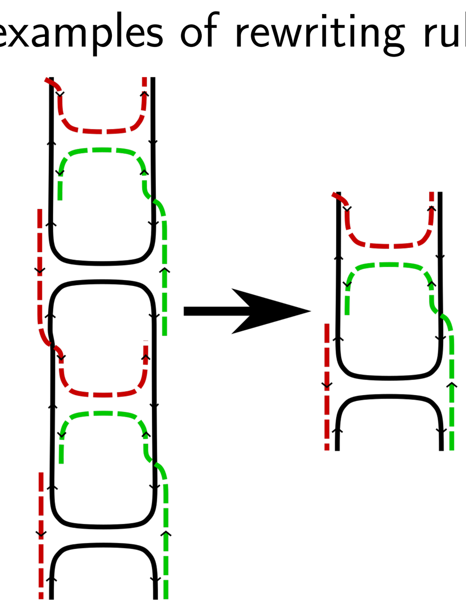


Figure 11: $\alpha_i\beta_i\alpha_i\beta_i \to \alpha_i\beta_i$, i odd

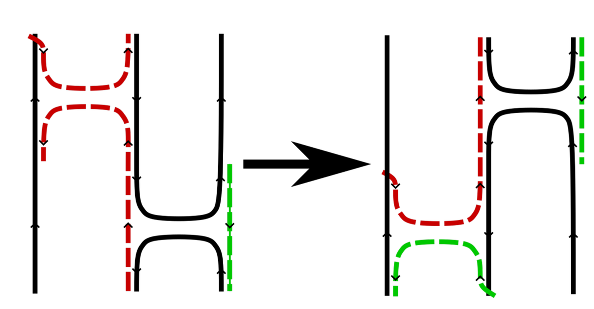


Figure 12: $\alpha_i\beta_{i+1} \to \beta_{i+1}\alpha_i$, i odd

Results

With software for algebraic computation, GAP, we solve the word problem for $n \leq 6$ and list all elements of the origami monoid, $\mathcal{O}_n$ [4]. For $2 \leq n \leq 6$ we found $\mathcal{O}_n$ to be finite, and the number of elements are 6, 44, 293, 2179, and 19086, respectively, representing distinct rectangular DNA origami structures. This computation also provided an internal structure of the ideals within the monoid.

Algebraic descriptions of higher-ordered structures in 3D, such as those depicted in Figure 13 are of future interest.

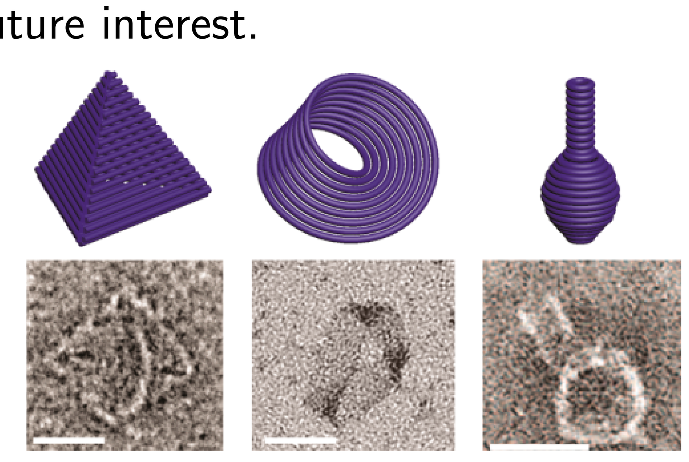


Figure 13: 3D structures can also be constructed using DNA origami techniques [2]

[1] Abramsky, S. *Temperley-Lieb algebra: from knot theory to logic and computation via quantum mechanics.* arXiv:0910.2737 (2009).

[2] Hong, F.; Zhang, F.; Liu, Y.; Yan, Y. *DNA Origami: Scaffolds for Creating Higher Order Structures.* Chem. Rev. 117, 20, 12584-12640 (2017).

[3] Rothemund, P. W. *Folding DNA to Create Nanoscale Shapes and Patterns.* Nature, 440. 297-302 (2006).

[4] The GAP Group, *GAP – Groups, Algorithms, and Programming, Version 4.9.3*; 2018, (www.gap-system.org).