Coloring Invariant for Topological Circuits in Folded Linear Chains

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Abstract: Circuit topology is a mathematical approach that categorizes the arrangement of contacts within a folded linear chain, such as a protein molecule or the genome. Theses linear biomolecular chains often fold into complex 3D architectures with critical entanglements and local or global structural symmetries stabilised by formation of intrachain contacts. Here, we adapt and apply the algebraic structure of quandles to classify and distinguish chain topologies within the framework of circuit topology. We systematically study the basic circuit topology motifs and define quandle/bondle coloring for them. Next, we explore the implications of circuit topology operations that enable building complex topologies from basic motifs for the quandle coloring approach.

Keywords: circuit topology; folded linear chains; quandle; bondle; coloring invariant

1. Introduction

Folded linear molecular chains typically fold via formation of intra-chain bonds that fix chain entanglement; examples include base–base interactions in nucleic acids and residue–residue interactions in proteins [1–3]. During the folding process, interactions form progressively until the chain reaches its final topology. Formation of an interaction may facilitate or hinder formation of subsequent interactions depending on the topological relations between them. Functionally critical entanglements and local or global structural symmetries are then stabilised by the formation of intrachain contacts. Motivated by the physics of folding, circuit topology has been developed to categorize the arrangement of intra-chain interactions (so-called contacts) and chain crossings in a folded linear chain [4]. While being mathematically rigorous, the topological picture is intuitive and simple and provides quantitative measures that can be readily used to relate topology to other properties of folded chain systems [5]. A growing number of studies have recently been conducted in which implications of circuit topology for folding and unfolding dynamics of polymer chains have been investigated [5].

The relation between circuit topology and the well-established knot theory is being studied [6]. While circuit topology complements knot theory by addressing interactions, tools developed by knot theorists might prove useful in strengthening circuit topology. Various coloring schemes have been developed by knot theorists that might be extended to classify topological circuits. Recently, a quandle coloring approach has been developed for protein analysis, which can in principle be adapted to resolve the space of possible circuit topologies [7,8]. The aim of this article is to use algebraic structures of quandles to study circuit topology. Using knot theory tools, we construct an invariant which we use to classify and distinguish chain topologies within the framework of circuit topology. The article is organized as follows. In Section 2, we review the basics of circuit topology. Section 3 reviews the basics of quandles, singquandle, and bondles with examples. In
Section 4, we define an invariant of circuit topology. This invariant is then used to tell when two circuit topologies are not topologically equivalent. In Section 5, we apply the bondle counting invariant to generalized circuit topologies. Section 6 explores the implications of circuit topology operations that enable building complex topologies from basic motifs for the quandle coloring approach.

2. Review of Circuit Topology

Let us consider a linear polymer made of \( n \) monomers. The simplest folded chain is a chain which has one contact \( C_{ij} \) that connects distinct monomers \( i \) and \( j \), \( (j > i) \) and forms a loop which corresponds to the interval \([i, j]\). Monomers \( i \) and \( j \) are then considered contact sites associated with contact \( C_{ij} \). Similarly, a folded polymer can be formed with \( m \) contacts from \( 2m \) contact sites. Any two contacts \( C_{ij} \) and \( C_{rs} \), will then be in one of the below circuit topology relations:

- **Series:** \( C_{ij}SC_{rs} ⇔ [i, j] ∩ [r, s] ⊂ \{i, j, r, s\} \)
- **Parallel:** \( C_{ij}PC_{rs} ⇔ [i, j] ⊂ [r, s] \)
- **Cross:** \( C_{ij}XC_{rs} ⇔ [i, j] ∩ [r, s] \notin \{\{i, j\}, [r, s]\} ∪ \mathcal{P}(\{i, j, r, s\}) \).

Mathematically, it means that two intervals, \( i \) to \( j \) and \( r \) to \( s \), are either not overlapping or partly overlapping, or one is entirely inside of another, where \( \mathcal{P} \) denotes the power set i.e., all subsets of a set including the null set \( \emptyset \). Note that the P (parallel) relation is not symmetric and thus gives rise to a hierarchy of contacts. The definition of P relation can however be adjusted to ensure symmetry if needed.

Contacts as defined above “glue” two chain segments together and thus restrict their physical motion. Two chain segments may also be “softly glued” by entanglement leading to their limited physical mobility. Circuit topology relations can be extended to categorize pairwise relation of these so-called “soft contacts” or s-contacts (in contrast to contacts defined above which are “hard”, thus termed h-contacts). A simple loop made of one twist of a polymer chain, is not stable, and opens up by thermal fluctuations. However, if a polymer chain is threaded through a loop, the resulting structure gain significant stability. A loop can be threaded in only two directions, either up or down (see Figure 1), which lead to thumb knot or figure eight knot, correspondingly. These two knots are s-contacts, the simplest, most basic entangled units in circuit topology.

![Figure 1. Thumb knot (top); and figure eight knot (bottom). These configurations are termed as s-contacts in the language of circuit topology.](image)

In circuit topology, s-contacts are not defined as 2D projections and should be viewed as 3D structures (despite the illustrations in the figure above, which are inevitably 2D). Similar to h-contacts, a pair of s-contacts can be arranged in parallel, series, and cross arrangements. One can use this bottom-up construction approach to generate diverse...
knots. Three and more s-contacts can be considered as a system of pairs of s-contacts. It can be shown that the relation between two s-contacts is not affected by other s-contacts. Interestingly, one can define contact sites for a s-contact, in analogy with contact sites of a h-contact [6]. Contact sites can then be labeled (e.g., letters) and the labels can be used to code circuit topology by string of labels, ordered as they appear when one walks along the polymer chain. We define a circuit as a segment of a string that consists only of pairs of labels (or letters) (for further information, please see [6]).

3. Overview of Quandles, Singquandle, and Bondles

In this section, we review the basics of quandles, singquandles, and bondles and give some examples. We advice the reader to consult [7,9,10] for more on the diagrammatic leading to the definitions of a quandle, a singquandle and a bondle.

**Definition 1.** A quandle is a set $X$ with two binary operations $\ast, \ast^{-1} : X \times X \to X$ such that the following three conditions are satisfied.

1. For all $x \in X$, $x \ast x = x$.
2. For all $x, y \in X$, $(x \ast y) \ast^{-1} y = x = (x \ast^{-1} y) \ast y$.
3. For all $x, y, z \in X$, $(x \ast y) \ast z = (x \ast z) \ast (y \ast z)$.

Here are a few typical examples of quandles:

- Any set $X$ with $x \ast y = x = x \ast^{-1} y$ is a quandle (called trivial quandle).
- The set $\mathbb{Z}_n$ of integers modulo $n$ with operation $x \ast y = -x + 2y = x \ast^{-1} y$ is a quandle.
- Any group $G$ with $x \ast y = yxy^{-1}$ and $x \ast^{-1} y = y^{-1}xy$ is a quandle.

Quandles were introduced independently in the 1980s by Joyce and Matveev [11,12] and have been used extensively to construct invariants of knots in the 3-space and knotted surfaces in 4-space (see [10] for more details). Now, we give the definition of an oriented singquandle, which leads us to the notion of a bondle below.

**Definition 2.** Let $(X, \ast)$ be a quandle. Let $R_1$ and $R_2$ be two maps from $X \times X$ to $X$. The quadruple $(X, \ast, R_1, R_2)$ is called an oriented singquandle if the following axioms are satisfied for all $a, b, c \in X$:

\[
\begin{align*}
R_1(a \ast^{-1} b, c) \ast b &= R_1(a, c \ast b), \\
R_2(a \ast^{-1} b, c) &= R_2(a, c \ast b) \ast^{-1} b, \\
(b \ast^{-1} R_1(a, c)) \ast a &= (b \ast R_2(a, c)) \ast^{-1} c, \\
R_2(a, b) &= R_1(b, a \ast b), \\
R_1(a, b) \ast R_2(a, b) &= R_2(b, a \ast b).
\end{align*}
\]

The following family of singquandles constructed over the set $\mathbb{Z}_n$, of integers modulo $n$, was given by [13] which we use below.

**Example 1.** Let $n$ be a positive integer, let $a$ be an invertible element in $\mathbb{Z}_n$, and let $\beta, \gamma \in \mathbb{Z}_n$. Then, the binary operations $x \ast y = ax + (1 - a)y$, $R_1(x, y) = \beta x + \gamma y$, and $R_2(x, y) = \alpha \gamma x + (\beta + \gamma - \alpha \gamma)y$ make the quadruple $(\mathbb{Z}_n, \ast, R_1, R_2)$ into an oriented singquandle.

Oriented singquandles have been used to construct invariants of singular knots and links (see, e.g., [9,13–15] for more details). Now, we have all the necessary ingredients to give the definition of an oriented bondle which was introduced by [7].
Definition 3. An oriented bondle is a quandle with operation * and choices for functions $R_1(x, y)$, $R_2(x, y)$, and $R_3(x, y)$ such that they satisfy conditions 1–5 of Definition 2 and the additional conditions:

$$R_3(y, x \ast^{-1} z) = R_3(y \ast z, x) \ast^{-1} z,$$

$$R_3(x, y \ast z) = R_3(x \ast^{-1} z, y) \ast z,$$

$$(z \ast^{-1} R_3(x, y)) \ast x = (z \ast^{-1} y) \ast R_3(y, x),$$

$$R_3(x, y) \ast^{-1} y = R_3(x \ast^{-1} R_3(y, x), y).$$

Definition 4. A coloring of a circuit topology $X$ is a function $f : R \rightarrow B$, where $B$ is a fixed oriented bondle and $R$ is the set of semiarcs in a fixed circuit topology $X$, satisfying the conditions in Figure 2.

The following family of oriented bondles was given by [7].

Example 2. Let $n$ be a positive odd integer greater than or equal to 3 and let $a$ be an invertible element of $\mathbb{Z}_n$. Consider the quandle $(\mathbb{Z}_n, \ast)$ with $x \ast y = ax + (1 - a)y$ and inverse operation $x \ast^{-1} y = a^{-1}x + (1 - a^{-1})y$. Let $m$ be an element in $\mathbb{Z}_n$ and let $R_3$ be given by $R_3(x, y) = mx + (1 - m)y$. Then, the map $R_3$ satisfies Equations 6–9 if and only if $m(m - 1) = 0 \in \mathbb{Z}_n$.

We use this example later for some specific values of $n$ and $m$ when we discuss the bondle counting invariant of a circuit topology $X$ by a bondle $B$. Bondles were introduced by [7] and used to distinguish the topological types of proteins. Furthermore, an enhancement of the coloring invariants of folded molecular chains by bondles was introduced and investigated by [8], who used Boltzmann weights to construct a state-sum invariant of folded molecular chains.

4. Coloring Invariant for Circuit Topology

In this section, we define an invariant of circuit topology. Given two circuit topologies and a choice of bondle, we can count the number of distinct colorings of each circuit topology by the chosen bondle, and, if those numbers are distinct, we know the two circuit topologies are not topologically equivalent.

We must first define the set of colorings of a circuit topology $X$ by a fixed bondle $B$. 

![Figure 2. Coloring rule at a positive crossing and negative crossing (top); parallel bond (bottom left); and anti-parallel bond (bottom right).](image-url)
Definition 5. The set of colorings of a circuit topology $X$ by a bondle $B$ is the set denoted by $Col_B(X)$.

From the set of colorings of a circuit topology $X$ by a bondle $B$, we can define the following computable invariant.

Definition 6. Let $X$ be a circuit topology and $B$ by a bondle. Then, the bondle counting invariant of the circuit topology $X$ by bondle $B$ is defined by

$$\Phi_B(X) = |Col_B(X)|.$$ 

This invariant counts the number of possible colorings of a circuit topology by a fixed bondle. We now use the bondle counting invariant to distinguish the arrangement of two intra-chain contacts (h-contacts) of the following types: parallel, series, and cross. We follow the rules in Figure 2 at crossings and bonds. Let $(B, *, R_1, R_2, R_3)$ be an oriented bondle. We first consider two intra-chain contacts arranged in parallel. We denote this arrangement by $P$ (see Figure 3).

$$z = R_3(R_3(x, y), z), \quad y = R_3(z, R_3(x, y)).$$

Figure 3. The diagram $P$ of a parallel arrangement of two h-contacts.

From this arrangement, we obtain the following coloring equations:

$$z = R_3(R_3(x, y), z), \quad y = R_3(z, R_3(x, y)).$$

Next, we consider the arrangement of two h-contacts in series. We denote this arrangement by $S$ (see Figure 4).

$$y = R_3(x, y), \quad z = R_3(R_3(x, y), z).$$

Figure 4. The diagram $S$ of a series arrangement of two h-contacts.

From $S$, we obtain the following coloring equations:

$$y = R_3(x, y), \quad z = R_3(R_3(y, x), z).$$

Lastly, we consider the arrangement of two h-contacts in cross. We denote this arrangement by $X$ (see Figure 5).
This system of equations has 10 solutions. Therefore, \( \Phi \) compute the solutions of the coloring equations. Using this bondle, the coloring equations for in Figure 6. Again, using the same bondle structure, we can distinguish the arrangement to each other, whereby posing restrictions on the movement of the chain. as shown (the 10 solutions: solved in \( Z \) by \( x \) coloring equations. we use a specific bondle and compute the bondle counting invariant using the Figure 5. The diagram \( X \) of a cross arrangement of two h-contacts.

From \( X \), we obtain the following coloring equations:

\[
\begin{align*}
y &= R_3(R_3(x, y), z), \\
z &= R_3(y, x).
\end{align*}
\]

Now that we have extracted the coloring equations for each of the three arrangements, we use a specific bondle and compute the bondle counting invariant using the coloring equations.

Let \((B, *, R_1, R_2, R_3)\) be the oriented bondle with \( B = Z_{15} \) and operations defined by \( x * y = 4x + 12y = x + 3y \), \( R_1(x, y) = 10 + 14x + 12y \), \( R_2(x, y) = 10 + 3x + 8y \), \( R_3(x, y) = 10 + 10x + 10x^2 + 11y \). First, notice that we only need the map \( R_3 \) to compute the solutions of the coloring equations. Using this bondle, the coloring equations for the parallel arrangement become

\[
\begin{align*}
z &= R_3(R_3(x, y), z) = 10x^2 + 5x^3 + 10x^4 + 10xy + 10x^2y + 10y^2 + 11z, \\
y &= R_3(z, R_3(x, y)) = 5x + 5x^2 + y + 10z + 10z^2.
\end{align*}
\]

Independent computations by Mathematica and Maple gave 750 solutions. Therefore, \( \Phi_B(P) = 750 \). The coloring equations obtained from the series arrangement become

\[
\begin{align*}
y &= R_3(x, y) = 10 + 10x + 10x^2 + 11y, \\
z &= R_3(R_3(y, x), z) = 10x^2 + 10xy + 10y^2 + 10xy^2 + 5y^3 + 10y^4 + 11z.
\end{align*}
\]

Independent computations by Mathematica and Maple gave 375 solutions. Therefore, \( \Phi_B(S) = 375 \). Lastly, the coloring equations for the cross arrangement become

\[
\begin{align*}
y &= R_3(R_3(x, y), z) = 10x^2 + 5x^3 + 10x^4 + 10xy + 10x^2y + 10y^2 + 11z, \\
z &= R_3(y, x) = 10 + 11x + 10y + 10y^2.
\end{align*}
\]

Substituting the second equation in the first one gives the following equation to be solved in \( Z_{15} \):

\[
10 + 10x^2 + 11x + 9y + 10(10x^2 + 10x + 11y + 10)^2 + 5y^2 = 0.
\]

Computations by Mathematica and Maple independently gave 10 solutions. Since \( z \) is dependent of \( x \) and \( y \), we only give the possible values of the pairs \((x, y)\). We list the 10 solutions: \((0, 10), (2, 2), (3, 13), (5, 5), (6, 1), (8, 8), (9, 4), (11, 11), (12, 7), \) and \((14, 14)\). This system of equations has 10 solutions. Therefore, \( \Phi_B(X) = 10 \).

By computing the bondle counting invariant with the oriented bondle specified above, we can distinguish the above arrangements of two intra-chain contacts (h-contacts).

Furthermore, we can consider \( h-h \) interaction. An \( h-h \) interaction occurs when h-loops hook to each other, whereby posing restrictions on the movement of the chain. as shown in Figure 6. Again, using the same bondle structure, we can distinguish the arrangement
shown in Figure 6 from the \( h \)-contact circuit topologies. The coloring equations obtained from the \( h \)-interaction are listed below:

\[
\begin{align*}
y &= R_3(x, y) * R_3(z, u) = 10 + 12u + 10x + 10x^2 + 14y, \\
u &= R_3(z, u) * R_3(x, y) = 10 + 14u + 12y + 10z + 10z^2.
\end{align*}
\]

Using Mathematica and Maple independently, we obtained that this system of equations has 1125 solutions. Therefore, \( \Phi_B(hh) = 1125 \). If we consider the parallel arrangement of two \( h-h \) interactions we can distinguish this arrangement from the \( h-h \) interaction. Figure 7 presents the parallel arrangement of two \( h-h \) interactions.

![Figure 6. The diagram \( hh \) of an \( h-h \) interaction.](image)

![Figure 7. The diagram \( Phh \) of two \( h-h \) interactions arranged in \( P \).](image)

From the results in Figure 7, we obtain the following coloring equations:

\[
\begin{align*}
z &= R_3(R_3(y, x), z * R_3(x, y)) \\
    &= 10x^2 + 12y + 10xy + 10y^2 + 10xy^2 + 5y^3 + 10y^4 + 14z, \\
u &= R_3(z * R_3(x, y), R_3(y, x)) = x + 5y + 5y^2 + 10z + 10z^2, \\
y &= R_3(x, y) * z = 10 + 10x + 10x^2 + 14y + 12z, \\
v &= R_3(u, v) * R_3(v, w) = 10 + 10u + 10u^2 + 14v + 12w, \\
w &= R_3(R_3(v, u), w) * R_3(u, v) \\
    &= 10u^2 + 12v + 10uv + 10v^2 + 5v^3 + 10v^4 + 14w.
\end{align*}
\]

This system of equations has 375 solutions. Therefore, \( \Phi_B(Phh) = 375 \). Therefore, using this bondle structure, we can distinguish the \( h-h \) interaction from the parallel arrangement of two \( h-h \) interactions.

5. Extension to Soft Contacts

In this section, we apply the bondle counting invariant to generalized circuit topologies. We first compute the bondle counting invariant to distinguish an \( s \)-contact, \( s \)-contacts in series configuration, and \( s \)-contacts in cross configuration. We then select a different bondle to distinguish \( s \)-contacts in parallel from the other configurations. Let \((B, *, R_1, R_2, R_3)\) be the bondle \( B = \mathbb{Z}_{15} \) and with operations \( x * y = 2x - y, x *^{-1} y = 8x - 7y, R_1(x, y) = x, R_2(x, y) = y, \) and \( R_3(x, y) = 10x - 9y \). Now, consider the \( s \)-contact in Figure 8.
The s-contact has the following coloring equation by the given bondle:

\[ y = (x \ast y) \ast y = 3x + 13y. \]

This equation has 45 unique solutions. Therefore, \( \Phi_B(s) = 45 \). We now consider the arrangement of two s-contacts in series arrangement (see Figure 9).

This arrangement has the following coloring equations:

\[
\begin{align*}
  y &= (x \ast y) \ast y = 3x + 13y, \\
  z &= ((x \ast y) \ast x) \ast x = 5x + 11y, \\
  w &= (((z \ast y) \ast w) \ast (z \ast y)) = 13w + 12y + 6z.
\end{align*}
\]

Therefore, we have 135 solutions to this system of equations. Hence, \( \Phi_B(Ss) = 135 \). Next, we consider s-contacts in parallel arrangement (see Figure 10).

The arrangement has the following coloring equations:

\[
\begin{align*}
  y &= a \ast^{-1} w = 8a + 8w, \\
  z &= (x \ast y) \ast x = 3x + 13y, \\
  w &= (z \ast^{-1} w) \ast^{-1} z = 4w + 12z, \\
  a &= w \ast^{-1} z = 8w + 8z.
\end{align*}
\]

The system above has 135 solutions. Hence, \( \Phi_B(Ps) = 135 \). Note that the bondle counting invariant associated with our chosen bondle is unable to distinguish the s-contact in series and s-contact in parallel. We return to these two arrangement below in this section. Lastly, we consider two s-contacts in cross arrangement (see Figure 11).
Figure 10. The diagram $P_s$ of a parallel arrangement of two s-contacts.

Figure 11. The diagram $X_s$ of a cross arrangement of two s-contacts.

From this arrangement, we obtain the following coloring equations:

$$y = (x \ast y) \ast w = 14w + 4x + 13y,$$
$$z = (y \ast z) \ast a = 14a + 4y + 13z,$$
$$w = ((y \ast z) \ast a) \ast (x \ast y) = 13a + 13x + 9y + 11z,$$
$$a = (w \ast z) \ast (y \ast z) = 4w + 13y + 14z.$$

Therefore, this system has 15 solutions. Hence, $\Phi_B(X_s) = 15$.

6. Beyond s-Contacts and h-Contacts

In the previous sections we consider s-contacts and h-contacts separately. In this section, we explore the implications of circuit topology operations that enable building complex topologies from basic motifs for the quandle coloring approach. Let $(B, \ast, R_1, R_2, R_3)$ be the oriented bundle with $B = \mathbb{Z}_{15}$, $x \ast y = 2x - y$, $x^{-1} = 8x - 7y$, $R_1(x, y) = x$, $R_2(x, y) = y$, and $R_3(x, y) = 10x - 9y$. We first compute the bondle counting invariant for a s-contact with h-contacts in $P$ (see Figure 12 for an example).
Figure 12. The diagram $P_1$ of an s-contact with two h-contacts in $P$.

For this first arrangement, we obtain the following coloring equations:

\[
\begin{align*}
y &= R_3(x, y) = 10x - 9y, \\
v &= R_3(R_3(y, x), z) * u = 14u + 5y + 12z, \\
x &= R_3(z, R_3(y, x)) * (v * R_3(y, x)) = 13v + 3x + 10y + 5z, \\
z &= u * R_3(R_3(y, x), z) = 2u + 5y + 9z.
\end{align*}
\]

This system of equations has 225 solutions. Therefore, $\Phi_B(P_1) = 225$.

The arrangement of a s-contact with two h-contacts in $S$ (Figure 13) has the following coloring equations:

\[
\begin{align*}
y &= R_3(u, z) * v = 5u + 14v + 12z, \\
z &= v * R_3(u, z) = 5u + 2v + 9z, \\
u &= R_3(z, u) * x = 12u + 14x + 5z, \\
x &= R_3(y, x) * u = 14u + 12x + 5y.
\end{align*}
\]

This system has 75 solutions. Therefore, $\Phi_B(P_2) = 75$.

Figure 13. The diagram $P_2$ of an s-contact with two h-contacts in $S$. 
Lastly, if we consider the arrangement of a s-contact with two h-contacts in $X$ (see Figure 14), then this arrangement has the following coloring equations by bondle $(B, *, R_1, R_2, R_3)$ defined above:

$$
y = R_3(R_3(z, y * x), x * y) = 12x + 9y + 10z,$$
$$z = R_3(x * y, R_3(z, y * x)) * (R_3(y * x, z) * z) = 3x + 9y + 4z.
$$

This system has 15 solutions. Therefore, $\Phi_B(P_3) = 15$. From these results, we see that the bondle counting invariant can be used to distinguish these three arrangements of the s-contact with two h-contacts.

Figure 14. The diagram $P_3$ of an s-contact with two h-contacts in $X$.

7. Conclusions

We use and extend some tools of knot theory and extend them to study the topology of circuits. Precisely, we adapt and apply the algebraic structures quandles/bondles to study circuit topology. We define colorings and Boltzmann weights for them to systematically study the basic circuit topology motifs. Next, we explore the implications of circuit topology operations that enable building complex topologies from basic motifs for the quandle coloring approach. Thus, the extension of quandles to circuit topology allows differentiating between the topological structures that can appear. Although the bondle counting invariant seems to be a very effective invariant for distinguishing different circuit topologies, it could not distinguish the circuit topology of the s-contact in series and the s-contact in parallel. Since the set $Col_B(X)$ contains more information than just a cardinality, it seems likely that enhancements to the bondle counting invariant can be defined to extract more information from $Col_B(X)$.

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