Hierarchical Self-Assembly and Substitution Rules

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Hierarchical Self-Assembly and Substitution Rules

by

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A dissertation submitted in partial fulfillment
of the requirements for the degree of
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Dedication

To my wife Angela Hamilton.
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The process of developing and writing my dissertation did not go as expected, to say the least. While I have the impression that the same is true for several doctors, I cannot emphasize enough how important the support which I have received over the years has been to my academic growth and my mental health. I genuinely feel that I would not be where I am today without the following people and organizations.

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Abstract

A set of elementary building blocks undergoes self-assembly if local interactions govern how this set forms intricate structures. Self-assembly has been widely observed in nature, ranging from the field of crystallography to the study of viruses and multicellular organisms. A natural question is whether a model of self-assembly can capture the hierarchical growth seen in nature or in other fields of mathematics. In this work, we consider hierarchical growth in substitution rules; informally, a substitution rule describes the iterated process by which the polygons of a given set are individually enlarged and dissected. We develop the Polygonal Two-Handed Assembly Model (p-2HAM) where building blocks, or tiles, are polygons and growth occurs when tiles bind to one another via matching, complementary bonds on adjacent sides; the resulting assemblies can then be used to construct new, larger structures. The p-2HAM is based on a handful of well-studied models, notably the Two-Handed Assembly Model and the polygonal free-body Tile Assembly Model.

The primary focus of our work is to provide conditions which are either necessary or sufficient for the “bordered simulation” substitution rules. By this, we mean that a border made up of tiles is allowed to form around an assembly which then coordinates how the assembly interacts with other assemblies. In our main result, we provide a construction which gives a sufficient condition for bordered simulation. This condition is presented in graph theoretic terms and considers the adjacency of the polygons in the tilings associated to a given substitution rule. Alongside our results, we consider a collection of over one hundred substitution rules from various sources. We show that only the substitution rules in this collection which satisfy our sufficient condition admit bordered simulation. We conclude by considering open questions related to simulating substitution rules and to hierarchical growth in general.
Chapter 1
Introduction

Self-assembly generally describes a process regulated exclusively by local interactions wherein a set of elementary building blocks in a disordered state forms intricate structures [41]. Examples of self-assembly can be found everywhere in nature, especially when considering supramolecular chemistry and microbiological systems; see Figure 1.01. We say that a self-assembly process is *hierarchical* if highly intricate structures form only after smaller, intermediary structures have been constructed [10]. Hierarchical self-assembly has been observed within various microbiological settings [1, 4, 36] and has served as the design motivation for supramolecular experiments aimed at assembling complex structures given relatively few components [9, 29, 45, 50].

![Figure 1.01](image-url)  
**Figure 1.01.** Top: Visualization of a lipid molecule (leftmost) and soft membranes formed using this molecule. Bottom: Visualization of a protein molecule (leftmost) and rigid, crystal-like structures formed using this molecule [51]. See Appendix D for the copyright permission from Nature Communications regarding the use of this image.
1.1 Substitution Rules

Our motivation for studying hierarchical self-assembly is to determine the principles and underlying mechanisms associated with this kind of self-assembly. In particular, we wish to use or adapt a model of self-assembly to study the hierarchical growth associated with substitution rules. Informally, a substitution rule $R$ describes a method of “enlarging and dissecting” a given set of polygons called the prototiles of $R$ [12,19]. First, each prototile $X$ is dilated by a factor $\lambda > 1$, called the inflation factor of $R$. The resulting polygon, denoted $\lambda X$, is then “dissected” so that it becomes a set $T$ of polygons, each of which is congruent to a prototile of $R$. Then, this process can be repeated again on each of the polygons in $T$, and so on; see Figure 1.02. The set $T$ is called a tiling of $\lambda X$; we define tilings and substitution rules formally in Section 2.1. For now, we note that each set of polygons obtained by applying the above process $\ell$ times to a prototile $X$ is called a supertile (of order $\ell$).

![Figure 1.02. The Sphinx substitution rule $R$ [13] represented informally using the idea of “enlarging and dissecting” the leftmost polygon. This polygon is called a prototile of $R$; it is first enlarged (i.e., dilated) by a factor of 2. The resulting polygon is then “dissected” so that it becomes a set $T$ of polygons which are (elementwise) congruent to the prototile. We can repeat this process iteratively on each of the polygons in $T$, as shown on the right. See Appendix D for the copyright information of the Tiling Encyclopedia regarding the modification and use of this image.](image)
We focus on substitution rules in our work because we can infer a relatively simple form of hierarchical self-assembly from a given substitution rule $\mathcal{R}$. Indeed, we can consider the first iteration of “enlarging and dissecting” a prototile $X$ as assembling the polygon $\lambda X$ from a set of polygons. Because each of the polygons in this set is congruent to a prototile of $\mathcal{R}$, we can then use the idea above as a guide for assembling a supertile of order $\ell$ from isometric copies of the supertiles of order $\ell - 1$. See Figure 1.03 for a visual example of this concept. In Section 2.3, we formalize this concept by defining how a substitution rule is “simulated” within a specific model of self assembly which we discuss in the next section.

**Figure 1.03.** Visualization of the hierarchical exhibited by the Sphinx substitution rule $\mathcal{R}$ (Figure 1.02). Top: First, we consider the supertile of order 1 (right) as having been assembled from four polygons (left), each of which is congruent to the prototile of $\mathcal{R}$. Bottom: Using the idea of assembly above, we can then consider the supertile of order 2 (right) as having been assembled from four isometric copies of supertiles of order 1 (left).

Before continuing with the next section, we note that there are several ways to generalize the idea presented above for substitution rules [12, 13]. Substitution rules have been extensively studied because they tend to yield aperiodic tilings of the Euclidean plane or exhibit interesting geometric and algebraic properties [12–14, 43]. For simplicity, we require that the prototiles of a substitution rule be polygons which are “enlarged and dissected” as described above. In an attempt to capture all known substitution rules adhering to our requirements, we consider a collection of over one hundred substitution rules from the following sources: [12–14, 18–20, 43]. We present a sample of these substitution rules within the following chapters;
1.2 Tile Assembly Models

In order to formalize the self-assembly process which we associated to substitution rules in the previous section, we turn to some well-studied models for self-assembly. In particular, we consider tile assembly models (TAMs) whose elementary building blocks (i.e. tiles) are polygons which have been defined with rules for local interaction. The first of these TAMs was formalized by Winfree in his thesis and is called the abstract Tile Assembly Model (aTAM) [47]. This model, and most subsequent TAMs, is based on Wang tiles and uses tiles which are unit squares [41,47]. The aTAM was originally designed to model DNA tile self-assembly; the survey [10] summarizes the relationship between this model and experimental work. We refer the reader to the surveys [41,48,49] for a better background into the TAMs which arose from the aTAM and the line of research considered within this field of algorithmic self-assembly.

For our own research, we consider the Two-Handed Assembly Model (2HAM) [41] and informally describe it in this paragraph. As in the aTAM, tiles in this model are unit squares and structures made from these tiles are called assemblies. The side of each tile is assigned a glue or bond which is an element of a finite set $\Sigma$; each bond $a \in \Sigma$ is in turn associated to a positive integer called the strength of $a$. Self-assembly occurs within this model in the context of a tile assembly system (TAS) $\Gamma = (T_0, \theta)$ where $T_0$ is a finite set of tiles and $\theta > 0$ is the temperature parameter of $\Gamma$. The tiles in $T_0$ are considered unit assemblies which are producible by $\Gamma$ at step 0. In general, an assembly $\alpha$ is producible by $\Gamma$ at step $n \geq 1$ if two assemblies $\beta_1$ and $\beta_2$, which are assemblies producible at steps $j_1, j_2 < n$, can be placed next to each other such that (i) $\alpha$ is the union of $\beta_1$ and $\beta_2$ and (ii) the sum of the strengths of the matching bonds between $\beta_1$ and $\beta_2$ is greater than or equal to $\theta$. In this way, the temperature $\theta$ of a TAS serves as a bonding threshold. We note that placing assemblies next to each other more formally means copying each assembly and then translating each copy to be adjacent to the other. There is no restriction on the copying process; that is to say, each assembly producible by $\Gamma$ can be copied infinitely many times. Refer to Figure 1.04 for a visual example of the informal descriptions above.

Though the 2HAM may seem to be a relatively simple model, this model and the aTAM are computationally universal [41,47]. These two models, and similar models based on them, have several computational results and structural results on efficient shape construction which inform our work [2,3,6,8,26,31,37,38,41,44,49]. Nonetheless, we must generalize the 2HAM to work with substi-
tion rules because tiles in the 2HAM are unit squares and the polygons associated to substitution rules are arbitrary. And while there are several TAMs whose tiles are not unit squares [11, 15, 22, 27, 33], we turn to the polygonal free-body Tile Assembly Model (pfbTAM) [5] as a basis for generalizing the 2HAM. The pfbTAM is closer to the aTAM in its self-assembly dynamics but does not place a restriction on the shapes of its tiles nor on the isometries which can be applied to them. The model which we develop for the 2HAM and the pfbTAM is called the Polygonal Two-Handed Assembly Model (p-2HAM), and we define it formally in Section 2.2.

![Figure 1.04. Top: An example of a set of tiles in the Two-Handed Assembly Model. Bottom: A visualization of some assemblies which are producible by a TAS $\Gamma = (T_0, \theta = 2)$ where $T_0$ is the given set of tiles. In this example, bonds are represented visually by unique colors: red, blue, and yellow. The strength of each bond is represented by the number of colored notches depicted on the sides of each tile. Accordingly, the red and blue bonds have a strength of 2 and the yellow bond has a strength of 1. In the bottom left, we have two assemblies which form when two tiles bind together. Note that the strength of the matching bonds for these tiles is 2, as required by the temperature parameter $\theta$. Each of these two assemblies then binds to another tile, visualized in the bottom middle, by again using bonds whose strengths are greater than or equal to 2. On the bottom right, we then take the two assemblies from the middle and bind them together according to their matching yellow bonds. While the yellow bond only has a strength of 1, the fact that two of these bonds match allows us to meet the given temperature parameter $\theta$.](image)
We conclude this section by noting that there is some precedence for our consideration of hierarchical self-assembly in relation to the recursive nature of substitution rules. Specifically, [31] presents a simulation of the Chair substitution rule which captures the dynamics of this substitution rule in the same way that we described in Section 1.1. On the other hand, we note that the recursive formation of fractals within the context of tile self-assembly is similar to the aspect of hierarchical self-assembly which we aim to study. The existing work on fractals in the 2HAM and related models [16, 23–25, 35, 42] has provided a basis for our understanding of the hierarchical self-assembly of infinite structures and recursive assembly processes. Moreover, the constructions in [24,31] directly provide a basis for the construction associated with our main result (Section 4.2).

1.3 Overview of Results

In Chapter 2, we formalize all of the concepts presented thus far. Notably, we present two distinct notions of simulation associated to substitution rules: strict and bordered simulation. These notions are motivated by our attempt to capture the hierarchical self-assembly dynamics of substitution rules as described in Section 1.1. Bordered simulation is inspired by [24, 31] in particular.

In Chapter 3, we provide necessary conditions for the strict and bordered simulation of substitution rules. Among these conditions, we show that a p-2HAM tile assembly system with a temperature parameter of 1 cannot simulate any substitution rule. We also introduce the idea of describing the tilings of substitution rules in graph theoretic terms. We develop this idea into our main result in the next chapter. Lastly, we provide a small collection of necessary conditions for determining if a given substitution rule admits bordered simulation. These conditions are easy to check, and we give examples of substitution rules which fail to meet these conditions.

In Chapter 4, we develop the idea of “backtrack constructible graphs” from the necessary conditions in Chapter 3. After providing formal definitions and examples for this idea, we provide our main result: a sufficient condition for determining if a substitution rule admits bordered simulation. This condition is formalized in terms of the backtrack constructible graphs defined in Section 4.1, and the proofs that it is sufficient encompass all of Section 4.2.
As noted in Section 1.1, our discussion of tilings and substitution rules is restricted to polygons. To avoid confusion, we refrain from using the term “tile” when discussing tilings (Section 2.1) and use it exclusively in the context of tile assembly models (Section 2.2). Similarly, we use “corners” and “sides” instead of “vertices” and “edges”, respectively, when discussing polygons [20]. We borrow classic definitions related to graph theory from [46] and only consider simple graphs \( G = (V, E \subseteq (V)^2) \) in our definitions and results. Moreover, we use \( \text{dom} f \) to denote the domain of a given mapping \( f \).

We take \( \mathbb{Z}_{\geq 0} \) to be the set of non-negative integers and \( \mathbb{Z}^+ \) to be \( \mathbb{Z}_{\geq 0} \setminus \{0\} \). For \( n \in \mathbb{Z}^+ \), \( \mathbb{R}^n \) is the classic \( n \)-dimensional Euclidean space with a fixed origin; we focus on \( \mathbb{R}^2 \), and let \( \mathcal{G} \) denote the group of isometries on this space. We use standard definitions from topology and denote the boundary of a set \( S \subset \mathbb{R}^2 \) by \( \partial S \).

A set \( S \subset \mathbb{R}^2 \) is a (closed) topological disk [20] if it is homeomorphic to the set \( \{x \mid d(x, O) \leq 1\} \) where \( O \) is the origin of \( \mathbb{R}^2 \). Let \( S_1, S_2 \subset \mathbb{R}^2 \) be bounded sets; we say that \( S_1 \) is properly contained in \( S_2 \) if \( S_1 \subseteq S_2 \) and \( \partial S_1 \cap \partial S_2 = \emptyset \).

## 2.1 Tilings, Substitution Rules, and Graphs

Formally, a set \( P \subset \mathbb{R}^2 \) is a polygon if it is a topological disk whose boundary is the finite union of line segments, \( \{L_i\}_{i=1}^n \), such that for any \( i \neq j \), \( L_i \cap L_j \) contains at most one point which must be an endpoint of \( L_i \) and of \( L_j \). We call each \( L_i \) a side of \( P \) and call a point in \( L_i \cap L_j \) a corner of \( P \) if it exists. Two polygons \( P, P' \) are congruent, denoted \( P \cong P' \), if there exists an isometry \( I \in \mathcal{G} \) which bijectively maps the sides of \( P \) to those of \( P' \) (Figure 2.01). We use the requirement that the isometry \( I \) preserves sides in the context of self-assembly when discussing “equivalent tiles” (see Section 2.2). Note that our notion of congruence for polygons extends naturally to an equivalence relation on finite sets of polygons; we extend the use of \( \cong \) accordingly. For \( \kappa > 0 \), let \( \mu_\kappa \) denote the dilation centered at the origin with factor \( \kappa \). Given a polygon \( P \subset \mathbb{R}^2 \), we write \( \kappa P \) to mean the image \( \mu_\kappa(P) \). Observe that if \( L \) is a side of \( P \), then \( \mu_\kappa(L) \) is a
side of $\kappa P$; hence, there is a bijective correspondence between the sides of $P$ and the sides of $\kappa P$. We say that two polygons $P$ and $P'$ are similar if $P$ is isometric to $\kappa P'$ for some $\kappa > 0$; note that $P$ does not need to be congruent to $\kappa P'$ in order to be similar to $P'$. As with isometric equivalence and congruence, we can extend similarity naturally to an equivalence relation on finite sets of polygons.

![Figure 2.01](image)

**Figure 2.01.** Visual representation of a sample set of polygons. Note that while most of the polygons visualized here are congruent via isometry, the two L-shaped polygons on the left are isometric but not congruent. The top polygon has eight sides while the bottom one only has seven; these are labeled.

![Figure 2.02](image)

**Figure 2.02.** Three examples of finite tilings of sets in $\mathbb{R}^2$. Note that these tilings are generated from a subset of the polygons presented in Figure 2.01. We enumerate the polygons in the left and right tilings for later use.

We adapt some of the following definitions from [14, 19], modifying them to the context of polygons.
We use \( \{P_i\}_{i \geq 1} \) to denote a finite or countable set of polygons \( P_i \). We say that \( \{P_i\}_{i \geq 1} \) is a **packing** if the interiors of \( P_i \) and \( P_j \) are disjoint for any \( i \neq j \). Given a connected set \( S \subseteq \mathbb{R}^2 \), \( \{P_i\}_{i \geq 1} \) is a **covering** of \( S \) if \( \bigcup_{i \geq 1} P_i = S \). We call \( \{P_i\}_{i \geq 1} \) a **tiling** of \( S \) if it is packing and covering of \( S \); if \( \{P_i\}_{i \geq 1} \) is a finite set, then we say that it is a **finite tiling** of \( S \). Let \( \{Q_j\}_{j=1}^n \) be a finite set of polygons such that \( Q_{j_1} \not\approx Q_{j_2} \) for any \( j_1 \neq j_2 \). We say that \( \{P_i\}_{i \geq 1} \) is a tiling of \( S \) generated from \( \{Q_j\}_{j=1}^n \) if for each \( P \in \{P_i\}_{i \geq 1} \), there exists \( Q \in \{Q_j\}_{j=1}^n \) such that \( P \sim Q \). See Figure 2.02 for examples.

**Definition 2.1.1.** A **substitution rule** is a 3-tuple \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) where

- \( \mathcal{P} = \{X_i\}_{i=1}^m \) is a finite set of polygons, called **prototiles**, such that \( X_{i_1} \not\approx X_{i_2} \) for any pair \( i_1 \neq i_2 \),
- \( \lambda > 1 \) is called the **inflation factor**, and
- \( \mathcal{S} = \{T_i\}_{i=1}^m \) is a set where each \( T_i = \{Y_{i,j}\}_{j=1}^{k_i} \) is a finite tiling of \( \lambda X_i \) generated from \( \mathcal{P} \).

Let \( \lambda \mathcal{P} \) denote the set \( \{\lambda X_i\}_{i=1}^m \). For each \( 1 \leq i \leq n \) and each \( 1 \leq j \leq k_i \), write that \( Y_{i,j} = I_{i,j}(X_{i,j}) \) for some \( I_{i,j} \in \mathcal{G} \) and some \( X_{i,j} \in \mathcal{P} \). The **substitution associated with** \( \mathcal{R} \) is a map \( \sigma_{\mathcal{R}} : \mathcal{P} \rightarrow \lambda \mathcal{P} \) where \( \sigma_{\mathcal{R}}(X_i) = \lambda X_i = \bigcup_{j=1}^{k_i} Y_{i,j} \) and \( \sigma_{\mathcal{R}} \) has the following property: for each \( I_{i,j} \) and each \( \ell \in \mathbb{Z}^+ \), there exists an isometry \( I_{i,j}^{(\ell)} \in \mathcal{G} \) such that \( \lambda^\ell I_{i,j}(X_{i,j}) = I_{i,j}^{(\ell)}(\lambda^\ell X_{i,j}) \).

![Figure 2.03](image-url)

**Figure 2.03.** Diagrams for the (a) Chair and (b) Pinwheel substitution rules [13]. Note that the inflation factor for the Chair is 2 while the inflation factor for the Pinwheel substitution rule is \( \sqrt{5} \). We do not often write the inflation factor since it can be calculated from the prototiles and tilings of a substitution rule.

Substitutions \( \sigma_{\mathcal{R}} \) are typically denoted by \( \sigma \) when \( \mathcal{R} \) is unambiguous and are often implied by \( \mathcal{R} \) rather than being explicitly defined. We use diagrams like those in Figures 2.03–2.04 to formally present substitution rules because such diagrams provide all of the information associated with a given substitution rule in a concise manner; this approach is standard [12–14, 18–20, 43]. In accordance with the copyright license of the Tiling Encyclopedia [13], we indicate here that we have reproduced and modified substitution diagrams from the Encyclopedia throughout this work; please see Appendix D.
Given a substitution rule $R$, observe that we can apply $\sigma$ repeatedly to formalize the “enlarge and dissect” process described in Section 1.1. Indeed, we define $\sigma^\ell(X)$ recursively for $X \in \mathcal{P}$ and $\ell \in \mathbb{Z}^+$ as follows:

$$
\sigma^\ell(X) = \sigma^{\ell-1}(\sigma(X)) = \sigma^{\ell-1}\left(\bigcup_{j=1}^{k_i} Y_{i,j}\right) = \sigma^{\ell-1}\left(\bigcup_{j=1}^{k_i} I_{i,j}(X_{i,j})\right) = \bigcup_{j=1}^{k_i} I_{i,j}^{(\ell-1)}(\sigma^{\ell-1}(X_{i,j}))
$$

where $\sigma^0(X) = X$ for any prototile $X \in \mathcal{P}$ by convention. We call $\sigma^\ell(X)$ a supertile (of order $\ell$), and note that it is a tiling of $\lambda^\ell X$ generated from $\mathcal{P}$; see Figure 2.06 for examples of supertiles of the Pentiamond AC Factor 2 and T2000 substitution rules [13] from Figures 2.04 and 2.05.

![Figure 2.04. The Pentiamond AC Factor 2 substitution rule [13]. Note that this substitution rule has two prototiles and that the tilings associated with this substitution rule are generated from both prototiles.](image1)

![Figure 2.05. The T2000 substitution rule [13]. Note that one tiling of this substitution rule is a singleton. While this may occur numerous times in other substitution rules, observe that there must always be a tiling which is not a singleton because the inflation factor of a substitution rule is strictly greater than 1.](image2)

The remaining definitions are necessary for our discussions on self-assembly and simulation. Let $\{P_i\}_{i \geq 1}$ be a tiling of $S \subseteq \mathbb{R}^2$. We say that $P \neq P' \in \{P_i\}_{i \geq 1}$ are corner neighbors if $P \cap P' \neq \emptyset$ and side neighbors if they have at least one pair of overlapping sides; note that side neighbors are always corner neighbors. Now suppose that $\{P_i\}_{i=1}^n$ is a finite tiling of $S$, and note that $S$ must be bounded. A polygon $P \in \{P_i\}_{i=1}^n$ is a boundary polygon of $\{P_i\}_{i=1}^n$ if it has at least one side which is a subset of $\partial(\bigcup_{i=1}^n P_i)$; such sides are called boundary sides of $\{P_i\}_{i=1}^n$. Boundary corners of $\{P_i\}_{i=1}^n$ are defined likewise.
Figure 2.06. Examples of supertiles of (a) Pentiamond AC Factor 2 and (b) T2000. In (a), we have the supertile $\sigma^2(X_1)$ on the right and $\sigma^2(X_2)$ on the left. In (b), we have the supertile $\sigma^3(X_1)$ on the right and $\sigma^3(X_2)$ on the left. Because of how the T2000 substitution rule is defined, note that $\sigma^3(X_1) = \sigma^2(X_2)$ and $\sigma^3(X_2) = \sigma^4(X_1)$.

Figure 2.07. The adjacency graphs of the labeled tilings in Figure 2.02. As stated previously, given the corner adjacency graph $G(T) = (T, E)$ and the side adjacency graph $\overline{G}(T) = (T, \overline{E})$, we visualize the edges in $E$ with solid lines and the edges in $E \setminus \overline{E}$ with dashed lines.

Let $\{P_i\}_{i \geq 1}$ be a tiling of $S \subseteq \mathbb{R}^2$. The corner adjacency graph induced from $\{P_i\}_{i \geq 1}$ is a graph $G(\{P_i\}_{i \geq 1}) = (V, E)$ where $V = \{P_i\}_{i \geq 1}$ and $\{P, P'\} \in E$ if $P$ is a corner neighbor of $P'$ (i.e., $P \cap P' \neq \emptyset$). On the other hand, the side adjacency graph induced from $\{P_i\}_{i \geq 1}$ is a graph $\overline{G}(\{P_i\}_{i \geq 1}) = (\{P_i\}_{i \geq 1}, \overline{E})$ where $\{P, P'\} \in \overline{E}$ if $P$ is a side neighbor of $P'$ (i.e., $P$ and $P'$ have at least one pair of overlapping sides). Since $\overline{G}(\{P_i\}_{i \geq 1})$ is a spanning subgraph of $G(\{P_i\}_{i \geq 1})$, we often draw both graphs simultaneously using solid lines to visualize edges in $E$ and dashed lines to visualize edges in $E \setminus \overline{E}$; see
Figure 2.07 for examples. Note that the graph $\overline{G}(T)$ is always planar but the graph $G(T)$ may not be. Moreover, observe that if $T$ is topologically connected, then $G(T)$ is connected in the graph theoretic sense. In the context of the finite tilings $T \in S$ of a substitution rule $R = (P, \lambda, S)$, note that both $G(T)$ and $\overline{G}(T)$ are connected since $\bigcup T$ is a topological disk; Figure 2.08 for examples.

Figure 2.08. Top: The adjacency graphs of the tilings of the (a) Chair and (b) Pinwheel substitution rules. Bottom: The adjacency graphs of the two tilings of the (c) Pentiamond AC Factor 2 substitution rule.

2.2 The Polygonal Two-Handed Assembly Model (p-2HAM)

The definitions and notation in this section are based on related notions in [5, 30, 41]. Let $\Sigma^+$ be a finite set and define the complementary set $\Sigma^- = \{-a \mid a \in \Sigma^+\}$. Let $\nu \notin \Sigma^+ \cup \Sigma^-$ be an element called the empty bond. Then $\Sigma = \Sigma^+ \cup \Sigma^- \cup \{\nu\}$ is a set of bonds. For $a \in \Sigma^+$, we define that $-(a) = a$ and refer to the pair of bonds $a$ and $-a$ by $\pm a$. A mapping $s : \Sigma \to \mathbb{Z}^\geq 0$ is a strength function if $s(a) = 0$ implies that $a = \nu$ and $s(a) = s(-a)$ for any $a \neq \nu$. We call $s(a)$ the strength of bond $a \in \Sigma$.

A tile is an ordered pair $t = (P, g)$ where $P$ is a polygon with sides $\{L_i\}_{i=1}^n$ and $g : \{L_i\}_{i=1}^n \to \Sigma$ is a bond mapping which associates a bond to each side of $P$; see Figure 2.09 for examples. Two tiles $t_1 = (P_1, g_1)$ and $t_2 = (P_2, g_2)$ are equivalent, denoted $t_1 \sim t_2$, if $P_1 \cong P_2$ with an associated isometry $I \in G$ such that $I(P_1) = P_2$ and $g_1 = g_2 \circ I$. Note that $g_1 = g_2 \circ I$ is well-defined because $P_1 \cong P_2$ requires that $I \in G$ bijectively maps the sides of $P_1$ to those of $P_2$. Clearly $\sim$ is an equivalence relation; the equivalence classes induced by $\sim$ are called tile types and denoted as $[t]$ for a fixed tile $t$.  

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Figure 2.09. Examples of tiles given a set of bonds $\Sigma = \{a, b, c, -a, -b, -c, \nu\}$ and a strength function $s : \Sigma \rightarrow \mathbb{Z}^{\geq 0}$ that is defined as follows for non-empty bonds: $s(a) = s(-a) = 1$ and $s(b) = s(-b) = s(c) = s(-c) = 2$. We note that sides without a bond are assigned the empty bond; we continue this practice with every figure which visualizes tiles unless otherwise stated. Observe that the large square tiles are equivalent; on the other hand, none of the right triangle tiles are equivalent despite having congruent associated polygons.

**Definition 2.2.1.** Let $S \subset \mathbb{R}^2$ be connected (and bounded) and $\mathcal{T}$ be a finite set of tile types. Let $\{t_i\}_{i=1}^n$ be a finite set of tiles $t_i = (P_i, g_i)$ such that $\{P_i\}_{i=1}^n$ is a tiling of $S$ and $[t_i] \in \mathcal{T}$. The map $\alpha : \{t_i\}_{i=1}^n \rightarrow \mathcal{T}$ is a configuration (of $S$ by $\mathcal{T}$) if $\alpha(t_i) = [t_i]$ for all $i$. We call $S = \bigcup_{i=1}^n P_i \subset \mathbb{R}^2$ the shape of $\alpha$. The binding graph of $\alpha$, denoted $G(\alpha) = (V_\alpha, E_\alpha)$, is a weighted graph with an associated function $\omega_\alpha : E_\alpha \rightarrow \mathbb{Z}^{\geq 0}$ where $V_\alpha = \{t_i\}_{i=1}^n$ and the following two conditions hold for any distinct $t, t' \in \{t_i\}_{i=1}^n$ using the notation $t = (P, g)$ and $t' = (P', g')$:

1. $\{t, t'\} \in E_\alpha$ if $P$ and $P'$ have at least one pair of coincident sides; and

2. Setting $q_\alpha(P, P') = \{L \mid L$ is a side of $P, g(L) \neq \nu,$ and $g(L) = -g'(L')$ for some side $L'$ of $P'$ coincident to $L\}$, we have that

\[ \omega_\alpha(\{t, t'\}) = \sum_{L \in q_\alpha(P, P')} s \circ g(L). \]

Informally, condition (2) in Definition 2.2.1 requires that $\omega_\alpha(\{t, t'\})$ equals the sum of the strength of the matching, complementary bonds associated to coincident pairs of sides. Note that $G(\alpha)$ in Definition 2.2.1
is isomorphic to a spanning subgraph of $\overline{G}(\{P_i\}_{i=1}^n)$ without the inclusion of weight function $\omega_\alpha$. Since $\{P_i\}_{i=1}^n$ is a finite tiling, we consider the tiles associated to boundary polygons of $\{P_i\}_{i=1}^n$ as boundary tiles of $\alpha$. We define the boundary corners and boundary sides of $\alpha$ likewise. See Figure 2.10 for examples of configurations.

![Figure 2.10](image)

**Figure 2.10.** Four examples of configurations; note that each tile in the domains of these four configurations is equivalent to some tile presented in Figure 2.09. We label the tiles in each configuration for later use.

For a connected graph $G = (V, E)$, recall that $K \subseteq E$ is called disconnecting set if $G' = (V, E \setminus K)$ has two or more components. Let $T$ be a finite set of tile types and $\theta \in \mathbb{Z}^+$. A (tile) assembly instance at temperature $\theta$ (over $T$) is a configuration $\alpha : \{t_i\}_{i=1}^n \rightarrow T$ with a connected binding graph $G(\alpha) = (V_\alpha, E_\alpha)$ such that for any disconnecting set $K \subseteq E_\alpha$,

$$\theta \leq \sum_{\{t,t'\} \in K} \omega_\alpha(\{t,t'\}).$$

We say that $\alpha$ is a unit (tile) assembly instance (over $T$) if $n = 1$; we often use “tile” and “unit assembly instance” interchangeably when discussing the latter. See Figures 2.10 for examples of assembly instances.
Let \( t_i = (P_i, g_i) \) for each tile in the domain of \( \alpha \) and \( \alpha' : \{ (P'_i, g'_i) \}_{i=1}^n \to \mathcal{T} \) be another assembly instance at temperature \( \theta \). We say that \( \alpha \) is equivalent to \( \alpha' \) if there exists an isometry \( I \in \mathcal{G} \) such that for all \( 1 \leq i \leq n \), \( I(P_i) = P'_i \) and \( g_i = g'_i \circ I \); i.e., each tile \( (P_i, g_i) \in \text{dom} \alpha \) is equivalent to \( (P'_i, g'_i) \in \text{dom} \alpha' \) via isometry \( I \). Since equivalence on assembly instances is a natural extension of \( \sim \), we denote \( \alpha \) equivalent to \( \alpha' \) by \( \alpha \sim \alpha' \). We call the equivalence class of \( \alpha \) an assembly at temperature \( \theta \) (over \( \mathcal{T} \)) and denote it by \( [\alpha] \). In particular, we say that \( [\alpha] \) is a unit assembly (over \( \mathcal{T} \)) if \( \alpha \) is a unit assembly instance.

![Figure 2.11](image_url)

**Figure 2.11.** The four binding graphs of the configurations from Figure 2.10. Note that we have labeled the edges with their respective weights according to Definition 2.2.1. In particular, note that the edge between tiles \( t_6 \) and \( t_7 \) has a weight of 0 despite the fact that these tiles have a pair of coincident sides. The reason for this is that the corresponding sides do not have matching, complementary bonds. The same holds for the edge between tiles \( t_9 \) and \( t_{10} \).

Given an assembly \( [\alpha] \), we simply call \( \alpha' \in [\alpha] \) an instance of \([\alpha]\). Unless we give specific conditions, we use \( \alpha \) to mean an arbitrary instance of \([\alpha]\) if we only give the latter. Recall that congruence extends to finite tilings; given the shape \( S \) of a configuration \( \beta \), there is a finite tiling of \( S \) by the polygons associated with the domain of \( \beta \). It follows that the notion of two configurations having congruent shapes is well-defined. Now note that any two instances of an assembly must have isomorphic binding graphs and congruent shapes. The shape class of an assembly \( [\alpha] \) is the equivalence class (under congruence) of the shapes of the instances of \([\alpha]\). We say that \([\alpha]\) covers \( S \subset \mathbb{R}^2 \) if every element in the shape class of \([\alpha]\) is isometric to \( S \).

Let \( \{ \beta_i \}_{i=1}^n \) be a finite set of configurations. A configuration \( \alpha \) is the sum of \( \{ \beta_i \}_{i=1}^n \) if \( \text{dom}(\beta_i) \cap \text{dom}(\beta_j) = \emptyset \) for \( i \neq j \) and \( \bigcup_{i=1}^n \text{dom}(\beta_i) = \text{dom}(\alpha) \). If each \( \beta_i \) is an assembly instance at temperature \( \theta \), then we define the set of connecting edges between \( \beta_i \) and \( \beta_j \), denoted \( K_\alpha(\beta_i, \beta_j) \subset E_\alpha \), for binding graph \( G(\alpha) = (V_\alpha, E_\alpha) \) as follows:

\[
K_\alpha(\beta_i, \beta_j) = \{ \{ t, t' \} \mid \{ t, t' \} \in E_\alpha \text{ where } 0 < \omega_\alpha(\{ t, t' \}), t \in \text{dom} \beta_i, \text{ and } t' \in \text{dom} \beta_j \}.
\]
Intuitively, $K_α(β_i, β_j)$ is the set of edges of $G(α)$ connecting $β_i$ and $β_j$ which contain non-empty matching, complementary bonds. In this context, we define a weighted graph called the connecting graph of $\{β_i\}_{i=1}^n$, denoted $G(\{β_i\}_{i=1}^n)$, as follows: the vertex set for $G(\{β_i\}_{i=1}^n)$ is $\{β_i\}_{i=1}^n$, and $\{β_i, β_j\}$ is in the edge set $E(\{β_i\}_{i=1}^n)$ if there exist $t, t' \in E_α$ such that $t \in dom β_i$ and $t' \in dom β_j$. Moreover, the weight function $ω : E(\{β_i\}_{i=1}^n) → Z^≥0$ is defined as follows:

$$ω(\{β_i, β_j\}) = \sum_{e ∈ K_α(β_i, β_j)} ω_α(e).$$

If $α$ is also an assembly instance at temperature $θ$, then we say that $\{β_i\}_{i=1}^n$ binds to form $α$. Moreover, we use $[β_1 ⊕ ⋯ ⊕ β_n]$, or simply $[Σ^n_{i=1} β_i]$, to denote the set $\{[α] | α$ is an assembly instance (at temperature $θ$) and $α$ is the sum of $β'_{n−1}, …, β'_n$ where each $β'_{i} ∈ [β_i]\}$. Unlike sums of assembly instances, note that $[Σ^n_{i=1} β_i]$, where each $β_{i} ∈ [β_i]\}$ is typically not a singleton (Figure 2.12). However, $[Σ^n_{i=1} β_i]$ is always finite because assembly instances have finite domains and these domains have finite sets of boundary sides. As an extension of our definitions for assembly instances, we refer to an assembly $[α] ∈ [Σ^n_{i=1} β_i]$ as an assembly sum of $\{[β_i]\}_{i=1}^n$ and also say that $\{[β_i]\}_{i=1}^n$ bind to form $[α]$. Frequently we say that the assemblies in the set $\{[β_i]\}_{i=1}^n$ “bind to each other” without specifying an assembly $[α] ∈ [Σ^n_{i=1} β_i]$ in order to imply that $[Σ^n_{i=1} β_i] ≠ \emptyset$ and to informally provide intuition for a process involving assemblies.

**Definition 2.2.2.** A tile assembly system (TAS) is an ordered pair $Γ = (T_0, θ)$ where $T_0$ is a finite set of tile types and $θ ∈ Z^+$. We recursively define the following sets of assemblies at temperature $θ$ over $T_0$ for each $n ∈ Z^+$: $T_n = \{[α] | [α] ∈ [β_1 ⊕ β_2]\}$ where $[β_1] ∈ T_{n−1}$ and $[β_2] ∈ T_m$ for some $m < n$. We use $T_∞$ to denote $∪_{n≥0} T_n$. An assembly $[α]$ is producible by $Γ$ (at step $n$) if $α ∈ T_n$ for some $n ≥ 0$ (i.e., $[α] ∈ T_∞$).

In Definition 2.2.2, note that it is possible for $T_{n_1} ∩ T_{n_2} ≠ \emptyset$ for $n_1 ≠ n_2$; in other words, it is possible for an assembly instance to be producible at different steps. Let $Γ = (T_0, θ)$ be a TAS and use $\{[α_i]\}_{i≥0}$ to denote finite or countable set of assemblies $[α_i]$ producible by $Γ$. We say that $\{[α_i]\}_{i≥0}$ is an assembly sequence (of $Γ$) if $[α_0] ∈ T_j$ for some $j ≥ 0$ and for all $i > 0$, $[α_i] ∈ T_{j+i}$ is such that $[α_i] ∈ [α_{i−1} ⊕ β_{i−1}]$ where $[β_{i−1}] ∈ T_k$ for some $k < j + i$. A finite assembly sequence $\{[α_i]\}_{i=0}^m$ of $Γ$ is nontrivial if $m > 0$. Now consider $A = \{B_η\}_{η=0}^∞$ where each set $B_η ⊂ T_∞$ is finite. We say that $A$ is an assembly chain (of $Γ$) if for each $η > 0$ and each assembly $[α] ∈ B_η$, there exists a finite assembly sequence $\{[α_i]\}_{i=0}^m$ such that $[α_0] ∈ B_{η−1}$ and $[α_m] = [α]$. Moreover, we say that each $B_η$ is an assembly block at level $η$ (of assembly chain $A$). See Figure 2.13 for examples of assembly sequences.
Figure 2.12. An example of two sums of unit assembly instances at temperature 2 which are not equivalent. Note that there are other sums of these unit assembly instances which are distinct from the two which have been presented.

Figure 2.13. Let $\Gamma = (\mathcal{T}_0, 1)$ be such that the tile types in $\mathcal{T}_0$ are visually defined on the right of the figure; we give two examples across the top and the bottom of assembly sequences of $\Gamma$. Note that we have vertically aligned the assemblies presented in the figure so that the leftmost assemblies belong to $\mathcal{T}_0$, the next two vertically aligned assemblies belong to $\mathcal{T}_1$, and so on.

2.3 Simulation of Substitution Rules

We define the notion of simulating a substitution rule $\mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S})$ with a tile assembly system $\Gamma = (\mathcal{T}_0, \theta)$ in this section. Motivated by the hierarchical self-assembly idea presented in Section 1.1, our goal is to capture the structural and dynamic aspects of a substitution rule with our definition of simulation so as to
replicate the “enlarge and dissect” process of $\mathcal{R}$:

- **Structural**: For each supertile $\sigma^\ell(X)$, there exist a finite set of producible assemblies by $\Gamma$ whose shape classes are (elementwise) similar to $\sigma^\ell(X)$.

- **Dynamic**: Only assemblies corresponding to supertiles of order $\ell - 1$ should be able to bind and form an assembly corresponding to $\sigma^\ell(X)$.

We also add the following restriction on $\Gamma$: all assemblies producible by $\Gamma$ must participate in simulation process above. Without this constraint, assemblies might exist which cannot be formed following dynamics of $\mathcal{R}$; see Example 2.3.1.

![Figure 2.14. The Square substitution rule.](image)

**Example 2.3.1.** Let $\mathcal{R}$ be the Square substitution rule (Figure 2.14), and let $X$ be the unique prototile of $\mathcal{R}$. Moreover, let $\Gamma = (\{[t]\}, 1)$ be a TAS where $[t]$ is visualized on the top left of Figure 2.15. Observe that the assemblies visualized on the top of Figure 2.15 are producible by $\Gamma$. By the definition of $\mathcal{R}$, these assemblies cover the supertiles $\sigma^0(X)$, $\sigma^1(X)$, and $\sigma^2(X)$ going from left to right. However, the assemblies visualized on the bottom of Figure 2.15 are also producible by $\Gamma$. In order to capture the dynamics of $\mathcal{R}$, $\Gamma$ should have assemblies corresponding to supertiles of order $\ell$ binding together to form an assembly corresponding to a supertile of order $\ell + 1$. If we try to define the assembly on the bottom left of Figure 2.15, denoted $[\alpha]$, as an assembly sum of assemblies associated with supertiles of $\mathcal{R}$, then either $[\alpha]$ is an assembly sum of five assemblies corresponding to $\sigma^0(X)$ or $[\alpha]$ is an assembly sum of an assembly corresponding to $\sigma^0(X)$ and an assembly corresponding to $\sigma^1(X)$. In either case, $[\alpha]$ is producible by $\Gamma$ but cannot be formed following the dynamics of $\mathcal{R}$ according to our description above. We can make similar observations for the assembly on the bottom right of of Figure 2.15.

Below, we present two formal definitions for our notion of simulation: “strict” and “bordered” simulation. The former definition naturally arises from the idea of converting the prototiles of a substitution rule into
Figure 2.15. Visualization of some producible assemblies for the TAS $\Gamma = (\mathcal{T}_0, 1)$ in Example 2.3.1 which attempts to simulate the Square substitution rule. In particular, the unit assembly on the top right is $[t]$, the only element in $\mathcal{T}_0$.

tiles in the context of self-assembly. The latter definition arises from the use of “border” or “grout” tiles to facilitate hierarchical growth in other tile assembly models [23, 24, 31]. Both notions of simulation follow the informal description of simulation at the beginning of this section.

**Definition 2.3.2.** Let $\Gamma = (\mathcal{T}_0, \theta)$ be a TAS and $\mathcal{R} = (\mathcal{P}, \lambda, S)$ be a substitution rule. We say that $\Gamma$ strictly simulates $\mathcal{R}$ if the conditions below hold for an assembly chain $\mathcal{A} = \{B_\ell\}_{\ell \geq 0}$ of $\Gamma$ (called the substitution chain of $\Gamma$) where $B_0 = \mathcal{T}_0$.

(1) Structures of $\mathcal{R}$:

For each $\ell \in \mathbb{Z}_{>0}$ and each prototile $X \in \mathcal{P}$, there exists a nonempty subset $B_\ell(X) \subseteq B_\ell$ such that each $[\alpha] \in B_\ell(X)$ covers $\lambda^\ell X$. Moreover,

$$B_\ell = \bigcup_{X \in \mathcal{P}} B_\ell(X).$$

(2) Dynamics of $\mathcal{R}$:
Suppose that \(\{[\alpha_i]\}_{i=0}^{m}\) is a nontrivial assembly sequence of \(\Gamma\) such that \([\alpha_0] \in B_\ell\) and \([\alpha_m] \in B_{\ell+1}\) for some \(\ell \geq 0\), and let \(X \in \mathcal{P}\) such that \([\alpha_m]\) covers \(\lambda^{\ell+1}X\). Then the following hold for \(0 \leq i \leq m\):

(a) \([\alpha_i] \in C_{\ell,i}\) where \(C_{\ell,0} = B_\ell\) and

\[
C_{\ell,i} = \{[\alpha] \mid [\alpha] \in [\beta_1 \oplus \beta_2] \text{ where } [\beta_1] \in C_{\ell,i-1} \text{ and } [\beta_2] \in C_{\ell,j} \text{ for some } j < i\} \text{ for } 0 < i \leq m.
\]

Note that each assembly in \(C_{\ell,i}\) is an assembly sum of assemblies in \(B_\ell\).

(b) \([\alpha_i]\) covers \(\lambda^\ell Z\) where \(Z\) is a (connected) subset of the tiling \(\{Y_j\}_{j=1}^{k}\) of \(\lambda X\) in \(\mathcal{S}\). It follows that each assembly in \(C_{\ell,m}\) is an assembly sum of \(k\) assemblies in \(B_\ell\).

(3) Participation in \(\mathcal{A}\):

If \([\alpha] \in \mathcal{T}_\infty \setminus \mathcal{T}_0\), then there exist \(\ell \in \mathbb{Z}_{\geq 0}\) and assembly sequence \(\{[\alpha_i]\}_{i=0}^{m}\) of \(\Gamma\) where \([\alpha_0] \in B_\ell\) and \([\alpha_m] \in B_{\ell+1}\) such that \([\alpha] = [\alpha_i]\) for some \(0 \leq i \leq m\).

If any TAS exists which strictly simulates \(\mathcal{R}\), then we say that \(\mathcal{R}\) admits strict simulation.

Note that conditions (2)(b) and (3) of Definitions 2.3.2 provide the necessary restrictions so that the only assemblies producible by \(\Gamma\) are those which participate the simulation process. We briefly discuss strict simulation more in Chapter 3 but do not focus on the concept much because we do not currently know of any substitution rule which admits strict simulation. In fact, it is unclear that such substitution rules exist.

To build intuition, we can consider bordered simulation to be a relaxation of strict simulation which still captures the structural and dynamic aspects of a substitution rule. Bordered simulation follows the same process as in strict simulation to produce assemblies whose shape classes are (elementwise) similar to a supertile \(\sigma^\ell(X)\). After such an assembly forms, tile types bind to it to create a “border” yielding an assembly whose shape class is also (elementwise) similar to \(\sigma^\ell(X)\). These bordered assemblies are then used to form supertiles of order \(\ell + 1\), repeating the process above. See Figure 2.16 for a visualization of this idea as applied to the Pinwheel substitution rule.

Before formally defining bordered simulation, we have to account for technical issues that may arise during border formation. Given an assembly instance \(\alpha\), a border should form around \(\alpha\) via tiles binding to the boundary sides of \(\alpha\). Moreover, the shape of the resulting assembly instance \(\alpha'\) should be similar to the shape of \(\alpha\), so the border must account for the difference in the sizes of \(\alpha\) and \(\alpha'\). Finally, when a tile binds to a boundary side of \(\alpha\), it should be adjacent to the respective boundary side of \(\alpha'\) (see Figure 2.16). To
meet these requirements, we require that the prototiles of a substitution rule be “star-shaped”. A polygon $P$ is star-shaped if there exists a point $x$ in $P$ such that for every point $x'$ in $P$, the line segment whose end points are $x$ and $x'$ is a subset of $P$.

**Figure 2.16.** Visualization of a border formation for the Pinwheel substitution rule, denoted $\mathcal{R}$. On the top left, we assume that there exists an assembly instance $\alpha$ whose shape is isometric to the tiling in $\mathcal{R}$. A border forms around $\alpha$ starting with the white tile binding to two boundary sides of $\alpha$; the arrows indicate the order in which the subsequent border tiles will bind. On the bottom left, we visualize the assembly instance $\alpha'$ resulting from a completed border having formed around $\alpha$. On the right, we visualize the sum of five assembly instances which are equivalent to $\alpha'$ (or are similarly defined). The idea is that these assembly instances can bind to one another via the boundary sides which they gained after a border formed.

Recall that a polygon is convex if every interior angle between two sides is less than or equal to $\pi$; a polygon which is not convex is concave. Note that every convex polygon is star-shaped, but not every concave polygon is star-shaped. Considering the above, we note that every prototile belonging to a substitution rule $\mathcal{R}$ in [12–14, 18–20, 43] is star-shaped. However, we suspect that it is easy to construct a substitution rule which adheres to Definition 2.1.1 and has a prototile that is not star-shaped.

**Definition 2.3.3.** Let $\Gamma = (\mathcal{T}_0, \theta)$ be a TAS and $\mathcal{R} = (\mathcal{P}, \lambda, S)$ be a substitution rule such that every $X \in \mathcal{P}$ is star-shaped. We say that $\Gamma$ simulates $\mathcal{R}$ with border if the conditions below hold for a proper subset $\mathcal{T}_B \subset \mathcal{T}_0$ (called the set of border tile types), an assembly chain $\mathcal{A} = \{B_\ell\}_{\ell=0}^\infty$ of $\Gamma$ (called the substitution chain of $\Gamma$) where $B_0 = \mathcal{T}_0 \setminus \mathcal{T}_B$, and a countable sequence of real numbers $\{\kappa_\ell\}_{\ell\geq 0}$ where $\kappa_0 = 1$ and $\kappa_\ell > 1$ when $\ell > 0$. We say that a tile $t$ is a border tile if $[t] \in \mathcal{T}_B$.

(1) Structures of $\mathcal{R}$:
For each $\ell \in \mathbb{Z}_{\geq 0}$ and each prototile $X \in \mathcal{P}$, there exists a nonempty subset $B_{\ell}(X) \subseteq B_\ell$ such that each $[\alpha] \in B_{\ell}(X)$ covers $X^\ell = \widehat{\kappa}_\ell X$ where $\widehat{\kappa}_\ell = \lambda^\ell \cdot \prod_{i=0}^{\ell} \kappa_i$. Moreover,

$$B_\ell = \bigcup_{X \in \mathcal{P}} B_{\ell}(X).$$

Note that we can define $X^\ell$ recursively for a given $X \in \mathcal{P}$: $X^0 = X$ and $X^\ell = \kappa_\ell (\lambda X^{\ell-1})$ if $\ell > 0$.

(2) Dynamics of $\mathcal{R}$:

Suppose that $\{[\alpha_i]\}_{i=0}^m$ is an assembly sequence of $\Gamma$ such that $[\alpha_0] \in B_\ell$ and $[\alpha_m] \in B_{\ell+1}$ for some $\ell \geq 0$. Let $X \in \mathcal{P}$ such that $[\alpha_m]$ covers $X^{\ell+1} = \kappa_{\ell+1}(\lambda X^\ell)$. Then there exists $0 \leq u < m$ such that $[\alpha_u] \text{ covers } \lambda X^\ell = \lambda(\widehat{\kappa}_\ell X)$ and the following hold:

(a) For $0 \leq i \leq u$, $[\alpha_i] \in C_{\ell,i}$, where $C_{\ell,0} = B_\ell$ and

$$C_{\ell,i} = \{[\alpha] \mid [\alpha] \in [\beta_1 \oplus \beta_2] \text{ where } [\beta_1] \in C_{\ell,i-1} \text{ and } [\beta_2] \in C_{\ell,j} \text{ for some } j < i\} \text{ for } 0 < i \leq u.$$  

Note that each assembly in $C_{\ell,i}$ is an assembly sum of assemblies in $B_\ell$.

(b) For $0 \leq i \leq u$, $[\alpha_i]$ covers $\widehat{\kappa}_\ell Z$ where $Z$ is a (connected) subset of the tiling $\{Y_j\}_{j=1}^k$ of $\lambda X$ in $\mathcal{S}$.

It follows that each assembly in $C_{\ell,u}$ is an assembly sum of $k$ assemblies in $B_\ell$.

(c) For $u < i \leq m$, $[\alpha_i] \in D_{\ell,i-p}$ where $D_{\ell,0} = \{[\alpha_u]\}$ and

$$D_{\ell,j} = \{[\alpha] \mid [\alpha] \in [\beta_1 \oplus \beta_2] \text{ where } [\beta_1] \in D_{\ell,j-1} \text{ and } [\beta_2] \in \mathcal{T}_B\} \text{ for } 0 < j \leq m - p.$$  

Note that each assembly in $D_{\ell,j}$ is an assembly sum of $[\alpha_u]$ and $j$ border tile types.

(d) For $u \leq i < m$, if configuration $\gamma$ is the sum of an instance of $[\alpha_i]$ and $\beta$ for some assembly $[\beta] \in \mathcal{T}_\infty \setminus \mathcal{T}_B$, then $\gamma$ is not an assembly instance at temperature $\theta$. Moreover, each element in the shape class of each $[\alpha_i]$ is a topological disk.

(e) If $\alpha_u$ and $\alpha_m$ are instances of their respective assemblies such that $\alpha_m$ is the sum of $\alpha_u$ and $(m-u)$ border tiles, then the shape of $\alpha_u$ is properly contained in $\alpha_m$.

We call $[\alpha_u]$ the unbordered assembly of $\{[\alpha_i]\}_{i=0}^m$ in this context.

(3) Participation in $\mathcal{A}$:

If $[\alpha] \in \mathcal{T}_\infty \setminus \mathcal{T}_0$, then there exist $\ell \in \mathbb{Z}_{\geq 0}$ and assembly sequence $\{[\alpha_i]\}_{i=0}^m$ of $\Gamma$ where $[\alpha_0] \in B_\ell$ and $[\alpha_m] \in B_{\ell+1}$ such that $[\alpha] = [\alpha_i]$ for some $0 \leq i \leq m$. 

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If any TAS exists which simulates $\mathcal{R}$ with border, then we say that $\mathcal{R}$ admits bordered simulation.

Informally, condition (2)(d) of Definition 2.3.3 states that assemblies $[\alpha_i]$, for $u \leq i < m$, can only bind to border tile types in order to yield elements of the next assembly block. Moreover, the binding of border tiles in this context cannot create holes in the topological sense. We infer from condition (3) that the sum of two border tiles is not an assembly instance (at temperature $\theta$), and thus border tile types cannot form assemblies outside of the substitution chain of $\Gamma$.

The terms in the sequence $\{\kappa_\ell\}_{\ell \geq 0}$ serve as dilation factors in condition (1). In particular, these dilation factors represent the increase in size that occurs when border tile types bind around an unbordered assembly to produce an assembly associated with a supertile of order $\ell + 1$; see condition (2). Note that $\kappa_0 = 1$ because no border is necessary for assemblies associated to the supertiles of order 0 (i.e., assemblies in $B_0$). On the other hand, $\kappa_\ell > 1$ for $\ell > 0$ because a border is required in order to yield an assembly corresponding to a supertile of order $\ell > 0$.

Observe that condition (2)(b) of Definition 2.3.3 mirrors condition (2)(b) of Definition 2.3.2. Condition (2) and the fact that $B_0 = \mathcal{T}_0 \setminus \mathcal{T}_B$ allow our definition of bordered simulation to approximate strict simulation while permitting assembly sequences from assembly block $B_\ell$ to $B_{\ell+1}$ to incorporate the formation of a border. Unlike with strict simulation however, there are several examples of substitution rules which admit bordered simulation; see Example 2.3.6 at the end of this chapter.

**Remark 2.3.4.** Condition (2)(e) of Definition 2.3.3 implies that the boundary tiles (up to equivalence) of each $[\alpha]$ in $B_\ell$ are border tiles (i.e., elements of $[t] \in \mathcal{T}_B$) if $\ell > 0$. This requirement matches our intuition about how the border should form around an assembly which covers $\lambda X^{\ell-1}$, namely unbordered assembly $[\alpha_u]$. Condition (2) also implies that the boundary tiles (up to equivalence) of an assembly $[\alpha] \in \mathcal{T}_\infty$ are all border tiles if $[\alpha]$ is an assembly sum of assemblies in $B_\ell$ for $\ell > 0$. Using condition (3), observe the following:

If there exists an assembly sequence $\{[\alpha_i]\}_{i=0}^m$ of $\Gamma$ where $[\alpha_0] \in B_\ell$ for $\ell > 0$ and $[\alpha_m] \in B_{\ell+1}$ such that $[\gamma] = [\alpha_i]$ for some $0 \leq i \leq m$, then every boundary tile (up to equivalence) of $[\gamma]$ is a border tile.

**Remark 2.3.5.** In the context of Definition 2.3.3, note that an assembly sequence from an assembly block $B_\ell$ to $B_{\ell+1}$ is always nontrivial because the formation of a border is required. However, the formation of multiple borders, one after the other, around an assembly is possible; see our comments below. We note that
eventually this formation process must end because \( \mathcal{P} \) is finite and \( \lambda > 1 \). There must be a prototile \( X_\ast \in \mathcal{P} \) such that the tiling in \( \mathcal{S} \) of \( \lambda X_\ast \) is not a singleton.

Suppose that there exists a prototile \( X \in \mathcal{P} \) such that the tiling \( T \in \mathcal{S} \) of \( \lambda X \) is a singleton. Let \( X' \in \mathcal{P} \) be congruent to the single element in \( T \) and \( [\alpha] \in B_\ell(X) \subset B_\ell \) for some \( \ell > 1 \). By the definition of an assembly chain, there exists an assembly sequence \( \{[\alpha_i]_{i=0}^m \} \) such that \( [\alpha_0] \in B_{\ell-1} \) and \( [\alpha_m] = [\alpha] \).

Using condition (2)(b), observe that \( u = 0 \) and \( [\alpha_0] \) covers \( (X')^{\ell-1} \). Since \( \ell > 1 \), the boundary tiles (up to equivalence) of \( [\alpha_0] \in B_{\ell-1} \) are also border tiles, and \( [\alpha_0] \) is the last element in another assembly sequence starting at \( B_{\ell-2} \) which incorporates the formation of a border by condition (2)(c).

![Figure 2.17](image)

**Figure 2.17.** Left: An instance \( \alpha_u \) of the unbordered assembly of a given assembly sequence. Right: The tiling of the Square substitution rule (Figure 2.14) to which \( \alpha_u \) is associated, with its four squares enumerated. We write \( \alpha_u \) as the sum of four assembly instances whose assemblies belong to \( B_\ell \). We enumerate these assemblies by \( \{\zeta_i\}_{i=1}^4 \) so that \( \zeta_i \) corresponds to the polygon \( Y_i \) in the tiling on the right for \( 1 \leq i \leq 4 \). This enumeration and correspondence conveys the meaning of \( \zeta_i \) representing \( Y_i \) in \( \alpha_u \). We color coordinate the assemblies on the left and the polygons on the right for ease of visibility.

Before concluding this chapter with an example of bordered simulation, we formalize the idea of associating certain assembly instances with polygons in a tiling \( T \in \mathcal{S} \) of \( \lambda X \) for \( X \in \mathcal{P} \); see Figure 2.17 as a visual guide for the Square substitution rule (Figure 2.14). Let \( \Gamma = (\mathcal{T}_0, \theta) \) be a TAS which simulates a substitution rule \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) with border, using the notation of Definition 2.3.3. Let \( [\alpha] \) be the unbordered assembly of some assembly sequence \( \{[\alpha_i]_{i=0}^m \} \) of \( \Gamma \) where \( [\alpha_0] \in B_\ell \) for some \( \ell \geq 0 \) and \( [\alpha_m] \in B_{\ell+1} \) so that \( [\alpha] \) covers \( \lambda X^\ell = \lambda(\check{\kappa}_\ell X) \) for some \( X \in \mathcal{P} \). Let \( T = \{Y_j\}_{j=1}^k \) be the tiling of \( \lambda X \) in \( \mathcal{S} \). By conditions (2)(a) and (2)(b), choose \( \{\zeta_j\}_{j=1}^k \) so that \( \alpha \) is the sum of \( \{\zeta_j\}_{j=1}^k \) and each \( [\zeta_j] \in B_\ell \). We say that \( \zeta_j \) represents \( \alpha \).
Let \( \gamma \) be the shape of \( \zeta_j \) isometric to \( \tilde{\kappa}_\ell Y_j \) via some \( I \in \mathcal{G} \) and the shape of \( \alpha \) is isometric to \( \lambda X^\ell \) via the same isometry \( I \). Now suppose that \( \gamma \) is the sum of some \( W \subset \{ \zeta_j \}_{j=1}^4 \) such that \( [\gamma] \in T_\infty \), and let \( Z \subseteq T \) such that \( Z = \{ Y \mid Y \in \{ Y_j \}_{j=1}^4 \} \) such that there exists some \( \zeta \in W \) which represents \( Y \) in \( \alpha \). Then we say that \( \gamma \) represents \( Z \) in \( \alpha \), noting that \( Z \) is also a tiling and \( Z \) is connected because \( \gamma \) is an assembly instance. Letting \( [\alpha] = [\alpha_u] \) for \( 0 \leq u < m \), note that every instance of \( [\alpha_i] \) for \( 0 \leq i \leq u \) meet the requirements on \( \gamma \) by conditions (2)(a) and (2)(b).

**Example 2.3.6.** Let \( \mathcal{R} = (\{ X \}, 2, \{ \{ Y_j \}_{j=1}^4 \}) \) be the Square substitution rule (see Figure 2.14). In this example and its associated figures, we describe a TAS \( \Gamma = (T_0, 2) \) which simulates \( \mathcal{R} \) with border. A similar approach to ours is given in [31] for a different tile assembly model which incorporates “signals”; we discuss such TAMs further in Chapter 5. The full set \( T_0 \) is defined with diagrams in Appendix B; \( T_0 \) has 100 tile types, 96 of which belong to the set of border tile types \( T_B \). Moreover, the set of bonds \( \Sigma \) for \( T_0 \) has 42 elements (not including the empty bond \( \nu \)), and the strength function \( s : \Sigma \to \{ 0, 1 \} \) is defined trivially: \( s(a) = 1 \) if \( a \neq \nu \). For this specific example, \( \kappa_1 = \frac{5}{4} \); however, any \( \kappa_1 > 1 \) could have been chosen if \( T_B \) was modified appropriately.

We give an overview of the substitution chain \( \mathcal{A} \) of \( \Gamma \) associated with this simulation in Figure 2.18. We associate the four elements of an assembly block \( B_\ell \) with the four squares in the tiling \( T = \{ Y_j \}_{j=1}^4 \in \mathcal{S} \) of \( 2X \). If \( [\alpha] \) is the sum of the four distinct assemblies in \( B_\ell \) for \( \ell \geq 0 \), then any instance of \( [\alpha] \) is the sum of four assembly instances \( \{ \zeta_j \}_{j=1}^4 \), each of which represents of the four squares in \( T \). We have designed \( \Gamma \) so that the bijective correspondence between each assembly block and \( T \) also coordinates how the assemblies in \( B_\ell \) bind to each other. In particular, an assembly in \( B_\ell \) associated with square \( Y_j \) for \( 1 \leq j < 3 \) has two unique boundary bonds \( (a_{2j-1}, a_{2j}) \) which allow it to bind to the assembly in \( B_\ell \) associated with \( Y_{j+1} \). Additionally, an assembly in \( B_\ell \) associated with square \( Y_4 \) has two unique boundary bonds \( (a_5, a_6) \) which allow it to bind and complete the unbordered assembly associated with the tiling \( T \). The assemblies in \( B_\ell \) associated with \( Y_1 \) and \( Y_4 \) each have one boundary bond \( (a_7, a_8) \), respectively which are used to form the border. One of four border tile types, called “border starters”, binds to these two bonds to begin border formation. Once border formation is complete, the resulting assembly is an element in \( B_{\ell+1} \). Refer to Figure 2.19 as a visual guide.

In Figures 2.20–2.25, we visualize the formation of an instance of \( [\alpha] \in B_1 \) which corresponds to \( Y_1 \) from the assemblies in \( B_0 \). Note that the assembly instances which represent \( Y_1 \) through \( Y_4 \) bind to each other first via two bonds in \( \{ \pm a_1, \pm a_2, \ldots, \pm a_6 \} \), as in the general case. Similarly, the border begins to form
Figure 2.18. Visualization of the assembly chain associated with the TAS $\Gamma$ from Example 2.3.6. Each assembly block has four assemblies corresponding to the four squares in the tiling $T$ of the Square substitution rule (Figure 2.14). The assembly on the left is colored white to indicate that there are four assemblies within assembly block $B_0$. The four assemblies from $B_0$ bind to form the colored assembly in the middle of the figure; note that these four assemblies are assigned colors with respect to their corresponding polygon in the tiling $T$. The assembly visualization in the middle corresponds to $B_1$. As with $B_0$, we color the border tiles white in this visualization to indicate that there are four assemblies within assembly block $B_1$. These assemblies bind together within the assembly visualized on the right, and the process repeats infinitely.

around the resulting assembly instance one tile at a time starting with a “border starter” which is associated to $Y_1$ and binds to the boundary bonds $a_7$ and $a_8$. In this way, we follow the proposed design for assemblies in later blocks mentioned previously. Observe that conditions (1)–(3) of Definition 2.3.3 are met by design. In particular, condition (3) is met because each bond and each border tile type is associated with a specific purpose which is used during the simulation of $\mathcal{R}$. In the case of bonds, the function of a bond is to (i) bind assemblies associated with supertiles together, (ii) bind the “border starter” to an assembly, or (iii) bind border tile types to an assembly growing in a specific direction (with respect to the assembly). Hence all assemblies producible by $\Gamma$ participate in the simulation process of the substitution chain $\mathcal{A}$. 

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Figure 2.19. An overview of the four assemblies in assembly block $B_{\ell}$ for $\ell \geq 1$ associated with the four squares in the tiling $T$ of the Square substitution rule (Figure 2.14). The four inner, opaque squares in each of the assemblies indicate the assemblies from assembly block $B_{\ell-1}$. Each assembly in $B_{\ell}$ has two unique boundary bonds with which it binds to exactly one other assembly in $B_{\ell}$; these bonds are positioned according to their relative locations in each assembly. Two assemblies in $B_{\ell}$ bind together using these bonds. Afterwards, one of four border tile types, associated with a specific square in $T$, binds to the sum; these border tile types bind to bonds $a_7$ and $a_8$ which only appear in the assemblies associated to $Y_1$ and $Y_4$, respectively. The arrows around each assembly indicate how the border forms; in all four cases, the border formation ends in one unique L-shaped tile type.
Figure 2.20. Left: Visualization of a tile whose tile type belong to $\mathcal{T}_0$ for the TAS $\Gamma$ presented in Example 2.3.6. Right: An assembly instance which forms when the green tile on the left binds with to the red tile; we note that the tile type of the red tile also belongs to $\mathcal{T}_0$. As stated in Example 2.3.6, every bond in $\Sigma$ has a strength of 1. We note that the sum on the right is an assembly instance at temperature 2 because the green tile and the red tile have two matching, complementary pairs of bonds. The assembly containing the assembly instance on the right belongs to $\mathcal{T}_1$. 
Figure 2.21. The sum of the right assembly instance from Figure 2.20, the yellow tile, and the purple tile. Observe that the sum of the red, green and yellow tiles is an assembly instance at temperature 2 because the red and yellow tiles have two matching, complementary pairs of bonds. Similarly, the sum of these three tiles and the purple tile is also an assembly instance at temperature 2. It follows that the assembly containing this assembly instance belongs to $\mathcal{T}_3$. 
Figure 2.22. The sum of the assembly instance from Figure 2.21 and a rectangle border tile which we call a “border starter”. This border tile binds to the green and purple tiles; because these tiles do not have matching, complementary bonds, the border tile cannot bind to either of them until the assembly instance from Figure 2.21 has been completely formed. For ease of visualization, we have hidden the bonds on the non-boundary sides of the square tiles.
Figure 2.23. The sum of the assembly instance from Figure 2.22 and another rectangle border tile. Note that this new border tile (on the top left) binds to the previous border tile and to the assembly instance from Figure 2.21. Because each bond in $\Sigma$ has a strength of 1, it follows that this border tile could not bind until the first border tile had already bound. The arrows indicate how future border tiles will bind around this assembly instance. Note that this corresponds to the border formation description from Figure 2.19. We have hidden some more bonds for ease of visualization.
Figure 2.24. The assembly instance resulting from border tiles binding to the assembly instance in Figure 2.23. In this case, we have hidden all but the bonds on the boundary sides of the border tiles.
Figure 2.25. The assembly instance resulting from border tiles binding to the assembly instance in Figure 2.24. Note that the bonds $a_1$, $a_2$, $a_5$, and $a_8$ in the green square tile now appear in their corresponding locations on the boundary sides of the completed assembly. Thus, the assembly can now bind using these bonds just as the green square tile did.
Chapter 3

Necessary Conditions for Strict and Bordered Simulation

In this chapter, we present necessary conditions for strict and bordered simulation. Notably, we conclude that a TAS $\Gamma = (T_0, 1)$ cannot strictly simulate any substitution rule or simulate any substitution rule with border. If we state that a TAS $\Gamma$ simulates a substitution rule $R$ with border, we also assume that every prototile of $R$ is star-shaped even if this condition is not included explicitly. We separate the necessary conditions into two categories: conditions on tile assembly systems (Section 3.1) and conditions on substitution rules (Section 3.2). We present substitution rules alongside the latter conditions as examples which do not admit bordered. All of the results which we discuss here follow directly from our definitions in Section 2.3.

3.1 Tile Assembly Systems Which Simulate Substitution Rules

We begin with a lemma which provides a necessary condition for bordered simulation. Informally, Lemma 3.1.1 states that an assembly $[\alpha] \in B_\ell$ (for $\ell > 0$) must use the bonds on two or more boundary sides to bind with any assembly $[\beta]$ which is not a border tile type (i.e., $[\beta] \in T_\infty \setminus T_B$). If $\alpha$ is the sum of assembly instances $\{\beta_i\}_{i=1}^n$, recall the definition of the set of connecting edges between $\beta_i$ and $\beta_j$ from Section 2.2, denoted by $K_{\alpha}(\beta_i, \beta_j)$.

Lemma 3.1.1. Let $\Gamma = (T_0, \theta)$ be a TAS which simulates a substitution rule $R = (P, \lambda, S)$ with border and $A = \{B_\ell\}_{\ell=0}^\infty$ be the substitution chain of $\Gamma$. Then the following holds for any $\ell > 0$ and any $[\alpha] \in B_\ell$:

\[(\ast) \text{ If } [\gamma] \in T_\infty \text{ such that } \gamma \text{ is the sum of } \alpha \text{ and } \beta \text{ for some } [\beta] \in T_\infty \setminus T_B, \text{ then the set } K_{\gamma}(\alpha, \beta) \text{ does not contain any edge } e \text{ such that } \omega_{\gamma}(e) \geq \theta \text{ in } G(\gamma).\]

Proof. Let $\Gamma$, $R$, and $A$ be as given. Suppose that the result does not hold – i.e., there exist $\ell > 0$, $\alpha$, $\gamma$, and $\beta$ as above so that $K_{\gamma}(\alpha, \beta)$ contains at least one edge $e$ such that $\omega_{\gamma}(e) \geq \theta$ in $G(\gamma)$. Denote $e = \{t, t'\}$ such that $t \in \text{dom } \alpha$ and $t' \in \text{dom } \beta$. Because $\omega_{\gamma}(e) \geq \theta$, it follows that the sum of $t$ and $\beta$, denoted $\hat{\beta}$, is
an assembly instance at temperature \( \theta \). Moreover, note that \( \{\hat{\beta}\} \in \mathcal{T}_\infty \setminus \mathcal{T}_0 \) because the domain of \( \hat{\beta} \) contains at least \( t \) and \( t' \).

Because \( \{\alpha\} \in B_\ell \) for \( \ell > 0 \), the boundary tiles of \( \alpha \) are all border tiles by Remark 2.3.4; it follows that \( \{t\} \in \mathcal{T}_B \). By the definition of an assembly chain, we also have that there exists an assembly sequence \( \{[\alpha_i]\}_{i=0}^m \) of \( \Gamma \) such that \( [\alpha_0] \in B_{\ell-1} \) and \( [\alpha_m] = [\alpha] \). Using conditions (2)(a) and (2)(c) of Definition 2.3.3, choose assembly instances \( \alpha_i \) in their respective assemblies so that \( \alpha_{i+1} \) is the sum of \( \alpha_i \) and some appropriate assembly instance for all \( 0 \leq i < m \); thus, \( \text{dom} \alpha_i \subset \text{dom} \alpha_{i+1} \) by construction. Moreover, let \( 0 \leq u < m \) be such that \( [\alpha_u] \) is the unbordered assembly of \( \{[\alpha_i]\}_{i=0}^m \). We infer from condition (2)(c) that border tiles bind to an assembly instance one at time. It follows that there exists some \( u \leq i^* < m \) such that \( \text{dom} \alpha_{i^*+1} \setminus \text{dom} \alpha_{i^*} = \{t\} \). But because \( \text{sum of } \alpha_{i^*} \text{ and } t \) is an assembly instance at temperature \( \theta \), we also have that the sum of \( \alpha_{i^*} \) and \( \hat{\beta} \) is an assembly instance at temperature \( \theta \). However, this contradicts condition (2)(d); therefore, the result holds.

Proposition 3.1.2 provides an analogous necessary condition to Lemma 3.1.1 for strict simulation.

**Proposition 3.1.2.** Let \( \Gamma = (\mathcal{T}_0, \theta) \) be a TAS which strictly simulates a substitution rule \( R = (P, \lambda, S) \) and \( A = \{B_\ell\}_{\ell=0}^\infty \) be the substitution chain of \( \Gamma \). There exists \( L > 0 \) such that the following holds for any \( \ell > L \) and any \([\alpha]\) \( \in B_\ell \):

\( \star \) If \( [\gamma] \in \mathcal{T}_\infty \) such that \( \gamma \) is the sum of \( \alpha \) and \( \beta \) for some \([\beta]\) \( \in \mathcal{T}_\infty \), then the set \( K_\gamma(\alpha, \beta) \) does not contain any edge \( e \) such that \( \omega_\gamma(e) \geq \theta \) in \( G(\gamma) \).

**Proof.** Let \( \Gamma, \mathcal{R}, \) and \( A \) be as given. Suppose that no such \( L \) exists – i.e., there is an infinite subset \( Z \subset \mathbb{Z}^+ \) so that for each \( \ell \in Z \), there exist \([\alpha_\ell]\) \( \in B_\ell \) and \([\gamma_\ell]\) \( \in \mathcal{T}_\infty \) where \( \gamma_\ell \) is the sum of \( \alpha_\ell \) and \( \beta_\ell \) for some \([\beta_\ell]\) \( \in \mathcal{T}_\infty \) such that the set \( K_{\gamma_\ell}(\alpha_\ell, \beta_\ell) \) contains at least one edge \( e \) whose weight \( \omega_{\gamma_\ell}(e) \geq \theta \) in \( G(\gamma_\ell) \).

Below we generate a contradiction using the definition of strict simulation (Definition 2.3.2).

Let \( \ell \in Z \). By the definition of \( K_{\gamma_\ell}(\alpha_\ell, \beta_\ell) \), we can denote \( e \) by \( \{t_\ell, t'_\ell\} \) so that \( t'_\ell \in \text{dom} \beta_\ell \) and \( t_\ell \in \text{dom} \alpha_\ell \) in turn. Let \( \hat{\alpha}_\ell \) be the sum of assembly instance \( \alpha_\ell \) and \( t'_\ell \) so that \( \text{dom} \hat{\alpha}_\ell \subset \text{dom} \gamma_\ell \). Note that \( \hat{\alpha}_\ell \) is an assembly instance at temperature \( \theta \) because \( \alpha_\ell \) is an assembly instance and \( \omega_{\hat{\alpha}_\ell}(e) = \omega_{\alpha_\ell}(e) \geq \theta \).

Thus, \([\hat{\alpha}_\ell]\) \( \in \mathcal{T}_\infty \setminus \mathcal{T}_0 \); see Figure 3.01(a).

Let \( \{P_1\}_{i=0}^n \) be finite tiling of \( S \subset \mathbb{R}^2 \). We use \([S]_{\text{sim}}\) denote the equivalence class of \( S \) with respect to similarity, recalling that similarity extends to finite sets of polygons. Let \( Q_0 = \{[S]_{\text{sim}} \mid S \subset \mathbb{R}^2 \} \) is a connected subset of some \( \{Y_j\}_{j=1}^k \subset S \}. Because each tiling \( T \) in \( S \) is a finite set, the set of connected
subsets of \( T \) is also finite. It follows that \( Q_0 \) is finite because \( P \) and \( S \) are finite. On the other hand, recall that the shape of each \( \alpha_\ell \) is isometric to \( \lambda X \) for some \( X \in P \) by condition (1) of Definition 2.3.2. Let \( S_\ell \) be shape of \( \hat{\alpha}_\ell \) for \( \ell \in \mathbb{Z} \) and \( Q_1 = \{ [S] \mid S = S_\ell \text{ for some } \ell \in \mathbb{Z} \} \). Observe that \( Q_1 \) is infinite because the shape of each \( \alpha_\ell \) scales with \( \ell \) but the shape of each \( t'_\ell \) does not; see Figure 3.01(b).

\[
\alpha_\ell \quad \beta_\ell \quad t_\ell \quad \hat{\alpha}_\ell
\]

\[
\ell_1 \quad \ell_2 \quad \ell_3 \quad \ell_4 \quad \ldots
\]

**Figure 3.01.** (a) Visualization of \( \alpha_\ell \), \( \beta_\ell \), and \( \hat{\alpha}_\ell \) for the proof of Proposition 3.1.2. For ease of visibility, we color \( \alpha_\ell \) blue and \( \beta_\ell \) red, and note that the tiles \( t_\ell \) and \( t'_\ell \) are also denoted. (b) Visualization of \( \hat{\alpha}_{\ell_i} \) for \( i \geq 1 \). As indicated in the proof, the shapes of \( \alpha_{\ell_i} \) grows as \( \ell_i \) increases. However, since each \( t'_{\ell_i} \) is a tile, the shapes of these tiles do not change as \( \ell_i \) increases.

Choose \( L \in \mathbb{Z} \) so that \([S_L] \not\in Q_0\). Since \([\hat{\alpha}_L] \in T_\infty \setminus T_0\), there exists \( \ell \in \mathbb{Z}^{\geq 0} \) and assembly sequence \( \{[\alpha_i]\}_{i=0}^m \) of \( \Gamma \) where \([\alpha_0] \in B_\ell \) and \([\alpha_m] \in B_{\ell+1} \) such that \([\hat{\alpha}_L] = [\alpha_i] \) for some \( 0 \leq i \leq m \), by condition (3) of Definition 2.3.2. But by condition (2)(b), the shape class of \([\hat{\alpha}_L] = [\alpha_i] \) must be similar to the union of a connected subset of some \( \{Y_j\}_{j=1}^k \in S \), contradicting the fact that \([S_L] \not\in Q_0\).

The following corollary extends the results of Lemma 3.1.1 and Proposition 3.1.2. We conclude from Corollary 3.1.3 that after some level \( L > 0 \), sums of assemblies in \( B_\ell \) (where \( \ell > L \)) must bind to one another via the bonds on two or more boundary sides. In particular, sums of assembly instances corresponding to supertiles of order \( \ell \) must each use the bonds on two or more distinct boundary sides in order to bind with one another while forming an assembly instance corresponding to a supertile of order \( \ell + 1 \). This makes
By construction, of Definition 2.3.2, the assembly sequence \( \{ \alpha \} \geq 1 \) \( \lambda > \) \( \lambda \) holds.

Theorem 3.1.4. Let \( \Gamma = (T_0, \theta) \) be a TAS which strictly simulates a substitution rule \( R = (P, \lambda, S) \) (or simulates \( R \) with border, resp.) and \( A = \{ B_\ell \}_{\ell=0}^\infty \) be the substitution chain of \( \Gamma \). There exists \( L \geq 0 \) such that the following holds for any \( \ell > L \) and any \([\alpha] \in |\bigoplus_{i=1}^n \alpha_i|\) where each \([\alpha_i] \in B_\ell\):

\( \star \) If \([\gamma] \in T_\infty \) where \( \gamma \) is the sum of \( \alpha \) and \( \beta \) for some \([\beta] \in T_\infty \) (\([\beta] \in T_\infty \setminus T_B \), resp.), then \( K_\gamma(\alpha, \beta) \) does not contain any edge \( e \) such that \( \omega_\gamma(e) \geq \theta \) in \( G(\gamma) \).

Moreover, if \( \Gamma \) simulates \( R \) with border, then \( L = 0 \).

Proof. Let \( \Gamma \), \( R \), \( A \), and \([\alpha] \) be as given. Choose assembly instances \( \zeta_i \) be in their respective assemblies so that \( \text{dom} \zeta_i \subset \text{dom} \alpha \) for all \( 1 \leq i \leq n \). Then note that every boundary tile of \( \text{dom} \alpha \) is a boundary tile of \( \zeta_i \) for some \( 1 \leq i \leq n \). If \( \Gamma \) simulates \( R \) strictly, then we can repeat the contradiction arguments of Proposition 3.1.2, using some \([\zeta_i] \), to show that the result holds. On the other hand, if \( \Gamma \) simulates \( R \) strictly, then we can repeat the contradiction arguments of Proposition 3.1.2, using some \([\zeta_i] \), to show that the result holds.

\( \square \)

Theorem 3.1.4. Let \( R = (P, \lambda, S) \) be a substitution rule. If a TAS \( \Gamma = (T_0, \theta) \) strictly simulates \( R \) or simulates \( R \) with border, then \( \theta > 1 \).

Proof. Let \( R \) and \( \Gamma \) be as given; let \( A = \{ B_\ell \}_{\ell=0}^\infty \) be the substitution chain of \( \Gamma \). We only need to prove that there exist assemblies \([\alpha], [\beta], [\gamma] \in T_\infty \) which satisfy the criteria of Proposition 3.1.2 or Lemma 3.1.1, respectively. Indeed, any edge \( e \in K_\gamma(\alpha, \beta) \) has weight \( 0 < \omega_\gamma(e) \in \mathbb{Z}^+ \) by definition. Therefore, if there exists an edge \( e \in K_\gamma(\alpha, \beta) \) such that \( \omega_\gamma(e) < \theta \), then clearly \( \theta > 1 \). Before proceeding, note that because \( \lambda > 1 \), there exists some prototile \( X_\ast \in P \) such that the tiling in \( S \) of \( \lambda X_\ast \) is not a singleton.

(Strict Simulation) First assume that \( \Gamma \) strictly simulates \( R \). Let \( L \) be as in Proposition 3.1.2, and choose \( \ell > L \). Choose \([\alpha] \in B_{\ell+1} \) such that \([\alpha] \) covers \( \lambda^{\ell+1} X_\ast \). By the definition of an assembly chain, there exists an assembly sequence \( \{ [\alpha_i] \}_{i=0}^m \) such that \([\alpha_0] \in B_\ell \) and \([\alpha_m] = [\alpha] \). By our choice of \( X_\ast \) and condition (2) of Definition 2.3.2, the assembly sequence \( \{ [\alpha_i] \}_{i=0}^m \) is nontrivial; so, \([\alpha_1] \in [\alpha_0 \oplus \beta] \) for some \([\beta] \in B_\ell \).

By construction, \([\alpha_0], [\beta], \) and \([\alpha_1] \) satisfy the criteria of Proposition 3.1.2.
Now assume that \( \Gamma \) simulates \( \mathcal{R} \) with border. By Remark 2.3.4, all boundary tiles (up to equivalence) of \([\alpha] \in B_\ell\) are border tiles if \( \ell > 0 \). Thus, all assemblies in \( B_\ell \) for \( \ell > 0 \) must be elements of \( \mathcal{T}_\infty \setminus \mathcal{T}_0 \) (i.e., each \([\alpha] \in B_\ell\) is not unit assembly). Let \( \ell > 0 \), and choose \([\alpha] \in B_{\ell+1}\) such that \([\alpha]\) covers \( X_\ell^{\ell+1} \). We can repeat the arguments for strict simulation with our choice of \([\alpha] \in B_{\ell+1}\) to find suitable assemblies as above using condition (2) of Definition 2.3.3.

Theorem 3.1.4 is an immediate result of Lemma 3.1.1 and Proposition 3.1.2. The theorem equivalently states that a TAS \( \Gamma = (\mathcal{T}_0, \theta) \) cannot simulate a substitution rule, strictly or with border. Tile assembly systems with a temperature parameter \( \theta = 1 \) are often called “non-cooperative” [49] because only one pair of matching bonds on coincident boundary sides is sufficient for two assembly instances to bind. The computational and structural capabilities of non-cooperative tile assembly systems have been extensively studied in various tile assembly models [8, 11, 17, 22, 27, 30, 34, 37, 39, 41, 42]. In our context, it should not be surprising that “cooperation” (i.e., \( \theta > 1 \)) is necessary for a TAS to simulate a substitution rule because the simulation process continues indefinitely, and all assemblies producible by \( \Gamma \) must participate in the process. We conclude this section with a few necessary conditions for bordered simulation.

**Proposition 3.1.5.** Let \( \Gamma = (\mathcal{T}_0, \theta) \) be a TAS which simulates a substitution rule \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) with border. If \([\alpha] \in \mathcal{T}_\infty\), then the shape of each instance of \([\alpha]\) is a topological disk.

**Proof.** Let \( \mathcal{R} \) and \( \Gamma \) be as given and \( \mathcal{A} = \{B_\ell\}_{\ell=0}^\infty \) be the substitution chain of \( \Gamma \). Because all unit assemblies in \( \mathcal{T}_0 \) satisfy the result, we can just consider assemblies in \( \mathcal{T}_\infty \setminus \mathcal{T}_0 \). Furthermore, we can focus on the elements of an assembly sequence \( \{[\alpha_i]\}_{i=0}^m \) where \([\alpha_0] \in B_\ell \) for some \( \ell \geq 0 \) and \([\alpha_m] \in B_{\ell+1}\) by condition (3) of Definition 2.3.3. We use the notation of conditions (1) and (2) for \( \{[\alpha_i]\}_{i=0}^m \), letting \([\alpha_m]\) cover \( X_\ell^{\ell+1} \) for some \( X \in \mathcal{P} \). Let \([\alpha_u]\) be the unbordered assembly of \( \{[\alpha_i]\}_{i=0}^m \) for \( 0 \leq u < m \) and \( \alpha_0 \) be some fixed instance of its respective assembly. Using conditions (2)(a) and (2)(c), choose assembly instances \( \alpha_i \) in their respective assemblies so that \( \alpha_i \) is the sum of \( \alpha_{i-1} \) and some appropriate assembly instance for all \( i > 0 \); thus, \( \text{dom} \alpha_{i-1} \subset \text{dom} \alpha_i \) by construction. Note that the result holds for \( i = 0 \) and \( u \leq i \leq m \) by conditions (2)(d) and (2)(e). In particular, the previous statement and condition (2)(c) imply the following:

\((*)\) If \([\gamma] \in \mathcal{T}_\infty\) such that \( \gamma \) is the sum of \( \alpha \) and \( \beta \) where \([\alpha] \in \mathcal{T}_\infty\) and \([\beta] \in \mathcal{T}_B\), then the shape of \( \alpha \) is a topological disk.
It suffices to show that the shape of each \( \alpha_i \), for \( 0 < i < u \), is a topological disk since any two elements of \( [\alpha_i] \) have congruent shapes (see Section 2.2).

**Figure 3.02.** Visualization of assembly instances \( \alpha_i \) and \( \alpha_u \) for the proof of Proposition 3.1.5. (a) If we assume that some assembly instance \( \alpha_i \) is not a topological disk, then because \( \alpha_u \) is a topological disk, there must be a set \( \{ \beta_j \}_{j=1}^k \) whose sum “fills” the hole in \( \alpha_i \). The assembly instance \( \alpha_i \) is visualized on the bottom with its hole. On top, \( \alpha_u \) is visualized and the dashed lines indicate the boundary of \( \alpha_i \). (b) If the sum of \( \gamma \) and some \( \beta \in T_\infty \) is an assembly instance (top), then it follows that the sum of \( \alpha_i \) and \( \beta \in T_\infty \) is also an assembly instance (bottom). The boundary sides of \( \gamma \) are also boundary sides of \( \alpha_i \). (c) Because \( \alpha_u \) is an instance of the unbordered assembly of an assembly sequence, \( \alpha_u \) binds with at least one border tile \( \beta \). But then the assembly instance \( \gamma' \) must also be able to bind to \( \beta \) since the boundary sides of \( \alpha_u \) are also boundary sides of \( \gamma' \).

Assume that the shape of \( \alpha_i \) is not a topological disk for some \( 0 < i^* < u \). Recall that the shape of an assembly instance is a connected, finite union of polygons within \( \mathbb{R}^2 \). Because the shape of \( \alpha_u \) is a topological disk, there exists at least one finite set of polygons \( \{ P_j \}_{j=1}^n \) in the shape of \( \alpha_u \) such that \( \{ P_j \}_{j=1}^n \) is a tiling of a topological disk \( S \subset \mathbb{R}^2 \) and \( \{ P_j \}_{j=1}^n \) is missing from the shape of \( \alpha_i \), thus creating a hole; see Figure 3.02(a). By condition (2)(a), there exist assembly instances \( \{ \beta_j \}_{j=1}^k \) where \( [\beta_j] \in B_\ell \) such that the union of the shapes of \( \{ \beta_j \}_{j=1}^k \) is \( S \) and \( \text{dom } \beta_j \subset \text{dom } \alpha_u \) for each \( j \) because every \( [\alpha_i] \) is an assembly sum of assemblies in \( B_\ell \).
Let configuration \( \gamma \) be the sum of \( \alpha_{i^*} \) and \( \{ \beta_j \}_{j=1}^k \), and note that \( [\gamma] \in T_\infty \) because \( \alpha_{i^*}, \beta_j, \) and \( \alpha_u \) are assembly instances and \( \dom \gamma, \dom \alpha_{i^*}, \dom \beta_j \subset \dom \alpha_u \) for \( 1 \leq j \leq k \). Moreover, observe that if an assembly instance is the sum of \( \gamma \) and \( \beta \) for any \( [\beta] \in T_\infty \), then the sum of \( \alpha_{i^*} \) and \( \beta \) must also be an assembly instance because only the boundary tiles of \( \gamma \) allow it to bind to \( \beta \), and these same tiles are present in \( \alpha_{i^*} \); see Figure 3.02(b). From this observation and \( \{ [\alpha_i] \}_{i=0}^m \), we infer that there exists an assembly instance \( \gamma' \) (at temperature \( \theta \)) such that \( \dom \alpha_u \setminus \dom \gamma' = \bigcup_{j=1}^n \dom \beta_j \).

Choose a unit assembly instance \( \beta \) such that \( [\beta] \in T_B \) and \( \alpha_{u+1} \) is the sum of \( \alpha_u \) and \( \beta \). Then the sum of \( \gamma' \) and \( \beta \) is also an assembly instance at temperature \( \theta \); see Figure 3.02(c). But this contradicts observation (\( \ast \)) because the shape of \( \gamma' \) is not a topological disk. It follows that no such index \( 0 < i^* < u \) exists, and thus the result holds.

We conclude from Proposition 3.1.5 that assembly instances cannot have holes in the context of bordered simulation. This verifies our intuition about where the boundary tiles of an assembly instance should be located. As implied in Section 2.2, assembly instances bind to one another via boundary tiles, so this proposition gives us insight about how assemblies bind to each other.

The next few results provide necessary conditions on an assembly instance \( \alpha \) can bind to two assembly instances \( \beta_1 \) and \( \beta_2 \) when the latter assembly instances satisfy certain criteria. We use Propositions 3.1.6 and 3.1.7 to prove the results in Section 3.2. Meanwhile, Corollaries 3.1.8 and 3.1.9 provide the motivation for the definitions in Chapter 4.

**Proposition 3.1.6.** Let \( \Gamma = (T_0, \theta) \) be a TAS which simulates a substitution rule \( \mathcal{R} = (\mathcal{P}, \lambda, S) \) with border and \( A = \{ B_\ell \}_{\ell=0}^\infty \) be the substitution chain of \( \Gamma \). Let \( [\alpha] \in T_\infty \), and suppose that configuration \( \gamma \) is the sum of \( \alpha, \beta_1, \) and \( \beta_2 \) where \( [\beta_1] \in T_B \) and \( [\beta_2] \in T_\infty \setminus T_B \). Then for \( k = 1 \) or \( k = 2 \),

\[
\sum_{e \in K_\gamma(\alpha, \beta_k)} \omega_\gamma(e) < \theta.
\]

**Proof.** Let \( \mathcal{R}, \Gamma, A, \gamma, \) and all assemblies be as given. Suppose that the result does not hold; that is to say, we assume that

\[
\sum_{e \in K_\gamma(\alpha, \beta_k)} \omega_\gamma(e) \geq \theta
\]

for both \( k = 1 \) and \( k = 2 \). Let \( \gamma' \) be the sum of \( \alpha \) and \( \beta_1 \) so that \( \dom \alpha, \dom \beta_1 \subset \dom \gamma' \subset \dom \gamma \). Because \( \alpha, \beta_1, \) and \( \beta_2 \) are assembly instances (at temperature \( \theta \)), observe that \( \gamma \) and \( \gamma' \) are also assembly
instances at temperature $\theta$ using our assumption above. Moreover, $[\gamma'] \in \mathcal{T}_\infty \setminus \mathcal{T}_0$ because $[\gamma']$ is an assembly sum of $[\alpha] \in \mathcal{T}_\infty$ and $[\beta_1] \in \mathcal{T}_B$.

Recall that $B_0 = \mathcal{T}_0 \setminus \mathcal{T}_B$. It follows that $[\alpha] \not\in \mathcal{T}_B$ because otherwise $[\gamma'] \in \mathcal{T}_\infty \setminus \mathcal{T}_0$ would contradict condition (3) of Definition 2.3.3. Now suppose that $[\alpha] \in \mathcal{T}_0 \setminus \mathcal{T}_B$. Because $[\gamma']$ is an assembly sum of $[\alpha] \in \mathcal{T}_0 \setminus \mathcal{T}_B$ and $[\beta_1] \in \mathcal{T}_B$, we infer from conditions (2)(a) and (3) that there exists an assembly sequence $\{[\alpha_i]\}_{i=0}^m$ of $\Gamma$ where $[\alpha_0] \in B_0$ and $[\alpha_m] \in B_1$ such that $[\gamma'] = [\alpha_i]$ for some $0 < i^* \leq m$. Let $[\alpha_u]$ be the unbordered assembly of $\{[\alpha_i]\}_{i=0}^m$ for $0 \leq u < m$; note that $u < i^* \leq m$ because $[\gamma']$ is not an assembly sum of assemblies in $B_0 = \mathcal{T}_0 \setminus \mathcal{T}_B$. We infer from Remark 2.3.4 that $i^* \neq m$ because there is a boundary tile of $\gamma'$, in $\text{dom} \alpha \subset \text{dom} \gamma'$, which is not a border tile. But $u < i^* < m$ contradicts condition (2)(d) because $[\beta_2] \in \mathcal{T}_\infty \setminus \mathcal{T}_B$ and assembly instance $\gamma$ is the sum of $\gamma'$ and $\beta_2$. Thus, $[\alpha] \in \mathcal{T}_\infty \setminus \mathcal{T}_0$.

By condition (3) of Definition 2.3.3, there exists $\ell \in \mathbb{Z}_{\geq 0}$ and assembly sequence $\{[\alpha_i]\}_{i=0}^m$ of $\Gamma$ where $[\alpha_0] \in B_\ell$ and $[\alpha_m] \in B_{\ell+1}$ such that $[\alpha] = [\alpha_i]$ for some $0 \leq i^* \leq m$. Let $0 \leq u < m$ be as in the context of condition (2). Because $[\gamma']$ is an assembly sum of $[\alpha]$ and $[\beta_1] \in \mathcal{T}_B$, we infer from condition (2)(c) that $u \leq i^* < m$, adjusting assembly sequence $\{[\alpha_i]\}_{i=0}^m$ if necessary to exclude $m$ (see Remark 2.3.5). But as above, $u \leq i^* < m$ contradicts condition (2)(d) because $[\beta_2] \in \mathcal{T}_\infty \setminus \mathcal{T}_B$ and assembly instance $\gamma'$ is the sum of $\alpha$ and $\beta_2$. Thus, the result holds.

We can draw several conclusions from Proposition 3.1.6 because $[\alpha]$ in the statement can be any assembly in $\mathcal{T}_\infty$. For example, a border tile type cannot bind to an assembly $[\alpha]$ in $B_\ell$ (for some $\ell \geq 0$) unless $[\alpha]$ is the unbordered assembly of some assembly sequence $\{[\alpha_i]\}_{i=0}^m$ where $[\alpha_0] \in B_\ell$ and $[\alpha_m] \in B_{\ell+1}$, implying that $[\alpha] = [\alpha_0]$. In general, this means that the first border tiles to bind to an instance $\alpha$ of the unbordered assembly of an assembly sequence $\{[\alpha_i]\}_{i=0}^m$ must bind at least two instances, $\beta_1$ and $\beta_2$, of elements $B_\ell$ which are “within” $\alpha$ (i.e., $\text{dom} \beta_1, \text{dom} \beta_2 \subset \text{dom} \alpha$).

**Proposition 3.1.7.** Let $\Gamma = (\mathcal{T}_0, \theta)$ be a TAS which simulates a substitution rule $\mathcal{R} = (\mathcal{P}, \lambda, S)$ with border and $A = \{B_\ell\}_{\ell=0}^\infty$ be the substitution chain of $\Gamma$. Let $[\alpha] \in B_\ell$ for $\ell \geq 0$ and $[\gamma] \in \mathcal{T}_\infty$ such that $\gamma$ is the sum of $\alpha$, $\beta_1$, and $\beta_2$ where $[\beta_k] \in \mathcal{T}_\infty \setminus \mathcal{T}_B$ for $k = 1, 2$. If $K_\gamma(\beta_1, \beta_2) = \emptyset$, then there exist two edges $e_k = \{t_k, t_k'\} \in K_\gamma(\alpha, \beta_k)$ for $k = 1, 2$ such that $t_1 = t_2 \in \text{dom} \alpha$ and for $k = 1, 2$

$$\sum_{e \in K_\gamma(\alpha, \beta_k) \setminus \{e_k\}} \omega_\gamma(e) < \theta.$$ 

**Proof.** Let $\mathcal{R}$, $\Gamma$, $A$, and all assemblies be as given. When $\ell = 0$, note that the proof is trivial because $[\alpha]$ is a unit assembly in $\mathcal{T}_0 \setminus \mathcal{T}_B$. So suppose that $\ell > 0$. Since $\gamma$, $\alpha$, $\beta_1$, and $\beta_2$ are all assembly instances at
temperature $\theta$ but $K_\gamma(\beta_1, \beta_2) = \emptyset$, it follows that

$$\sum_{e \in K_\gamma(\alpha, \beta_k)} \omega_\gamma(e) \geq \theta \text{ for } k = 1, 2.$$  

Since $\ell > 0$, the boundary tiles of $\alpha$ are all border tiles by Remark 2.3.4. For $k = 1, 2$, let $n_k = |K_\gamma(\alpha, \beta_k)|$ and $Z_k = \{t_k^i\}_{i=1}^{n_k}$ be boundary border tiles of $\alpha$ such that $\{t_j, t'_j\} \in K_\gamma(\alpha, \beta_k)$ for some $t' \in \text{dom } \beta_k$.

By the definition of an assembly chain, there exists an assembly sequence $\{[\alpha_i]\}_{i=0}^{m}$ of $\Gamma$ where $[\alpha_0] \in B_{\ell-1}$ and $[\alpha_m] = [\alpha]$. Let $[\alpha_u]$ be the unbordered assembly of $\{[\alpha_i]\}_{i=0}^{m}$ for $0 \leq u < m$. Using conditions (2)(a) and (2)(c) of Definition 2.3.3, choose assembly instances $\alpha_i$ in their respective assemblies so that $\alpha_i$ is the sum of $\alpha_{i-1}$ and some appropriate assembly instance for all $i > 0$; thus, dom $\alpha_{i-1} \subset$ dom $\alpha_i$ by construction. We infer from condition (2)(c) that border tiles bind to an assembly instance one at a time. In other words for $u < i \leq m$, dom $\alpha_i \setminus$ dom $\alpha_{i-1} = \{t\}$ where $[t] \in T_B$. Let $t^* \in$ dom $\alpha_m \setminus$ dom $\alpha_{m-1}$. We show the result holds by using contradiction to progressively eliminate all other possibilities.

(Case I) Assume that there exist no two edges $e_k = \{t_k, t_k'\} \in K_\gamma(\alpha, \beta_k)$ for $k = 1, 2$ such that $t_1 = t_2 \in$ dom $\alpha$. Then the sets $Z_k$ for $k = 1, 2$ are mutually disjoint. If $t^* \notin Z_k$ for both $k = 1$ and $k = 2$, then this implies that the sum of $\alpha_{m-1}$ and $\beta_1$ is an assembly instance at temperature $\theta$ because

$$\sum_{e \in K_\gamma(\alpha, \beta_1)} \omega_\gamma(e) \geq \theta.$$  

This contradicts condition (2)(d) of Definition 2.3.3 since $[\beta_1] \in T_\infty \setminus T_B$. By assumption, $t^* \notin Z_k$ for either $k = 1$ or $k = 2$; without loss of generality, assume that $t^* \notin Z_2$. Then the contradiction of condition (2)(d) above still holds.

(Case II) Assume that for any two edges $e_k = \{t_k, t_k'\} \in K_\gamma(\alpha, \beta_i)$ for $k = 1, 2$ such that $t_1 = t_2 \in$ dom $\alpha$ and

$$\sum_{e \in K_\gamma(\alpha, \beta_k) \setminus \{e_k\}} \omega_\gamma(e) \geq \theta$$

for both $k = 1$ and $k = 2$. We can repeat the arguments in Case I if $t^* \notin Z_k$ for both $k = 1, 2$ or if $t^*$ is in one set but not the other. If $t^* \in Z_k$ for both $k = 1, 2$, then the sum of $\alpha_{m-1}$ and $\beta_1$ is an assembly instance at temperature $\theta$ by assumption. But this contradicts condition (2)(d) again.

(Case III) Assume that for any two edges $e_k = \{t_k, t_k'\} \in K_\gamma(\alpha, \beta_i)$ for $k = 1, 2$ such that $t_1 = t_2 \in$ dom $\alpha$ and

$$\sum_{e \in K_\gamma(\alpha, \beta_k) \setminus \{e_k\}} \omega_\gamma(e) \geq \theta$$

for both $k = 1$ and $k = 2$. We can repeat the arguments in Case II if $t^* \notin Z_k$ for both $k = 1, 2$ or if $t^*$ is in one set but not the other. If $t^* \in Z_k$ for both $k = 1, 2$, then the sum of $\alpha_{m-1}$ and $\beta_1$ is an assembly instance at temperature $\theta$ by assumption. But this contradicts condition (2)(d) again.
for either $k = 1$ or $k = 2$. Without loss of generality, suppose that the above holds for $k = 1$. We repeat the arguments of Case I and Case II for $t^*$. □

**Corollary 3.1.8.** Let $\Gamma = (T_0, \theta)$ be a TAS which simulates a substitution rule $R = (P, \lambda, S)$ with border and $A = \{B_\ell\}_{\ell=0}^\infty$ be the substitution chain of $\Gamma$. There exists $L > 0$ so that the following holds for any $\ell > L$ and any $[\alpha] \in B_\ell$:

(⋆) Suppose that $[\gamma] \in T_\infty$ such that $\gamma$ is the sum of $\alpha$, $\beta^1$, and $\beta^2$ where $[\beta^k]$ is an assembly sum of assemblies in $B_\ell$ for $k = 1, 2$. If $K_{\gamma}(\beta^1, \beta^2) = \emptyset$, then the shapes of $\beta^1$ and $\beta^2$ have at least one pair of coincident boundary corners.

**Proof.** Let $R$, $\Gamma$, and $A$ be as given. Suppose that no such $L$ exists – i.e., there is an infinite subset $Z \subset \mathbb{Z}^+$ so that for each $\ell \in Z$, there exist $[\alpha_\ell]$, $[\gamma_\ell]$, $[\beta^1_\ell]$, and $[\beta^2_\ell]$ as above so that $K_{\gamma_\ell}(\beta^1_\ell, \beta^2_\ell) = \emptyset$ but $\beta^1_\ell$ and $\beta^2_\ell$ do not have any coincident boundary corners.

Let $\ell \in Z$; by Proposition 3.1.7, that there exists a boundary tile $t_\ell \in \text{dom } \alpha_\ell$ such that $[t_\ell, t^h_\ell] \in K_{\gamma_\ell}(\alpha_\ell, \beta^h_\ell)$ for $k = 1, 2$. Note that $[t_\ell] \in T_B$ because $\ell > 0$ by Remark 2.3.4. By our assumption, it follows that there exists a nonempty sequence of boundary sides of $t \in \text{dom } \alpha$ such that the first side is adjacent to a boundary corner of $\beta^1_\ell$ and the last is adjacent to a boundary corner of $\beta^2_\ell$; see Figure 3.03.

As in the proof of Proposition 3.1.2, we use $[S]_{\text{sim}}$ denote the equivalence class of a tiling $S$ with respect to similarity. Let $Q_0 = \{[S]_{\text{sim}} \mid S \subset \mathbb{R}^2 \text{ is a connected subset of some } T \in S\}$; $Q_0$ is finite because $P$ is finite and each tiling in $S$ is also finite. On the other hand, let $S_\ell$ be the shape of $\gamma_\ell$ for $\ell \in Z$ and $Q_1 = \{[S]_{\text{sim}} \mid S = S_\ell \text{ for some } \ell \in Z\}$. Observe that $Q_1$ is infinite because the shapes of $\alpha_\ell$, $\beta^1_\ell$, and $\beta^2_\ell$ scale with $\ell$ but the shape of each $t_\ell$ does not.
Choose \( L \in \mathcal{Z} \) so that \([S_L]_{\text{sim}} \not\in \mathcal{Q}_0\). From the conditions on \( \alpha_{\ell}, \beta_{\ell}^1, \text{ and } \beta_{\ell}^2 \), note that \([\gamma_{\ell}]\) is an assembly sum of assemblies in \( B_{\ell} \). We infer from conditions (2)(b) and (3) of Definition 2.3.3 that the shape of \( \gamma_{\ell} \) must be similar to the union of a connected subset of some \( \{Y_j\}_{j=1}^k \in \mathcal{S} \). But this contradicts the fact that \([S_L]_{\text{sim}} \not\in \mathcal{Q}_0\). Therefore, the result holds.

\[\square\]

**Corollary 3.1.9.** Let \( \Gamma = (T_0, \theta) \) be a TAS which simulates a substitution rule \( \mathcal{R} = (P, \lambda, \mathcal{S}) \) with border and \( A = \{B_\ell\}_{\ell=0}^\infty \) be the substitution chain of \( \Gamma \). There exists \( L > 0 \) such that the following holds for any \( \ell > L \) and any \([\alpha] \in B_{\ell} \):

\((*)\) Suppose that \([\gamma] \in \mathcal{T}_\infty \) such that \( \gamma \) is the sum of \( \alpha \) and \( W = \{\beta^k\}_{k=1}^n \) where \( n \geq 3 \) and each \([\beta^k]\) is an assembly sum of assemblies in \( B_{\ell} \). Then \( K_{\gamma}(\beta^j, \beta^k) \neq \emptyset \) for some \( j \neq k \).

**Proof.** Let \( \mathcal{R}, \Gamma, \text{ and } A \) be as given. Suppose that the result does not hold – i.e., there is an infinite subset \( \mathcal{Z} \subset \mathcal{Z}^+ \) so that for each \( \ell \in \mathcal{Z} \), there exist \([\alpha_{\ell}], [\gamma_{\ell}] \), and \( W_\ell = \{\beta^k\}_{k=1}^n \) (with \( n \geq 3 \)) as above so that \( K_{\gamma_{\ell}}(\beta^j_{\ell}, \beta^k_{\ell}) = \emptyset \) whenever \( j \neq k \).

Let \( L > 0 \) be as in Corollary 3.1.8, and choose \( \ell > L \) large enough such that any boundary (border) tile of \( \alpha \) is adjacent to at most two assembly instances in \( W_\ell \). Note that this is possible because each pair of distinct \( \beta^j_{\ell} \) and \( \beta^k_{\ell} \) in \( W \) satisfy the conditions of Corollary 3.1.8 and because \( \alpha_{\ell} \) and all assembly instances in \( W_\ell \) scale with \( \ell \) but border tiles do not. Then observe that there must be at least three distinct boundary (border) tiles \( t_1, t_2, t_3 \in \text{dom } \alpha \) which satisfy the conditions of Proposition 3.1.7 for distinct pairs of assembly instances in \( W_\ell \).

By definition of an assembly chain, there exists an assembly sequence \( \{[\alpha'_u]\}_{u=0}^m \) of \( \Gamma \) where \([\alpha_0]\) \( \in B_{\ell-1} \) and \([\alpha'_m] = [\alpha_{\ell}] \). Let \([\alpha'_u]\) be the unbordered assembly of \( \{[\alpha'_u]\}_{u=0}^m \) for \( 0 \leq u < m \). Using conditions (2)(a) and (2)(c) of Definition 2.3.3, choose assembly instances \( \alpha'_i \) in their respective assemblies so that \( \alpha'_i \) is the sum of \( \alpha'_{i-1} \) and some appropriate assembly instance for all \( i > 0 \); thus, \( \text{dom } \alpha'_{i-1} \subset \text{dom } \alpha'_i \) by construction. We infer from condition (2)(c) that border tiles bind to an assembly instance one at time. In other words for \( u < i \leq m \), \( \text{dom } \alpha'_i \setminus \text{dom } \alpha'_{i-1} = \{t\} \) where \([t] \in \mathcal{T}_B \). Let \( t^* \in \text{dom } \alpha'_m \setminus \text{dom } \alpha'_{m-1} = \text{dom } \alpha_{\ell} \setminus \text{dom } \alpha'_{m-1} \). Because \( t_1, t_2, \text{ and } t_3 \) are all distinct, \( t^* \) is equal to at most one of these tiles. But then it follows that some pair of assembly instances in \( W_\ell \) must be able to bind to \( \alpha'_{m-1} \), contradicting condition (2)(d). Therefore, the result holds.

\[\square\]
3.2 Bordered Simulation and Adjacency Graphs

We shift our attention to the corner and side adjacency graphs of a tiling $T \in S$ for a given substitution rule $R = (P, \lambda, S)$. From Section 2.1, we know that the corner adjacency graph and side adjacency graphs of $T$, $(G(T)$ and $\overline{G}(T)$, respectively) are connected because $T$ is a tiling of a polygon $\lambda X$ for some $X \in P$. Moreover, recall that $\overline{G}(T)$ is a spanning subgraph of $G(T)$ and that vertices in $G(T)$ are polygons in $T$.

We begin with a proposition that gives us a necessary condition for bordered simulation which is easily verifiable.

**Proposition 3.2.1.** Let $R = (P, \lambda, S)$ be a substitution rule such that every $X \in P$ is star-shaped. If there exists $T \in S$ and $v$ in $G(T) = (V, E)$ such that the subgraph of $G(T)$ induced by $V \setminus v$ has two or more components, then $R$ does not admit bordered simulation.

**Proof.** Let $R = (P, \lambda, S)$, $T \in S$, and $v \in V = T$ be as given above, but suppose that the result does not hold; that is, suppose that there exists some TAS $\Gamma = (T_0, \theta)$ which simulates $R$ with border. Let $A = \{B_\ell\}_{\ell=0}^\infty$ be the substitution chain of $\Gamma$ where $[\alpha_0] \in B_0$, $[\alpha_m] \in B_{\ell+1}$, and $[\alpha_m]$ covers $X^{\ell}$ (using the notation of Definition 2.3.3):

If $\alpha$ is an instance of the unbordered assembly of $\{\alpha_i\}_{i=1}^m$ and $\alpha$ is the sum of $\{\zeta_j\}_{j=1}^k$ such that each $[\zeta_j] \in B_\ell$, then no tile $\in \text{dom} \alpha$ can be adjacent to both domains of the assembly instance representing $v_1$ and the assembly instance representing $v_2$ in $\alpha$.

Note that we can choose such an $\ell$ because each pair of vertices $v_1$ and $v_2$ belong to different components in $G'$ and thus have no coincident corners. In other words, there is at least one side of $v$ separating any such pair $v_1$ and $v_2$.

Let $\alpha$ and $\{\zeta_j\}_{j=1}^k$ be as above and $\zeta \in \{\zeta_j\}_{j=1}^k$ represent $v$. Because the subgraph of $G(T)$ induced by $V \setminus v$ has two or more components and $\alpha$ is an assembly instance at temperature $\theta$, we observe the following: $K_\gamma(\zeta', \zeta'') = \emptyset$ for any $\zeta', \zeta'' \in \{\zeta_j\}_{j=1}^k \setminus \{\zeta\}$ which represent two vertices $v'$ and $v''$, respectively, belonging to different components in $G'$. Indeed, the vertices $v', v'' \in V = T$ do not have coincident sides, so
the assembly instances which represent them in $\alpha$ cannot have adjacent, matching, and complementary bonds. It follows that $\zeta$ induces a partition on $\{\zeta_j\}_{j=1}^k$ where subsets in the partition correspond to the components of $G'$. But since $[\alpha] \in T_\infty$, the sums of these subsets must themselves by assembly instances at temperature $\theta$. Let $v_1$ and $v_2$ belong to different components in $G'$ and $\zeta_i \in \{\zeta_j\}_{j=1}^k$ represent $v_i$ for $i = 1, 2$. Then, there exist sums $\beta_i$ of nonempty, mutually disjoint subsets of $\{\zeta_j\}_{j=1}^k \{\zeta\}$ for $i = 1, 2$ such that $\text{dom} \zeta_i \subset \text{dom} \beta_i \subset \text{dom} \alpha$, $[\beta_i] \in T_\infty$, the sum of $\beta_i$ and $\zeta$ is also an assembly instance at temperature $\theta$, and $K_\gamma(\beta_1, \beta_2) = \emptyset$.

Let $\gamma$ be the sum of $\beta_1$, $\beta_2$, and $\alpha$, and note that $\gamma$ is an assembly instance at temperature $\theta$. More importantly, $[\gamma] \in T_\infty$ because $\beta_1$ and $\beta_2$ bind to $\alpha$ independent of each other. Clearly $\beta_i \in T_\infty \setminus T_0$ for $i = 1, 2$, and $K_\gamma(\beta_1, \beta_2) = \emptyset$ as noted above. By our choice of $\ell$, there is no tile $t \in \text{dom} \alpha$ for which there exist edges $\{t, t_i\} \in K_\gamma(\alpha, \beta_i)$ with $t_i \in \text{dom} \beta_i$ for both $i = 1$ and $i = 2$. But by Proposition 3.1.7, such a tile must exist; contradiction. Therefore, the result holds.

Figure 3.04. The Domino Variant substitution rule [13] and its associated corner and side adjacency graphs. Let $T$ be the tiling of this substitution rule, and note that subgraph of $G(T)$ induced by removing polygon 3 is disconnected. Thus, the Domino Variant substitution rule does not admit bordered simulation by Proposition 3.2.1.

With adjacency graphs in mind, the definitions we provide in this section and in Section 4.1 are given for a connected graph $G = (V, E)$ and a connected spanning subgraph $H = (V, E)$ of $G$. As with corner and side adjacency graphs, we often draw $G$ and $H$ simultaneously, using solid lines to visualize edges in $\overline{E}$ and dashed lines to visualize edges in $E \setminus \overline{E}$; see Figure 3.05 for examples. For a vertex $v$ of a graph $G$, we use $d_G(v)$ to denote the degree of $v$ in $G$.

Definition 3.2.2. Let $G = (V, E)$ be a connected graph, $H = (V, \overline{E})$ be a connected spanning subgraph of $G$, and $v \in V$. We call $v$ a pier (vertex) of $H$ in $G$ if $d_H(v) = 1$ but $d_G(v) > 1$. On the other hand, $v$ is a bridge (vertex) of $H$ in $G$ if the subgraph of $H$ induced by $V \setminus \{v\}$ has two or more components and
the subgraph of $G$ induced by $V \setminus \{v\}$ is connected. We say that $v$ bridges $v_1$ and $v_2$ in $H$ if the following hold: (1) $v$ is a bridge of $H$ in $G$, (2) $v_1$ and $v_2$ are adjacent to $v$ in $G$, and (3) $v_1$ and $v_2$ belong to different components in the subgraph of $H$ induced by $V \setminus \{v\}$.

Figure 3.05. A graph $G$ and a spanning subgraph $H$ of $G$ on 10 vertices; we use solid lines to denote edges in $H$ and dashed lines to denote edges in $G$ but not $H$. By definition, note that $v_1$ and $v_8$ are piers of $H$ in $G$. On the other hand, $v_2$, $v_7$, $v_9$, and $v_{10}$ are all bridges of $H$ in $G$.

Note that if $|V| > 2$ and $v$ is a pier of $H$ in $G$ and $\{v, v'\} \in E$, then $v'$ is a bridge of $H$ in $G$ by definition. Our consideration of pier vertices is partially based on the study of “pier fractals” and their self-assembly [16]. We provide examples of both piers and bridges in Figure 3.05. For a tiling $T \in \mathcal{S}$, note that any pier of $\overline{G}(T)$ in $G(T)$ must be a boundary polygon of $T$ because $\bigcup T$ is a polygon. Similarly, any bridge $v$ of $\overline{G}(T)$ in $G(T)$ must have at least two corners which are boundary corners of $T$. Furthermore, if two polygons $x, y \in T \setminus \{v\}$ are corner neighbors but belong to different components in the subgraph of $\overline{G}(T)$ induced by $T \setminus \{v\}$, then observe that $x$ and $y$ must be adjacent to $v$ via one of its boundary corners. It follows that $v$ bridges $x$ and $y$ for any two such $x, y \in T$ by definition.

With the next two results, we find the piers and bridges of $\overline{G}(T)$ in $G(T)$ (for $T \in \mathcal{S}$) are related to necessary conditions for substitution rules $\mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S})$ which admit bordered substitution. Informally, Proposition 3.2.3 states that if there exists a bridge $v$ of $\overline{G}(T)$ in $G(T)$ for a tiling $T \in \mathcal{S}$ of $X \in \mathcal{P}$ and an assembly instance $\beta$ represents $v$ in (an instance of) some unbordered assembly whose shape covers $\lambda X^\ell$, then the border must begin forming adjacent to $\beta$. Corollary 3.2.4 states that the same is true if $v$ is a pier of $\overline{G}(T)$ in $G(T)$ instead. The subsequent corollary of these results gives us another easily verifiable condition for bordered simulation like the one in Proposition 3.2.1.
For Proposition 3.2.3 and Corollary 3.2.4, we adopt the following notation using conditions (2)(a) and (2)(b) of Definition 2.3.3: Let \( \alpha \) be an instance of the unbordered assembly of an assembly sequence \( \{(\alpha_i)\}_{i=0}^m \) of \( \Gamma \) and \( [\gamma] \in T_\infty \) where \( [\alpha_0] \in B_\ell \) for some \( \ell \geq 0 \) and \( [\alpha_m] \in B_{\ell+1} \). Let \( X \in \mathcal{P} \) be such that the shape of \( \alpha \) is isometric to \( \lambda X^\ell \) and \( T = \{(Y_j)_{j=1}^k \} \in \mathcal{S} \) be the tiling of \( \lambda X \). We write \( \alpha = \bigcup_{j=1}^k \zeta_j \) to denote that \( \alpha \) is the sum of \( \{\zeta_j\}_{j=1}^k \) where \( [\zeta_j] \in B_\ell \) for \( 1 \leq j \leq k \).

**Proposition 3.2.3.** Let \( \Gamma = (T_0, \theta) \) be a TAS which simulates a substitution rule \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) with border and \( \mathcal{A} = \{B_\ell\}_{\ell=0}^\infty \) be the substitution chain of \( \Gamma \). Let \( T = \{(Y_j)_{j=1}^k \} \in \mathcal{S} \) be the tiling of \( \lambda X \) for some \( X \in \mathcal{P} \). If \( v \) in \( G(T) = (V, E) \) is a bridge of \( \overline{G}(T) = (V, \overline{E}) \), then there exist \( L > 0 \) such that condition (*) holds for any assembly sequence \( \{(\alpha_i)\}_{i=0}^m \) of \( \Gamma \) where \( [\alpha_0] \in B_\ell \) for some \( \ell > L \), \([\alpha_m] \in B_{\ell+1} \), and \([\alpha_m]\) covers \( X^{\ell+1} \).

\[ (*) \text{ If } [\gamma] \in T_\infty \text{ such that } \gamma \text{ is the sum of } \alpha \text{ and } \beta \text{ where } \alpha = \bigcup_{j=1}^k \zeta_j \text{ is an instance of the unbordered assembly of } \{(\alpha_i)\}_{i=0}^m \text{ and } [\beta] \in T_\mathcal{B}, \text{ then there exist } v_1, v_2 \in V \text{ bridged by } v \text{ such that } \]

\[
\sum_{e \in K_\gamma(\alpha, \beta) \setminus K_\gamma(\beta, \zeta^i)} \omega_\gamma(e) < \theta \text{ for } \ell = 1, 2 \text{ where } \zeta^i \in \{\zeta_j\}_{j=1}^k \text{ represents } v_\ell.
\]

Moreover, the subgraph of \( G(T) \) induced by \( V \setminus \{v\} \) has exactly two components.

**Proof.** Let \( \mathcal{R}, \Gamma, \mathcal{A}, \) and \( T \) be as given. Let \( v \in V \) be a bridge of \( \overline{G}(T) \) in \( G(T) \), but suppose that the result does not hold – i.e., there exists an infinite subset \( Z \subset \mathbb{Z}^+ \) such that for each \( \ell \in Z \) and each pair of vertices \( v_1 \) and \( v_2 \) bridged by \( v \), there exist \( \alpha = \bigcup_{j=1}^k \zeta_j, \beta, \gamma, \) and \( \zeta^i \) as in the statement where

\[
\sum_{e \in K_\gamma(\alpha, \beta) \setminus K_\gamma(\beta, \zeta^i)} \omega_\gamma(e) \geq \theta \text{ for } \ell = 1 \text{ or } 2.
\]

Let \( \ell \in Z \) large enough such that for any border tile \( \beta' \) (i.e., \([\beta'] \in T_\mathcal{B}\)), if the sum of \( \beta' \) and \( \alpha \) is an assembly instance at temperature \( \theta \), then \( \ell \in \text{dom } \beta' \) is adjacent to at most two assembly instances in \( \{\zeta_j\}_{j=1}^k \). Note that this is possible because the shapes of each \( \zeta_j \) scale with the levels of the assembly blocks of \( \mathcal{A} \) while shapes of border tiles do not. Furthermore, the shape of \( \alpha \) is a topological disk by Proposition 3.1.5, so a border tile \( \beta' \) can either be adjacent to one assembly instance of \( \{\zeta_j\}_{j=1}^k \) or two. We infer from the above and Proposition 3.1.6 that \( \beta \) must be adjacent to two assembly instances of \( \{\zeta_j\}_{j=1}^k \) since \([\beta] \in T_\mathcal{B}\). Moreover, \( \beta \) must bind to both of these assembly instances since \( \gamma \) is an assembly instance at temperature \( \theta \).
Let $\zeta \in \{\zeta_j\}_{j=1}^k$ represent $v$ in $\alpha$. Let $G'$ be the subgraph of $\overline{G}(T)$ induced by $V \setminus \{v\}$. Because $v$ is a bridge of $\overline{G}(T)$ in $G(T)$, $G'$ has two or more components. Repeating the arguments in the proof of Proposition 3.2.1, we observe that if $\zeta', \zeta'' \in \{\zeta_j\}_{j=1}^k \setminus \{\zeta\}$ which represent two vertices $v'$ and $v''$, respectively, belonging to different components in $G'$, then $K_\gamma(\zeta', \zeta'') = \emptyset$ because such vertices have no coincident sides. It follows that there exists a partition $\{W_i\}_{i=1}^n$ of $\{\zeta_j\}_{j=1}^k \setminus \{\zeta\}$ corresponding to the $n \geq 2$ components of $G'$. Because $\alpha$ is an assembly instance (at temperature $\theta$), observe that each sum $\gamma_i$ of $W_i$ is an assembly instance (at temperature $\theta$). Moreover, each $[\gamma_i] \in T_\infty$ because $[\alpha] \in T_\infty$ and the elements of $W_i$ bind to form $\gamma_i$ independently of each other subset $W \neq W_i$.

By Proposition 3.1.6, observe that $\beta$ cannot be adjacent to two assembly instances in one subset $W \in \{W_i\}_{i=1}^n$ because the sum of $W$ and $\zeta$ is an assembly instance at temperature $\theta$. It follows that $\beta$ must be adjacent to some $\zeta' \in W' \in \{W_i\}_{i=1}^n$ and either to $\zeta$ or to $\zeta'' \in W'' \neq W'$ in $\{W_i\}_{i=1}^n$. The former case contradicts Proposition 3.1.6 because there is at least some other $W'' \neq W'$ which can bind to $\zeta$. In the latter case, we apply our contradiction assumption: since $W'$ and $W''$ correspond to separate components in $G'$,

$$\sum_{e \in K_\gamma(\alpha, \beta) \setminus K_\gamma(\beta, \zeta')} \omega_\gamma(e) \geq \theta \quad \text{or} \quad \sum_{e \in K_\gamma(\alpha, \beta) \setminus K_\gamma(\beta, \zeta'')} \omega_\gamma(e) \geq \theta$$

because $\zeta'$ and $\zeta''$ must represents two vertices $v'$ and $v''$, respectively, which are bridged by $v$. But $\beta$ binds to $\zeta''$ or $\zeta'$, respectively, by our assumption. In either case, we contradict Proposition 3.1.6 again; therefore, the result holds. Also, observe that the arguments above imply that there are at most two components in $G'$.

\[\square\]

**Corollary 3.2.4.** Let $\Gamma = (T_0, \theta) \in R = (P, \lambda, S)$ be a TAS which simulates a substitution rule $R = (P, \lambda, S)$ with border and $A = \{B_\ell\}_{\ell=0}^\infty$ be the substitution chain of $\Gamma$. Let $T = \{Y_j\}_{j=1}^k \in S$ be the tiling of $\lambda X$ for some $X \in P$. If $v$ in $G(T) = (V, E)$ is a pier of $\overline{G}(T) = (V, \overline{E})$, then there exist $\ell > 0$ such that condition $(\star)$ holds for any assembly sequence $\{[\alpha_i]\}_{i=0}^m$ of $\Gamma$ where $[\alpha_0] \in B_\ell$ for some $\ell > L$, $[\alpha_m] \in B_{\ell+1}$, and $[\alpha_m]$ covers $X^{\ell+1}$.

$(\star)$ If $[\gamma] \in T_\infty$ is such that $\gamma$ is the sum of $\alpha$ and $\beta$ where $\alpha = \bigsqcup_{j=1}^k \zeta_j$ is an instance of the unbordered assembly of $\{[\alpha_i]\}_{i=0}^m$ and $[\beta] \in T_B$, then

$$\sum_{e \in K_\gamma(\alpha, \beta) \setminus K_\gamma(\beta, \zeta)} \omega_\gamma(e) < \theta \quad \text{where} \quad \zeta \in \{\zeta_j\}_{j=1}^k \text{ represents } v.$$
Proof. Suppose that \( G \) is a connected graph, \( H \) is connected spanning subgraph of \( G \), and \( v \) is a pier of \( H \) in \( G \). Then by definition, the unique neighbor in \( H \) of \( v \) is a bridge of \( H \) in \( G \). By this observation, the result follows immediately from Proposition 3.2.3.

Corollary 3.2.5. Let \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) be a substitution rule such that every \( X \in \mathcal{P} \) is star-shaped. If either of the following holds for some \( T \in \mathcal{S} \), then \( \mathcal{R} \) does not admit bordered simulation: (i) there exist three (or more) piers of \( \overline{G}(T) \) in \( G(T) \), or (ii) there exist two (or more) non-adjacent vertices in \( G(T) \), each of which are either a pier or a bridge of \( \overline{G}(T) \).

Proof. This result follows from the proof of Proposition 3.2.3, the proof of Proposition 3.1.6, and the following observation: because each \( T \in \mathcal{S} \) is a tiling of a polygon, every boundary corner of \( T \) is the intersection of exactly two boundary sides.

\[ \text{Figure 3.06. The Triangle substitution rule and its associated corner and side adjacency graphs. Let } T \text{ be the tiling of this substitution rule, and note that there are three piers of } \overline{G}(T) \text{ in } G(T): \text{ polygons 1, 2, and 4. By Corollary 3.2.5, it follows that this substitution rule does not admit bordered simulation.} \]

In Figures 3.04 and 3.06, we give some examples of substitution rules which satisfy the criteria of Proposition 3.2.1 and Corollary 3.2.5, respectively. We also note that most of the substitution rules presented in [43] satisfy the criteria of one the aforementioned results. We consider all of the substitution rules in [12–14, 18–20, 43] which do not satisfy the criteria for these results in Chapter 4 with the exception of one substitution rule: the Trapezotriangular substitution rule (Figure 3.07). While this substitution rule does not satisfy the conditions for Proposition 3.2.1 or Corollary 3.2.5, we observe that this substitution rule does not admit bordered simulation. This observation follows from Corollaries 3.1.8 and 3.1.9 and from the proof of Proposition 3.2.1. Indeed, if we suppose that the Trapezotriangular substitution rule does admit bordered simulation, we can arrive at contradictions while analyzing how an assembly can be associated with a supertile \( \sigma^f(X_1) \).
Figure 3.07. The Trapezotriangular substitution rule [13] and its associated corner and side adjacency graphs.
Chapter 4
Sufficient Conditions for Bordered Simulation

In this chapter, we provide a sufficient condition for determining if a substitution rule \( R = (P, \lambda, S) \) admits bordered simulation. This condition is placed upon the corner and side adjacency graphs of the tilings in \( S \) and is inspired by the results in Sections 3.1 and 3.2. In Section 4.1, we present the concept of “backtrack constructible” graphs and then relate this concept to the tilings in \( S \) to define the aforementioned condition. We then formalize our condition and present proof that it is sufficient in Section 4.2. Note that the set of bonds \( \Sigma \) and the strength function \( s : \Sigma \to \mathbb{Z}_{\geq 0} \) for TAS \( \Gamma = (T_0, \theta) \) are often implied for proofs involving arbitrary tile assembly systems (e.g., Section 3.1). However, both \( \Sigma \) and \( s \) must be explicitly defined alongside \( T_0 \) when proving the existence of a TAS \( \Gamma \) (e.g., Example 2.3.6).

4.1 Backtrack Constructible Graphs

We begin by defining the notion of a spanning subgraph being “backtrack connected” within its parent graph. This notion is motivated by our concept of a TAS \( \Gamma \) simulating a substitution rule \( R \) with border from Section 2.3. Specifically, Definition 4.1.1 is based on Proposition 3.1.7 and Corollary 3.1.9. As in Section 3.2, the definitions in this section are given for a connected graph \( G = (V, E) \) and a connected spanning subgraph \( H = (V, E) \) of \( G \), which we visualize simultaneously. Because we only consider simple graphs, we denote a path \( p \) in \( G \) by \( p = v_0v_1 \cdots v_n \) and call \( v_0 \) and \( v_n \) the endpoints of \( p \). A path is trivial if it visits one vertex \( v \in V \) and Hamiltonian if it visits every vertex of \( G \).

**Definition 4.1.1.** Let \( G = (V, E) \) be a connected graph and \( H = (V, E) \) be a connected spanning subgraph of \( G \). A path \( p = v_0 \cdots v_n \) in \( H \) is \( G \)-backtrack if for all \( i > 1 \), there exists \( j < i - 1 \) such that \( \{v_i, v_j\} \in E \); we call such edges \( \{v_i, v_j\} \) the backtrack edges associated with \( p \). In this context, we denote \( v_n \) by \( \tau(p) \) and call this the target of \( p \). We say that \( H \) is \( G \)-backtrack connected (via \( p \)) if there exists a Hamiltonian path \( p \) in \( H \) which is \( G \)-backtrack.
Figure 4.01. A graph $G$ and a spanning subgraph $H$ of $G$ on seven vertices. Let $p_1 = v_1v_2v_3v_4$, $p_2 = v_3v_4v_5$, and $p_3 = v_6v_5v_4v_3$. Then note that $p_1$ and $p_3$ are $G$-backtrack paths in $H$ by definition. On the other hand, $p_2$ is not a $G$-backtrack path in $H$ because $v_3$ and $v_5$ are not adjacent in $G$. Also, note that the reverse path of $p_1$ is also $G$-backtrack path in $H$ but the reverse path of $p_3$ is not a $G$-backtrack path in $H$. If we denote the reverse path of $p_3$ by $p_3'$, then note that $p_3'$ starts at $v_3$ and visits $v_4$ and $v_5$ before $v_6$. Because $v_3$ and $v_5$ are not adjacent in $G$, $p_3'$ fails to be $G$-backtrack.

Figure 4.02. The adjacency graphs for (a) the tiling $T$ of the Pinwheel substitution rule and (b) the tiling $T_2$ of $\lambda X_2$ of the Pentiamond AC Factor 2 substitution rule. We note that $\overline{G}(T)$ is $G(T)$-backtrack connected and $\overline{G}(T_2)$ is $G(T_2)$-backtrack connected. We denote the associated paths for these tilings in red and enumerate the polygons (vertices) of these graphs in accordance to the order of the associated paths.

The intuition behind a $G$-backtrack path $p$ in $H$ is that as we move from $v_i$ to $v_{i+1}$ along $p$, we are always able to “see” some previous vertex other than $v_i$ through a backtrack edge in $G$; in other words, the $p$ bends back on itself within $G$ via backtrack edges. In Figures 4.01 and 4.02, we give some examples of $G$-backtrack paths in $H$. If $p$ is also a Hamiltonian path in $H$ and there exists a bridge $v$ of $H$ in $G$, then the subgraph of $H$ induced by $V \setminus \{v\}$ has exactly two components and each endpoint of $p$ must belong to a distinct component. Similarly, if there exists a pier $v$ of $H$ in $G$, then $v$ is an endpoint of $p$ because $d_H(v) = 1$. In Remark 4.1.2 we make a similar observation about Hamiltonian, $G$-backtrack paths in $H$. Note that a path in $H$ with one or two vertices is vacuously $G$-backtrack.

Remark 4.1.2. Let $G = (V, E)$ be a connected graph and $H = (V, \overline{E})$ be a connected spanning subgraph of
Suppose that there exists a pair of vertices $x_1$ and $x_2$ adjacent in $H$ such that the subgraph of $G$ induced by $V \setminus \{x_1, x_2\}$ has two or more components; in this case, we call $\{x_1, x_2\}$ a a **choke-hold pair in $H$**. If $p = v_0 \cdots v_n$ is a path in $H$ such that $v_0 \in \{x_1, x_2\}$, then $p$ can visit the vertices in at most two components. The same is true if $p$ is $G$-backtrack and $v_0 \notin \{x_1, x_2\}$. If $v_0$ belongs to one component and $p$ visits a vertex in a second component, then $p$ must visit $x_1$ or $x_2$; without loss of generality, suppose $p$ visits $x_1$. Since there are no edges in $G$ between vertices in these distinct components by assumption, it follows that $p$ must also visit $x_2$ to satisfy the backtrack edge adjacency requirement of Definition 4.1.1 before visiting any vertices in the second component. Now suppose that $p$ is a Hamiltonian, $G$-backtrack path in $H$; then the subgraph $G'$ of $G$ induced by $V \setminus \{x_1, x_2\}$ has exactly two components. Moreover, if $v_0 \notin \{x_1, x_2\}$ and $v_n \notin \{x_1, x_2\}$, then $v_0$ and $v_1$ cannot be in the same component of $G'$ because $p$ is Hamiltonian.

In Definition 4.1.3, we consider the situation where some of the backtrack edges associated with a $G$-backtrack path in $H$ are edges in $\mathcal{E}$. The existence of such edges is an inherently stronger condition than the one in Definition 4.1.1 since these edges entangle $p$ within $H$.

**Figure 4.03.** The adjacency graphs for (a) the tiling $T$ of the Chair substitution rule and (b) the tiling $T_1$ of $\lambda X_1$ of the Pentiamond AC Factor 2 substitution rule. We note that $G(T)$ is $G(T)$-backtrack connected and $\overline{G}(T_1)$ is $G(T_1)$-backtrack connected. We denote the associated paths for these tilings in red and enumerate the polygons (vertices) of these graphs in accordance to the order of the associated paths. Moreover, we note that the Hamiltonian, $G(T)$-backtrack path $p$ in $\overline{G}(T)$ is robust up to polygon (vertex) 4. On the other hand, the Hamiltonian, $G(T_1)$-backtrack path $p'$ in $\overline{G}(T_1)$ is only robust up to polygon (vertex) 3 because there is no edge in $\overline{G}(T_1)$ from polygon 4 to a polygon before 3.

**Definition 4.1.3.** Let $G = (V, E)$ be a connected graph, $H = (V, \mathcal{E})$ be a connected spanning subgraph of $G$, and $p = v_0 \cdots v_n$ be a nontrivial, $G$-backtrack path in $H$. We say that $p$ is **robust up to** $v_r$ for $1 \leq r \leq n$ if there exists a set of indices $J = \{i_1, i_2, \ldots, i_m = r\}$ such that $\{v_0, v_{i_1}\} \in \mathcal{E}$ and for $1 < j \leq m$, there exists $k < i_{j-1}$ so that $\{v_k, v_{i_j}\} \in \mathcal{E}$. We call such edges $\{v_0, v_{i_1}\}$ and $\{v_{k}, v_{i_j}\}$ robust backtrack edges.
associated with $p$.

Any nontrivial $G$-backtrack path $p = v_0v_1\cdots v_n$ in $H$ is at least robust up to $v_1$. For the purpose of notation, we say that a trivial path $p = v_0$ is robust up to $v_0$. Thus, any $G$-backtrack path $p$ in $H$ is robust up to $v_r$ for some index $r$. We always take $1 \leq r \leq n$ to be as large as possible given a $G$-backtrack path $p$ so that $p$ is robust up to $v_r$. Note that it is always possible to find such a maximal $r$ since $G$ and $H$ are finite simple graphs.

For use in later definitions, we define $\epsilon(p) = \{\{x, y\} \mid x, y \in V \text{ are consecutive in } p \text{ or } \{x, y\} \in \overline{E} \text{ is a robust backtrack edge associated to } p\}$. Informally, $\epsilon(p) \subseteq \overline{E}$ represents the set of edges in $\overline{E}$ which are necessary for $p = v_0\cdots v_n$ to be $G$-backtrack and robust up to $v_r$. Note that $\epsilon(p) = \emptyset$ when $p$ is a trivial path. Additionally, we define the set $\pi(p)$ as follows and note that it is also well-defined by the previous paragraph: $\pi(p) = \{v_i \mid i < r \text{ or } i = n\}$; we call vertices in $\pi(p)$ robust vertices of $p$.

We pause here to consider the substitution rules in [12–14, 18–20, 43], recalling from Section 2.3 that every one of these substitution rules has star-shaped prototiles. Let $R = (\mathcal{P}, \lambda, \mathcal{S})$ be such a substitution rule, and suppose that $R$ does not satisfy the criteria of Proposition 3.2.1 nor of Corollary 3.2.5. Then a tiling $T \in \mathcal{S}$ frequently has the following property: $\overline{G}(T)$ is $G(T)$-backtrack via a path $p$. In order to capture the tilings of substitution rules which do not have the property above, we generalize our notion of being backtrack connected to being “backtrack constructible”. The idea for this is to partition the vertex set of $H$ and extend the backtrack edge requirement to subsets in this partition. We start by defining a “backtrack partition” of the vertices in $H$.

**Definition 4.1.4.** Let $G = (V, E)$ be a connected graph, $H = (V, \overline{E})$ be a connected spanning subgraph of $G$, and $\Lambda = \{V_i\}_{i=0}^n$ be a partition of $V$. Let $G_i = (V_i, E_i)$ and $H_i = (V_i, \overline{E}_i)$ be the subgraphs of $G$ and $H$, respectively, induced from $V_i$ for each $0 \leq i \leq n$. We say that $\Lambda$ is a (stage 1) backtrack partition of $H$ if the following hold:

- For $0 \leq i \leq n$, there exists a Hamiltonian, $G_i$-backtrack path $p_i$ in $H_i$.

- The spanning subgraph $G^1(\Lambda) = (V, E^1(\Lambda))$ of $H$ is connected where $e = \{x, y\} \in E^1(\Lambda) \subseteq \overline{E}$ if (a) $\{x, y\} \in \epsilon(p_i)$ for some $0 \leq i \leq n$, or (b) $x \in \pi(p_i)$ and $y \in \pi(p_j)$ for $0 \leq i \neq j \leq n$.

We use $\overline{E}^1(\Lambda)$ to denote the set of such edges in $E^1(\Lambda)$ adhering to condition (2)(b) above. In this context, we say that each $H_i$ is a backtrack component (at stage 1).
In essence, a backtrack partition of $H$ consists of backtrack connected subgraphs (i.e., backtrack components) and the edges connecting their robust vertices to each other (i.e., binding edges). We formalize the idea of being “backtrack constructible” in Definition 4.1.5, noting that the technical requirements generalize the idea of a path bending back on itself in $G$. We also generalize the idea of robustness for backtrack paths afterwards.

**Definition 4.1.5.** Let $G = (V, E)$ be a connected graph and $H = (V, \overline{E})$ be a connected spanning subgraph of $G$. We say that $H$ is $G$-backtrack constructible (at stage 1) via $(f, \rho)$ if there exists a backtrack partition (at stage 1) $\Lambda = \{V_i\}_{i=0}^n$ of $V$ and a set of edges $\rho \subset \overline{E}$ such that conditions below hold, relabeling $\{V_i\}_{i=0}^n$ if necessary:

1. There exists a pair of edges $\{x_0, x_1\}, \{y_0, y_1\} \in \rho$ (denoted $C^1$) such that $x_i, y_i \in \pi(p_i), x_i \neq y_i$, and $x_i = \tau(p_i)$ or $y_i = \tau(p_i)$ for $i = 0, 1$. Note that if $i > 0$, this implies that $|V_0|, |V_1| > 0$.

2. For $i > 1$, there exist a pair of edges $\{x, x'\}, \{y, y'\} \in \rho$ (denoted $C^i$) such that $x, y \in \pi(p_i), x' \in \pi(p_{i-1})$, and the following hold:
   
   (a) If $|V_i| = 1$, then $y' \in \pi(p_j)$ for some $j < i - 1$ and $\{x', y'\} \in E$.
   
   (b) If $|V_i| > 1$, then $y' \in \pi(p_j)$ for some $j < i - 1$, $x \neq y$, and $x = \tau(p_i)$ or $y = \tau(p_i)$.

We call $\rho$ a (stage 1) route and call the pairs of edges $C^1$ (for $i > 0$) clumps (at stage 1). We use the notation $\rho = C^1 C^2 \cdots C^k$ accordingly; we denote $V_n$ by $\tau(\rho)$ and call this the target of $\rho$. A clump $C^i$ forks to $V_k$ for $k < i - 1$ if there exists $z, z' \in C^i$ such that $z \in V_i$ and $z' \in V_k$. In this situation, we call $V_{i-1}$ and $V_k$ the (stage 1) predecessors of $V_i$; otherwise we simply call $V_{i-1}$ the (stage 1) predecessor of $V_i$.

We say that $\rho$ is robust up to $V_r$ for $1 \leq r \leq n$ if there exists a set of indices $J = \{i_1 = 1, i_2, \ldots, i_m = r\}$ such that for $1 < j \leq m$, there exists $k < i_{j-1}$ so that $C^i_{i_j}$ forks to $V_k$. By convention, we take $r$ to be as large as possible and define $\pi(\rho) = \{v \mid v \in V_i \text{ where } i < r \text{ or } i = n\}$. Moreover, we define the set of fastening edges of $(f, \rho)$, denoted by $e^1(f, \rho) \subset \overline{E}$, as follows: $\{x, y\} \in e^1(f, \rho)$ if (a) $\{x, y\} \in e(p_i)$ for some $0 \leq i \leq n$, or (b) $\{x, y\} \in C^i_{i_1}$ for $1 \leq i \leq n$.

Intuitively, a (stage 1) route $\rho$ generalizes a $G$-backtrack path, with clumps $C^1$ simultaneously replacing edges and backtrack edges. The set $e^1(f, \rho)$ identifies all of the edges of $H$ relevant to our generalization of backtrack connectedness. We give a detailed example of a spanning subgraph $H$ which is $G$-backtrack constructible (at stage 1) in Figure 4.04 using the adjacency graphs of the Extended Armchair substitution.
rule. Note that Definition 4.1.5 allows backtrack components $V_i$ to be singletons for $i > 1$ and also permits a partition of $V$ to be trivial (i.e., to have one backtrack component). We make use of this flexibility shortly when generalizing backtrack constructibility.

**Figure 4.04.** The Extended Armchair substitution rule and induced adjacency graphs. Let $T$ be the tiling of this substitution rule, and note that $\overline{G}(T)$ has three mutually disjoint choke-hold pairs. We infer from Remark 4.1.2 that $\overline{G}(T)$ is not $G(T)$-backtrack connected. On the other hand, note that the following paths are all $G(T)$-backtrack in $\overline{G}(T)$: $p_1 = 1 - 2 - 3 - 4 - 5 - 6$, $p_2 = 7 - 8$, and $p_3 = 9 - 10 - 11 - 12 - 13 - 14 - 15 - 16$. It follows that $\overline{G}(T)$ is $G(T)$-backtrack constructible at stage 1. The edges associated with $G(T)$-backtrack paths are indicated in red, and the edges associated with the (stage 1) route are in blue.

Having established the notion of graphs which are backtrack constructible at stage 1, we are now ready to extend our notion to a stage $\eta \geq 1$ in the same manner that we extended backtrack connectedness. We use subgraphs which are backtrack constructible at stage $\eta - 1$ to “build” a graph that is backtrack constructible at stage $\eta$ in the same way that backtrack connected subgraphs form a backtrack constructible graph at stage 1. Note that we reuse word choice and notation of Definitions 4.1.4 and 4.1.5, increasing the superscript of relevant mathematical objects as appropriate; in this way, Definition 4.1.6 naturally extends the two previous definitions.

**Definition 4.1.6.** Let $G = (V, E)$ be a connected graph, $H = (V, \overline{E})$ be a connected spanning subgraph of $G$, and $\Lambda = \{V_i\}_{i=0}^{n}$ be a partition of $V$. Let $G_i = (V_i, E_i)$ and $H_i = (V_i, \overline{E}_i)$ be the subgraphs of $G$ and
There exists a pair of edges $i > j$ for $0 \leq i \leq n$. We say that $\Lambda$ is a stage $\eta > 1$ backtrack partition of $H$ if the following hold:

- For $0 \leq i \leq n$, $H_i$ is $G_i$-backtrack constructible at stage $\eta - 1$ via $(\Lambda_i, \rho_i)$.

- The spanning subgraph $G^n(\Lambda) = (V, E^n(\Lambda))$ of $H$ is connected where $e = \{x, y\} \in E^n(\Lambda) \subset \overline{E}$ if (a) $e \in e^{n-1}(\Lambda_i, \rho_i)$ for some $0 \leq i \leq n$, or (b) $x \in \pi(\rho_i)$ and $y \in \pi(\rho_j)$ for $0 \leq i \neq j \leq n$.

We use $\overline{E}^\eta(\Lambda)$ to denote the set of such edges in $E^n(\Lambda)$ adhering to condition (2)(b) above. In this context, we say that each $H_i$ is a backtrack component at stage $\eta$.

We say that $H$ is $G$-backtrack constructible at stage $\eta$ via $(\Lambda, \rho)$ if there exists a stage $\eta$ backtrack partition $\Lambda = \{V_i\}_{i=0}^n$ of $V$ and a set of edges $\rho \subset \overline{E}^\eta(\Lambda)$ such that conditions below hold, relabeling $\{V_i\}_{i=0}^n$ if necessary:

1. There exists a pair of edges $\{x_0, x_1\}, \{y_0, y_1\} \in \rho$ (denoted $C_i^\rho$) such that $x_i, y_i \in \pi(\rho_i)$, $x_i \in V \in \Lambda_i$ and $y_i \in V' \in \Lambda_i$ such that $V \neq V'$, and $x_i \in \tau(\rho_i)$ or $y_i \in \tau(\rho_i)$ for $i = 0, 1$. Note that if $i > 0$, this implies that $|V_0|, |V_1| > 0$.

2. For $i > 1$, there exist a pair of edges $\{x, x'\}, \{y, y'\} \in \rho$ (denoted $C_i^\rho$) such that $x, y \in \pi(\rho_i)$, $x' \in \pi(\rho_{i-1})$, and the following hold:

   a) If $|V_i| = 1$, then $y' \in \pi(\rho_j)$ for some $j < i - 1$ and $\{x', y'\} \in E$.

   b) If $|V_i| > 1$, then $y' \in \pi(\rho_j)$ for some $j < i - 1$, $x \in V \in \Lambda_i$ and $y \in V' \in \Lambda_i$ such that $V \neq V'$, and $x \in \tau(\rho_i)$ or $y \in \tau(\rho_i)$.

We call $\rho$ a stage $\eta$ route and call the pairs of edges $C_i^\rho$ (for $i > 0$) clumps at stage $\eta$. We use the notation $\rho = C_1^n C_2^n \cdots C_n^n$ accordingly; we denote $V_n$ by $\tau(\rho)$ and this the target of $\rho$. A clump $C_i^\rho$ forks to $V_k$ for $k < i - 1$ if there exists $\{z, z'\} \in C_i^\rho$ such that $z \in V_i$ and $z' \in V_k$. In this situation, we call $V_{i-1}$ and $V_k$ the stage $\eta$ predecessors of $V_i$; otherwise we simply call $V_{i-1}$ the stage $\eta$ predecessor of $V_i$.

We say that $\rho$ is robust up to $V_r$ for $1 \leq r \leq n$ if there exists a set of indices $J = \{i_1 = 1, i_2, \ldots, i_m = r\}$ such that for $1 < j \leq m$, there exists $k < i_{j-1}$ so that $C_{i_j}^\rho$ forks to $V_k$. By convention, we take $r$ to be as large possible and define $\pi(\rho) = \{v \mid v \in V_i \text{ where } i < r \text{ or } i = n\}$. Moreover, we define the set of fastening edges of $(\Lambda, \rho)$, denoted by $e^n(\Lambda, \rho) \subset \overline{E}$, as follows: $\{x, y\} \in e^n(\Lambda, \rho)$ if (a) $e \in e^{n-1}(\Lambda_i, \rho_i)$ for some $0 \leq i \leq n$, or (b) $\{x, y\} \in C_i^\rho$ for $1 \leq i \leq n$. 58
For the purpose of notation, we say that a subgraph $H$ which is $G$-backtrack connected via a path $p$ is $G$-backtrack constructible at stage 0 via $(\Lambda = \{V\}, p)$, and we call the path $p$ a stage 0 route. Moreover, we take “$x \in \tau(p)$” to mean $x = \tau(p)$ when we use the former notation and denote $\epsilon(p)$ by $\epsilon^0(\{V\}, p)$. Observe that because partitions may be singletons, a graph which is $G$-backtrack constructible at stage $\eta$ is also $G$-backtrack constructible at every stage greater than $\eta$; we typically take $\eta$ to be the least possible. Thus, a graph which is $G$-backtrack constructible at stage $\eta$ may be “constructed” from subgraphs which are backtrack constructible at various stages less than $\eta$.

We turn our attention to substitution rules for the final definition in this section. We note that Definition 4.1.7 is motivated by the results in Chapter 3 like the rest of the definitions in this section.

**Definition 4.1.7.** Let $S \subset \mathbb{R}^2$ be bounded, and let $T$ be a finite tiling of $S$. We say that $T$ is backtrack constructible (at stage $\eta \geq 0$) if the following hold:

1. $G(T)$ is $G(T)$-backtrack constructible at stage $\eta \geq 0$ via $(\Lambda, \rho)$.

2. If $|T| > 1$, then there exist polygons $x_1 \neq x_2$ in $T$ such that $x_i$ has a boundary side $L_i$ of $T$ for $i = 1, 2$ and $L_1 \cap L_2 \neq \emptyset$. Moreover, $x_1 \in \pi(\rho) \setminus \tau(\rho)$ and $x_2 \in \tau(\rho)$.

In Section 4.2, we show that a substitution rule $\mathcal{R}$ admits bordered simulation if every tiling in $\mathcal{R}$ is backtrack constructible and if $\mathcal{R}$ satisfies some minor requirements. This is our main result, and we note that every substitution rule in [12–14, 18–20, 43] which fails to satisfy this sufficient condition can be shown to not admit bordered simulation using the results in Section 3.2. This includes the Trapezotriangular substitution rule (Figure 3.07).

### 4.2 Constructing Tile Assembly Systems for Bordered Simulation

We begin with two notions which we use in the constructions associated with our main result (Corollary 4.2.4).

**Definition 4.2.1.** A tiling $\{P_i\}_{i \geq 1}$ of $S \subset \mathbb{R}^2$ is sibling side-to-side if the following holds for any distinct $P, P' \in \{P_i\}_{i \geq 1}$: if a side $L$ of $P$ intersects a side $L'$ of $P'$ at more than one point, then $L$ and $L'$ are coincident.

Intuitively, sibling side-to-side tilings require that polygons only overlap at coincident sides. These tilings are more commonly called “sibling edge-to-edge” [19]; as stated in Chapter 2, we avoid the use of “edge”
in favor of "side" when discussing polygons. If \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) is a substitution rule and every supertile of \( \mathcal{R} \) is sibling side-to-side, then we say that \( \mathcal{R} \) admits sibling sides.

**Definition 4.2.2.** Let \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) be a substitution rule, and consider a polygon \( \lambda X \in \lambda \mathcal{P} \) and its tiling \( \{Y_j\}_{j=1}^k \in \mathcal{S} \). We say that the prototile \( X \in \mathcal{P} \) has hereditary sides if each side of \( \lambda X \) is the union of some boundary sides of \( \{Y_j\}_{j=1}^k \). If every prototile in \( \mathcal{P} \) has hereditary sides, then \( \mathcal{R} \) admits hereditary sides.

For our main result (Corollary 4.2.4), we require that a given substitution rule admits hereditary and sibling sides. As noted in [19], this requirement is quite mild because every substitution rule which we have encountered [12–14, 18–20, 43] can be modified to admit hereditary and sibling sides. By modifying a substitution rule \( \mathcal{R} \), we mean changing the sides of the prototiles of \( \mathcal{R} \) so that the \( \mathcal{R} \) satisfies our condition. Typically, this modification involves cutting the sides of one or more prototiles so that \( \mathcal{R} \) admits sibling sides; see Figure 4.05 for example. It may be easy to show that some substitution rule does not admit hereditary or sibling sides even with modification, but we do not know of such an example.

![Figure 4.05](image_url)

**Figure 4.05.** The Pinwheel Substitution Rule, modified to admit hereditary and sibling sides. Note that this modification is accomplished by cutting the long leg of prototile \( X \) in half.

In order to prove Corollary 4.2.4, we first construct a TAS \( \Gamma \) which simulates a substitution rule \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) with border under the assumption that all tilings in \( \mathcal{S} \) are backtrack constructible at stage 0 (Theorem 4.2.3). Then, we generalize this construction under the assumption that all tilings in \( \mathcal{S} \) are backtrack constructible at stage \( \eta \geq 0 \) (Corollary 4.2.4). The construction processes in these two results are heavily motivated by the constructions in [19, 31] and summarized below. We use the term “decorate” below to mean the process of assigning specific bonds to the sides of a given polygon.

1. Mark the polygons in each \( T \in \mathcal{S} \) according to the edges of stage 0 backtrack routes, then the stage 1 backtrack routes, and so on until the edges in all routes have corresponding markings. Then, use these markings to define the set of bonds \( \Sigma \).
2. Define and decorate the tile types which will belong to the assembly block at level 0 \((B_0)\) of the substitution chain \(A\) of the TAS \(\Gamma\) once it is fully constructed.

3. Create polygon templates for the border tiles based on the tilings \(T \in S\) and a fixed \(\kappa > 1\). These polygons will essentially fall into three categories: parallelograms, trapezoids, and concave polygons. Then, define and decorate the border tiles.

We provide examples for these construction processes in this section and in Appendix C. We also note that the TAS described in Example 2.3.6 follows this construction with a minor modification; we elaborate on this modification in Section C.1. As in Example 2.3.6, we uniquely associated each assembly in an assembly block \(B_\ell\) (at level \(\ell \geq 0\)) to a fixed polygon in a tiling \(T \in S\), if possible. In this way, the number of assemblies in associated to a prototile \(X \in \mathcal{P}\) will be the number of congruent images of \(X\) in all of the tilings of \(S\) if there are any; otherwise, there will only assembly associated to \(X\).

**Theorem 4.2.3.** Let \(\mathcal{R} = (\mathcal{P}, \lambda, S)\) be a substitution rule which admits hereditary and sibling sides such that every \(X \in \mathcal{P}\) is star-shaped. If every tiling \(T \in S\) is backtrack constructible at stage 0, then there exists a TAS \(\Gamma = (T_0, 2)\) which simulates \(\mathcal{R}\) with border.

**Proof.** Let \(\mathcal{R}\) be as given; for each \(T \in S\), there exists a Hamiltonian path \(p = v_0v_1 \cdots v_{|T|−1}\) which is \(G(T)\)-backtrack path in \(\overline{G}(T)\) by assumption. We denote the corner and side adjacency graphs for \(T \in S\) by \(G(T) = (T, E(T))\) and \(\overline{G}(T) = (T, \overline{E}(T))\) as is custom.

**Claim:** Let \(T \in S\) such that \(|T| > 2\) and \(2 \leq i < |T|\). Suppose that there does not exist any \(j < i − 1\) such that \({v_i, v_j}\) \(\in \overline{E}(T)\). Then there exist \(j < i − 1\) and two adjacent sides \(L_1\) and \(L_2\) of \(v_{i−1}\) such that \(L_1\) coincides with some side of \(v_j\) and \(L_2\) coincides with some side of \(v_i\).

**Proof of Claim.** Because \(p\) is \(G(T)\)-backtrack, there exists \(j < i − 1\) such that \({v_i, v_j}\) \(\in E(T)\). By assumption, \({v_i, v_j}\) \(\in E(T) \setminus \overline{E}(T)\); this implies that \(v_i\) and \(v_j\) coincide in at least one point. Relabeling if necessary, we choose \(j < i − 1\) to be as large as possible such that the statements above still hold. Recall that each \(v_k \in T\) is adjacent to \(v_{k−1}\) and \(v_{k+1}\) in \(\overline{G}(T)\), if they exist. If \({v_{i−1}, v_j}\) \(\not\in E(T)\), then observe that the polygons \({v_j, v_{j+1}, \ldots, v_{i−1}\} \) enclose a topological hole; see Figure 4.06(a). Similarly, if \({v_{i−1}, v_j}\) \(\in E(T) \setminus \overline{E}(T)\), then either \({v_j, v_{j+1}, \ldots, v_{i−1}\} \) or \({v_j, v_{i−1}, v_i}\) enclose a topological hole; see Figures 4.06(b) and 4.06(c), respectively. On the other hand, suppose that \(v_{i−1}\) intersects \(c\) but \(c\) is not a corner of a side of \(v_{i−1}\) which coincides with a side of \(v_i\). Then because \({v_{i−1}, v_i}\) \(\in \overline{E}(T)\) by assumption, \(v_{i−1}\) and \(v_i\) enclose a topological hole; see Figure 4.06(d).
Figure 4.06. Visualization of the four cases for the first claim of Theorem 4.2.3. In (a), we assume that a polygon $v_i$ is adjacent to the corner of some $v_j$ where $j < i - 1$, but $v_{i-1}$ and $v_j$ are not adjacent in $G(T)$. In (b) and (c), we assume that $v_i$, $v_{i-1}$, and $v_j$ are all corner adjacent, but $v_{i-1}$ and $v_j$ are not adjacent in $\overline{G(T)}$. In (d), we assume that there is a corner in $v_i \cap v_{i-1} \cap v_j$, but this corner is not an endpoint of a side of $v_{i-1}$ which coincides with a side of $v_i$. As visualized above, note that in all four cases the set of polygons $\{v_j, v_{j+1}, \ldots, v_i\}$ encloses a topological hole.

In any of the cases above, note that there must be some set of polygons $Z \subset T$ such that $\{v_0, \ldots, v_i\} \cup Z$ is a topological disk because $T$ is a tiling of polygon $\lambda X$ for some $X \in \mathcal{P}$. Note that no polygon in $Z$ can be adjacent to a polygon $v_k$ for $k > i$, and each polygon in $Z$ cannot be a boundary polygon of $T$. Since $p$ is Hamiltonian, it follows that $\tau(p) \in Z$; but this contradicts the assumption that $\tau(p)$ is a boundary polygon (see Definition 4.1.7). Therefore, the claim holds. ■

(Step 1, Mark Polygons.) As mentioned informally before this theorem, we use the markings which we assign here to define a set of bonds $\Sigma$. Given a tiling $T \in \mathcal{S}$, we assign markings to the polygons in $T$; in particular, we assign a marking to a polygon $v \in T$ and a corner of $v$. The set of markings which we employ is $\{\bigcirc, \oplus, \ominus, \bullet, \oslash, \triangleleft\}$. The last marking, $(\triangleright)$, is used to define bonds which allow border tiles to begin binding to an assembly. All other markings are used to define bonds which coordinate how assemblies bind together if they correspond to supertiles of $\mathcal{R}$; we elaborate on these bonds later in the proof. We also make use of the fact that every tiling in $\mathcal{S}$ is sibling side-to-side; this follows from our assumption that $\mathcal{R}$ admits sibling sides.

Let $T \in \mathcal{S}$; until we indicate otherwise, we suppose that $|T| \geq 2$. We progressively mark each $v_i \in T$ (for $1 < i < |T|$) according to the following conditions.

A. Suppose there exists $j < i - 1$ such that $\{v_i, v_j\} \in \overline{E}(T)$, and let $c \in v_i \cap v_j$ be a corner of a side $L$ of
Furthermore, the following hold:

B. Suppose that the condition above does not hold. Then by the claim above, there exist \( j < i - 1 \) and two adjacent sides \( L_1 \) and \( L_2 \) of \( v_{i-1} \) such that \( L_1 \) coincides with some side of \( v_j \) and \( L_2 \) coincides with some side of \( v_i \). Let \( e \) be the unique point \( i \in L_1 \cap L_2 \); note that \( e = v_j \cap v_{i-1} \cap v_i \). We use \((\oplus_i, e)\) to mark \( v_i \) and \((\ominus_i, e)\) to mark \( v_j \). Moreover, we mark \( v_{i-1} \) with both \((\ominus_i, e)\) and \((\ominus_i, e)\).

Note that if \( |T| = 2 \), then no elements of \( T \) have been marked yet.

By our marking process above, each \( v_i \) has one \((\ominus_i, e)\) or one \((\oplus_i, e)\) for \( 1 < i < |T| \). A corner \( e \) in \( v_i \) for \( 0 \leq i \leq |T| - 1 \) may be associated with multiple markings following the process above. However, if a polygon \( v_i \) has is marked with \((\ominus_i, c_1)\) and \((\ominus_{i+1}, c_2)\), then note that \( c_1 \neq c_2 \). If \( c = c_1 = c_2 \), then \( e \) would have to be a corner of three distinct sides of \( v_i \). Also, observe that each \( v_i \in T \) has at most one of each of the following markings: \((\ominus_{i+2}, e)\), \((\oplus_{i+1}, e)\), and \((\ominus_{i+1}, e)\).

For \( 0 < i < |T| \), let \( L_i \) and \( L_i' \) a pair of coincident sides of \( v_i \) and \( v_{i-1} \), respectively. Such a pair exists because \( \{v_{i-1}, v_i \} \in \overline{E}(T) \) by assumption. Recall by the above, that \( v_i \) has either \((\ominus_i, e)\) or \((\oplus_i, e)\) when \( i > 1 \) and otherwise \( v_i \) has neither marking. We mark each \( v_i \) according the following conditions.

C. Suppose that \( v_i \) is not marked with \((\ominus_i, c_1)\), \((\oplus_i, c_2)\), or \((\ominus_{i+1}, c_3)\) for any corners \( c_1, c_2, c_3 \in v_i \). Then let \( e \) be one corner of \( L \) and \( e' \) be other corner. We use \((\bullet_i, e)\) and \((\circ_i, e')\) to both \( v_i \) and \( v_{i-1} \), noting that \( e, e' \in v_i \cap v_{i-1} \).

D. Suppose that \( v_i \) is marked with \((\ominus_i, e)\) or \((\oplus_i, e)\), where \( e \) is some corner of \( v_j \). Further, suppose that \( v_i \) is either not marked with \((\ominus_{i+1}, \hat{e})\) or marked with \((\ominus_{i+1}, \hat{e})\) but \( \hat{e} = e \). Let \( e' \) be a corner of \( L \) such that \( e' \neq e \); we use \((\bullet_i, e')\) to mark both \( v_i \) and \( v_{i-1} \).

By our marking procedures thus far, observe that if \( v \in T \) is marked with \((x, c)\) for some marking \((x)\) and some \( c \in V \), then \( c \) is a corner of a side \( L \) of \( v \) which is coincident to some side \( L' \) of some \( v' \in T \). Furthermore, the following hold:

- The polygon \( v_0 \) is marked with \((\bullet_1, c_1)\) and either \((\ominus_2, c_2)\) or \((\ominus_1, c_2)\) for corners \( c_1 \neq c_2 \) in \( v_0 \cap v_1 \). Similarly, \( v_1 \) is marked with \((\bullet_1, c_1)\) and either \((\ominus_2, c_2)\) or \((\ominus_1, c_2)\), respectively.
- For \( 1 < i < |T| \), \( v_i \) is marked with \((\ominus_i, c)\) or \((\oplus_i, c)\) such that \( c \in v_i \cap v_j \) for some \( 0 \leq j \leq i - 1 \). Also, \( v_i \) is marked with \((\ominus_{i+1}, c')\) or \((\bullet_i, c')\) for some \( c' \neq c \) in \( v_i \cap v_{i-1} \).
Thus, each \( v_i \) for \( 0 < i < \|T\| \) has at least one marking in common with \( v_{i-1} \) and another marking in common with \( v_j \) for \( j \leq i - 1 \). Before completing the marking process, we introduce some notation which we use in Step 3 for designing border tile types in \( T_0 \). Let \( 0 \leq i \leq \|T\| - 1 \); we select one corner \( c \) of \( v_i \) by the following process of elimination:

1. If possible, choose \( c \) such that \( v_i \) is marked with \( (\oplus_{i+1}, c) \) and \( (\ominus_{i+1}, c) \).

2. If no corner was chosen above, choose \( c \) such that \( v_i \) is marked with \( (\ominus_1, c) \) or \( (\ominus_i, c) \).

3. If no corner \( c \) has been chosen yet, then note that \( i = 1 \) or \( i = 2 \). In this case, choose \( c \) such that \( v_i \) is marked with \( (\circ_1, c) \) or \( (\ominus_2, c) \).

We denote the corner \( c \) of \( v_i \) chosen above by \( c(v_i) \). If \( i = 0 \), then \( c \in v_0 \cap v_1 \); otherwise, note that \( c \) is a corner in \( v_i \cap v_j \) for some \( j \leq i - 1 \). In Step 3, we use \( c(v_i) \) to determine how the border forms around an assembly instance associated with \( v_i \).

We conclude the marking process by marking two boundary polygons of \( T \) with \( \ominus \). There exist boundary polygons \( x_1 \neq x_2 \) in \( T \) such that \( x_i \) has a boundary side \( L_i \) for \( i = 1, 2 \) and \( L_1 \cap L_2 \neq \emptyset \) because \( T \) is backtrack constructible by assumption. Moreover, \( x_1 \in \pi(p) \), and \( x_2 = \tau(p) \) because \( T \) is backtrack constructible at stage 0. Let \( c(T) \) be the unique corner in \( L_1 \cap L_2 \subset x_1 \cap x_2 \); we use \( (\ominus_l, c(T)) \) to mark both \( x_1 \) and \( x_2 \). We make use of the notation \( c(T) \) in Step 3 when defining the border tile types in \( T_0 \) which are the first to bind. Observe that all markings appear exactly twice in \( T \): once in each of two corner neighbors \( v, v' \in T \). Moreover, if the marking is not \( (\ominus_l, c) \), then \( v \) and \( v' \) are side neighbors. We use \( M_T \) to denote the set of markings we assigned to polygons in \( T \).

Now, we consider the tilings in \( S \) which are singletons. We repetitively apply the marking procedure below on singleton tilings in \( S \) until every singleton tiling \( T \in S \) has a marking \( (\ominus_l, c(T)) \) on its unique element \( v \). We note that at least one singleton tiling in \( S \) satisfies the conditions of the procedure (at first) because \( \lambda > 1 \).

- Suppose that \( v \in T \) is congruent to a prototile \( \hat{X} \in \mathcal{P} \) such that the tiling \( \hat{T} \in S \) of \( \lambda \hat{X} \) has a polygon marked with \( (\ominus_l, c(\hat{T})) \). Because \( v \cong \hat{X} \), there exists an isometry \( I \in \mathcal{G} \) which bijectively maps the sides of \( v \) onto those of \( \hat{X} \). We use \( c(T) \) to denote a corner of \( v \) such that \( \mu_\lambda \circ I(c(T)) = c(\hat{T}) \); we mark \( v \) with \( (\ominus_l, c(T)) \).

After marking polygons for each tiling \( T \in S \), we incrementally define the set of bonds \( \Sigma \) for our TAS \( \Gamma = (T_0, 2) \) in the remainder of this step. Along the way, we describe the purpose of and define notation for
each bond. We begin by converting the markings above into bonds in \( \Sigma \) and then define other bonds which are used for border formation during the simulation process.

First, let \( T \in S, X \in P \) such that \( T \) is the tiling of \( \lambda X \), and \( 0 < i < |T| \). If \((\bullet_i, c) \in M_T \), then there exists a unique bond in \( \Sigma \) associated to \((\bullet_i, c)\); we denote this bond by \( a_X(\bullet_i) \). Likewise, if the markings \((\odot_i, c), (\oplus_i, c), (\ominus_i, c), \) or \((\ominus_{i+1}, c)\) are in \( M_T \), then there exist unique associated bonds in \( \Sigma \) for each; these bonds are denoted using the same convention for \( a_X(\bullet_i) \). On the other hand, there exist two unique bonds in \( \Sigma \) associated to \((\infty, c)\) regardless of however many times it appears in \( T \); we denote these bonds by \( a_X(\infty_1) \) and \( a_X(\infty_2) \).

Next, we define the following two sets for each \( X \in P \):

- \( B(X) = \{ Y \mid y \in T \text{ for some } T \in S \text{ such that } Y \cong X \}; \text{ let } n_X = |B(X)|. \)
- \( S(X) = \{ L \mid L \text{ is a boundary side of the tiling } T \in S \text{ of } \lambda X \}; \text{ let } m_X = |S(X)|. \)

If \( X \in P \) such that \( B(X) = \emptyset \), then there are \( m_X \) bonds in \( \Sigma \) associated with each side in \( S(X) \); we denote these bonds by \( a_X(L\lambda), \) where \( 1 \leq k \leq m_X. \) For each \( X \in P \) such that \( B(X) \neq \emptyset \), there exist \( n_X \cdot m_X \) bonds in \( \Sigma \) associated with each unique pair \((Y, L)\) where \( Y \in B(X) \) and \( L \in S(X) \). We denote these bonds by \( a_X(Y_j, L\lambda), \) where \( 1 \leq j \leq n_X \) and \( 1 \leq k \leq m_X. \) While the bonds associated with the markings coordinate how assemblies bind to each other, the bonds described in this paragraph coordinate how the border forms around each assembly. In addition to the bonds above, there are \( n_X \) bonds in \( \Sigma \) for each \( X \in P \); we denote these bonds by \( a_X(Y_j), \) where \( 1 \leq j \leq n_X. \) These bonds also coordinate how the border forms, but they are distinct from those above and are not always assigned to tile types in \( T_0. \)

Observe that the number of bonds described thus far is finite because the number of markings for a tiling \( T \in S \) is finite and because the sets \( B(X) \) and \( S(X) \) are also finite for a prototile \( X \in P \). There exist three more elements in \( \Sigma \) which do not depend on a specific prototile \( X \in P \): \( a(\perp), a(-), \) and the empty bond \( \nu. \) The bond \( a(\perp) \) is used for all tilings \( T \in S \) to indicate boundary corners which are not associated with a marking in \( M_T. \) Similarly, the bond \( a(-) \) is used for all tilings to indicate boundary sides. We conclude the definition of \( \Sigma \) by noting that the strength function \( s : \Sigma \to \{ 0, 1 \} \) is defined trivially as in Example 2.3.6: \( s(a) = 1 \) if \( a \neq \nu. \)

(Step 2, Define \( B_0 \) Tiles.) From this point forward, we use \( |L| \) to denote the length of a line segment \( L \subset \mathbb{R}^2. \) In order to construct \( T_0 \) using the bonds in \( \Sigma \), we need to define the polygons associated with the tile types in \( T_0. \) To this end, choose \( \delta > 0 \) such that \( 2 \delta < \min\{|L| \mid L \text{ is a side of some } X \in P\}. \) Because
$\mathcal{P}$ is finite and the set of sides for a polygon is also finite, such a $\delta > 0$ exists. We replace each side $L$ of each $X \in \mathcal{P}$ with three line segments $L'_1$, $L'_2$, and $L'_3$ such that $L = L'_1 \cup L'_2 \cup L'_3$, $|L'_1| = |L'_3| = \delta$, and $|L'_2| = |L| - 2\delta > 0$. Informally, we cut the sides of each $X \in \mathcal{P}$ so that each corner of $X$ is adjacent to two sides of length $\delta$ after modification. Later in this step, we will assign bonds associated to the markings from Step 1 to the sides of length $\delta$ which we just described. Given $X \in \mathcal{P}$, let $X'$ be the polygon resulting from the modification above. While $X' \not\equiv X$ by construction, $X'$ coincides with $X$. We denote the set of polygons resulting from this modification process by $\mathcal{P}'$. See Figure 4.07(a) for an example considering the only prototile of the modified Pinwheel substitution rule $\mathcal{R}_P = (\{X_P\}, \sqrt{5}, \{T_P\})$ (Figure 4.05). We use this substitution rule as an example throughout this proof, and then elaborate on the associated construction in Section C.2.

Figure 4.07. An example of the side modification in Step 2 of the proof of Theorem 4.2.3 using the modified Pinwheel substitution rule $\mathcal{R}$ (Figure 4.05). On the top left, we start with the original prototile of $\mathcal{R}$ and an enumeration $\{L_i\}_{i=1}^4$ of its sides. We choose $\delta > 0$ such that $2\delta < \min\{L_i\}_{i=1}^4$. On the bottom left, we have the resulting polygon $X'$ with the sides of length $\delta$ labeled according to their length. On the right, we observe that the tiling $T'$ constructed from the tiling $T$ of $\mathcal{R}$ is still sibling side-to-side.

Let $T = \{Y_j\}_{j=1}^k \in S$ be a tiling of $\lambda X$ for some $X \in \mathcal{P}$, and let $T' = \{Y'_j\}_{j=1}^k$ be a tiling of $\lambda X'$ generated from $\mathcal{P}'$ such that each $Y \in T$ coincides with some $Y' \in T'$. Informally, we consider $T'$ as having been constructed from $T$ by replacing each $Y \in T$ with its modified counterpart. Note that each corner of a polygon $Y \in T$ is also a corner of the corresponding polygon $Y' \in T'$ by construction. Moreover, observe that $T'$ is sibling side-to-side because $T$ is sibling side-to-side and because the modification made in the previous paragraph was uniformly applied to each polygon in $\mathcal{P}$. Also note that $T'$ is a tiling of both $\lambda X$
and \( \lambda X' \). Let \( T' \) be defined as above for each \( T \in \mathcal{S} \) and use \( \mathcal{S}' \) to denote the set of all tilings \( T' \). It follows that the substitution rule \( \mathcal{R}' = (\mathcal{P}', \lambda, \mathcal{S}') \) is not only well-defined but \( \mathcal{R}' \) also admits hereditary and sibling sides such that every \( X \in \mathcal{P} \) is star-shaped. Below, we use the polygons in each tiling \( T' \in \mathcal{S}' \) as templates for the tiles types in \( \mathcal{T}_0 \) which correspond to the prototiles of \( \mathcal{R} \). Rather than defining \( \mathcal{T}_0 \) directly however, we incrementally define a set \( \mathcal{T} \) of tiles which are distinct up to equivalence. In particular, we “add” tiles to \( \mathcal{T} \) in this step and the next while explaining their purpose. At the end, we will have a set \( \mathcal{T} \) which is well-defined and finite; then, we simply let \( \mathcal{T}_0 = \{[t] \mid t \in \mathcal{T}\} \).

First, we create a set of side markings based on the construction above and the markings from Step 1. So, let \( T \in \mathcal{S} \); for each \( Y \in T \), let \( Y' \in T' \) denote the polygon which coincides with \( Y \). If \(|T| = 1\), then the unique element \( Y \in T \) has \((\times, c)\) marked for some corner \( c \). By our construction above, there exist two sides \( L'_1 \) and \( L'_2 \) of \( Y' \) which have length \( \delta \) and intersect at \( c \); we mark each \( L'_i \) with \((\times_i)\) for \( i = 1, 2 \). If \(|T| \geq 2\), then \((\times, c)\) is marked twice: once each in two boundary polygons \( Y_1 \) and \( Y_2 \) which are corner adjacent via \( c \). In particular, \( Y_1 \) has a boundary side \( L_i \) for \( i = 1, 2 \) such that \( L_1 \cap L_2 = \{c\} \). By our construction above, there exist two unique boundary sides \( L'_1 \) and \( L'_2 \) of \( T' \) such that \( L'_i \) is a side of \( Y'_i \), \(|L'_i| = \delta\), and \( c \) is a corner of \( L'_i \) for \( i = 1, 2 \). We mark each \( L'_i \) with \((\times_i)\) for \( i = 1, 2 \). Now, let \((\times, c) \in \mathcal{M}_T\) such that \((\times) \neq (\times_i)\). From Step 1, there exist \( Y_1 \neq Y_2 \) in \( T \) such that a side \( L_1 \) of \( Y_1 \) coincides with a side \( L_2 \) of \( Y_2 \) and \( c \) is a corner of \( L_1 \) and \( L_2 \). By our construction above, there exist a unique pair of coincident sides \( L'_1 \) of \( Y'_1 \) and \( L'_2 \) of \( Y'_2 \) such that \(|L'_i| = \delta\), and \( c \) is a corner of \( L'_i \) for \( i = 1, 2 \); we mark each \( L'_i \) with \((\times)\) for \( i = 1, 2 \). Note that each marking from Step 1 has been transferred to exactly two sides of length \( \delta \) in \( T' \). We denote this new set of side markings by \( \mathcal{M}'_T \).

Next, we define the tiles in \( \mathcal{T} \) which correspond to prototiles in \( \mathcal{P} \). Let \( X \in \mathcal{P} \), and suppose that \( B(X) = \emptyset \); then there exists one tile \( t(X) = (X', g) \) in \( \mathcal{T} \) such that \( g \) maps every side of \( X' \) to \( \nu \). Because \( B(X) = \emptyset \), there does not exist any polygon \( Y \) in any tiling \( T \in \mathcal{S} \) such that \( Y \cong X \) by definition. So, the tile \( t(X) \in \mathcal{T} \) will not participate in the bordered simulation process associated with \( \Gamma \); we only include \( t(X) \) in \( \mathcal{T} \) for the sake of satisfying condition (1) of Definition 2.3.3. For each \( X \in \mathcal{P} \) such that \( B(X) \neq \emptyset \), there are \( n_X \) tiles in \( \mathcal{T} \) which correspond to \( X \). Rather than defining these tiles individually for each \( X \in \mathcal{P} \), we define tiles collectively for each tiling in \( \mathcal{S} \) below.

Let \( T \in \mathcal{S} \) and \( X \in \mathcal{P} \) such that \( T \) is the tiling of \( \lambda X \). For each \( Y \in T \), there exists a unique tile \( t(Y) = (Y', g[Y]) \) in \( \mathcal{T} \) associated with \( Y \). Below, we define the bond mappings \( g[Y] \) for the set of tiles \( \{t(Y)\}_{Y \in \mathcal{T}} \subset \mathcal{T} \); recall that every corner of \( Y \) is also a corner of \( Y' \) because of our construction in this step.

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1. Suppose that $Y' \in T'$ has a side $L$ which is not marked, and let $c_1$ and $c_2$ be the corners of $L$ in $Y'$.

   - If $c_1$ and $c_2$ are not corners of $Y \in T$ and $L$ is a boundary side of $T'$, then $g[Y](L) = a(-)$.
   - If the above criterion does not hold but $L$ is a boundary side of $T'$, then $g[Y](L) = a(\perp)$.
   - If neither of the criteria above hold, then $g[Y](L) = \nu$.

2. If $Y' \in T'$ has a side $L$ which is marked ($\bowtie_i$) for $i = 1$ or $i = 2$, then $g[Y](L) = a(\bowtie_i)$, respectively.

3. Suppose that $Y'_1 \neq Y'_2$ in $T'$ have sides $L_1$ and $L_2$, respectively, which are each marked with ($\times$) $\in \mathcal{M}_T \setminus \{(\bowtie_1), (\bowtie_2)\}$; this implies that $L_1$ coincides with $L_2$ by the marking processes above. Then, $g[Y_1](L_1) = a_X(\times)$ and $g[Y_2](L_2) = -a_X(\times)$. It does not matter how $L_1$ and $L_2$ are labeled within $T'$; rather, what matters is that the tiles $t(Y_1)$ and $t(Y_2)$ have matching, complementary bonds associated to these coincident sides.

As informally stated before the theorem, the tile types containing the tiles constructed above will be elements in the assembly block at level 0 of the substitution chain of $\Gamma$.

Now we make some observations about the tiles defined thus far. Let $T \in \mathcal{S}$ such that $|T| > 1$ and let $p = v_0v_1 \cdots v_{|T|-1}$ denote the Hamiltonian path in $\overline{G}(T)$ which is $G(T)$-backtrack. For each $v_i$ where $0 < i < |T|$, recall that $v_i$ has at least one marking in common with $v_{i-1}$ and another marking in common with $v_j$ where $j \leq i - 1$ (see Step 1). Because each of these markings has been converted into a bond with strength 1, we observe that the statements below hold.

- For $0 < i < |T|$, the sum of $\{t(v_j)\}_{j=0}^i$ is an assembly instance at temperature 2.

- For $0 \leq i_1 < i_2 \leq |T| - 1$, the following holds: if $\alpha$ is an assembly instance at temperature 2 and $\alpha$ is the sum of $t(v_{i_1}), t(v_{i_2})$, and some subset $W \subseteq \{t(v)\}_{v \in T} \setminus \{t(v_{i_1}), t(v_{i_2})\}$, then $\{t(v_j)\}_{j=i_1+1}^{i_2-1} \subseteq W$. Informally, this means that if $\alpha$ is an assembly instance at temperature 2 whose domain contains $t(v_{i_1})$ and $t(v_{i_2})$, then the domain of $\alpha$ must also contain $t(v_j)$ for every $j$ in between $i_1$ and $i_2$.

Let $X \in \mathcal{P}$ such that $T$ is the tiling of $\lambda X$ and $\alpha_T(0)$ denote the assembly instance at temperature 2 which is the sum of $\{t(v_j)\}_{j=0}^{|T|-1}$. Note that the shape of $\alpha_T(0)$ is $\bigcup T'$ and thus coincides with $\lambda X$. Furthermore, the set of bonds on the boundary sides of $\alpha_T(0)$ is $\{a(-), a(\perp), a_X(\bowtie_1), a_X(\bowtie_2)\}$ by construction. By the marking processes in Step 1 and this step, the bonds $a_X(\bowtie_1)$ and $a_X(\bowtie_2)$ only occur once each on some boundary sides $L_1$ and $L_2$ of $T'$. In particular, $L_1$ and $L_2$ are adjacent and $|L_1| = |L_2| = \delta$.
(Step 3, Define Border Tiles.) We begin our discussion on border tiles by considering how to form the assembly instances corresponding to supertiles of order 1 using the set of assembly instances \( \{ \alpha_T(0) \}_{T \in S} \) from Step 2. To this end, we choose \( \kappa > 1 \); once \( \Gamma \) is fully defined, \( \kappa \) will serve as \( \kappa_1 \) in Definition 2.3.3.

Figure 4.08. Left: The tiling \( T' \) of \( \lambda X \) constructed for the modified Pinwheel substitution rule \( \mathcal{R} \), with sides of length \( \delta \) adjacent to corners of \( \lambda X \) labeled. Because \( \lambda X \) is a convex polygon, it is star-shaped. Thus, given \( \kappa > 1 \), there exists a dilation \( \varphi_\kappa \) such that \( \varphi_\kappa(\lambda X) \) contains \( \lambda X \) and the line segments connecting each corner of \( \lambda X \) to its image under \( \varphi_\kappa \). Right: The tiling \( T' \) contained in \( \varphi_\kappa(\lambda X) \), with line segments of length \( \delta \) adjacent to corners of \( \varphi_\kappa(\lambda X) \) labeled. We use black arrows to indicate both transformation of the corners of \( \lambda X \) by the dilation \( \varphi_\kappa \) and the line segment connecting each corner to its image under \( \varphi_\kappa \). On the other hand, we use red arrows to connect the endpoints of the boundary sides labeled on the left with the line segments labeled on the right.

Let \( T \in S \) be the tiling of \( \lambda X \) for some \( X \in \mathcal{P} \) and \( T' \in S' \) be the tiling corresponding to \( T \) defined in Step 2; recall that \( T' \) is also a tiling of \( \lambda X \) and that \( \bigcup T' \) is the shape of \( \alpha_T(0) \). Because \( X \) is star-shaped, \( \lambda X \) is also star-shaped. It follows that there exists a dilation \( \varphi_\kappa \) centered inside \( \lambda X \) such that \( \varphi_\kappa(\lambda X) \) properly contains \( \lambda X \); thus \( \varphi_\kappa(\lambda X) \) contains the polygons in \( T \) and \( T' \). See Figure 4.08 for an example with the modified Pinwheel substitution rule. Let \( c \) be a boundary corner in \( T \), and recall that \( c \) is also a boundary corner in \( T' \). By the construction of \( T' \), \( c \) is in the intersection of two boundary sides of \( T' \) which have lengths equal to \( \delta \). If \( B(X) = \emptyset \), we will design a border tile \( t(X, c) \) in this step for each boundary corner \( c \) in \( T \) so that \( t(X, c) \) binds to \( \alpha_T(0) \) via the two boundary sides whose intersection contains \( c \). If \( B(X) \neq \emptyset \), we will design a border tile \( t(Y, c) \) similarly for each boundary corner \( c \) of \( T \) and each polygon \( Y \in B(X) \). In either case, these tiles will bind to \( \alpha_T(0) \) via the bonds \( a(\perp), a_X(\triangleright_1), \) or \( a_X(\triangleright_2) \).

Because \( |L| - 2\delta > 0 \) for each \( L \in S(X) \), we will also design border tiles whose polygons are parallelograms; these
tiles will fill in the rest of the border and will bind to \( \alpha_T(0) \) via the bond \( a(\cdot) \). Our motivation for designing these border tiles is based on the fact that the markings from Step 1 were originally associated with the corners of polygons in \( T \). These markings were then converted to side markings in Step 2, but the sides of length \( \delta \) which we marked were adjacent (after modification) the corners associated to the Step 1 markings. So, our goal in designing the border tiles in \( \mathbb{T} \) is to similarly use the corners of the polygon \( \varphi_\kappa(\lambda X) \) as reference points for placing bonds associated to the Step 1 markings on sides of length \( \delta \) once a border is formed around \( \alpha_T(0) \).

Figure 4.09. Given a corner \( c_k \) of the tiling \( T \), we visualize the line segments \( L_k, l_k, l_{k+1}, \) and \( L'_k \) and the trapezoid \( \text{Tr}_k \) defined by these four line segments.

In order to design border tiles mentioned above, we first define the polygons which will be the templates for these tiles. In doing so, we also specify some notation which we use later in this step. Fix an enumeration \( \{L_k\}_{k=1}^{m_X} \) of \( S(X) \) such that the boundary sides \( L_k \) and \( L_{k+1} \) of \( T \) are adjacent for \( 1 \leq k < m_X \). Note that this implies that \( L_{m_X} \) is adjacent to \( L_1 \) as well; we let \( c_1 \) be the boundary corner in \( L_{m_X} \cap L_1 \) and set \( c'_1 = \varphi_\kappa(c_{m_X}) \). We denote the boundary corner in \( L_k \cap L_{k+1} \) by \( c_{k+1} \) for \( 1 \leq k < m_X \) and set \( c'_{k+1} = \varphi_\kappa(c_{k+1}) \). Now let \( 1 \leq k \leq m_X \); we use \( k + 1 \) to mean \( (k \mod m_X) + 1 \) throughout so that the notation below is well-defined. We use \( l_k \) to denote the line segment whose endpoints are \( c_k \) and \( c'_k \); note that \( l_k \subset \varphi_\kappa(\lambda X) \) because \( \lambda X \) is star-shaped and that \( l_k \) is completely determined by dilation \( \varphi_\kappa(\lambda X) \) and the point \( c_k \). We set \( L'_k = \varphi_\kappa(L_k) \) and note that \( L_k \) and \( L'_k \) are parallel; see Figure 4.09. Let \( \text{Tr}_k \) denote the trapezoid whose sides are \( L_k, L'_k, l_k, \) and \( l_{k+1} \). Observe that \( \text{Tr}_k \) is a subset of \( \varphi_\kappa(\lambda X) \) because \( \lambda X \) is star-shaped. Recall that \( L_k \) is the union of three boundary sides of \( T' \), two of which are adjacent to the endpoints of \( L_k \) and have length \( \delta \). Let \( r_k \) be the remaining boundary side of \( T' \) which is a subset of \( L_k \) and note that \( |r_k| = |L_k| - 2\delta > 0 \); see Figure 4.10. Finally, let \( \varepsilon_k \) denote \( |L'_k| - |L_k| = (\kappa - 1)|L_k| \) and note that \( \varepsilon_k \) can also be calculated geometrically from \( l_k \) and \( l_{k+1} \). In other words, \( \varepsilon_k \) is also a function of the dilation \( \varphi_\kappa \). Having defined the above for \( 1 \leq k \leq m_X \), we also remark that the union of \( \lambda X \) and \( \bigcup_{k=1}^{m_X} \text{Tr}_k = \varphi_\kappa(\lambda X) \).
is exactly $\varphi_\kappa(\lambda X)$. In the next paragraph, we define polygons which are subsets of $\bigcup_{k=1}^{m_X} T_k$ in order to define the aforementioned border tiles.

**Figure 4.10.** Given a corner $c_k$ of the tiling $T$, we visualize the side $r_k$ of $T'$, the polygon $Q(T, c_k)$, and the parallelogram $P(T, L_k)$. We also label the side of $Q(T, c_k)$ which has length $\varepsilon_k$ and the pairs of line segments of length $\delta$ whose intersections contain $c_k, c'_k, c_{k+1}$, or $c'_{k+1}$ by their respective lengths. As in Figure 4.09, we use dashed lines to denote the line segments $l_k$ and $l_{k+1}$ although these are not labeled.

We define two polygons visually in Figure 4.10 for $1 \leq k \leq m_X$, a parallelogram $P(T, L_k)$ and a polygon $Q(T, c_k)$ which has seven sides. First, we enumerate the sides of $Q(T, c_k)$ by $\{\hat{L}_{k,\iota}\}_{\iota=1}^{7}$ such that $\hat{L}_{k,1}$ and $\hat{L}_{k,7}$ are adjacent. We describe most of these sides below using our enumeration.

- $\hat{L}_{k,1}$ and $\hat{L}_{k,2}$ coincide with the two boundary sides of $T'$ whose intersection is $c_k$; in particular, $\hat{L}_{k,1} \subset L_k$. This implies that $|\hat{L}_{k,1}| = |\hat{L}_{k,2}| = \delta$ by the construction of $T'$.

- $\hat{L}_{k,4}$ and $\hat{L}_{k,5}$ have $c'_{k-1}$ as an endpoint and are parallel and isometric to $\hat{L}_{k,2}$ and $\hat{L}_{k,1}$, respectively.

- $\hat{L}_{k,3}$ and $\hat{L}_{k,7}$ intersect $\partial \varphi_\kappa(\lambda X)$ at one point (each) and are parallel to $l_{k-1}$ and $l_k$, respectively.

Recall that $\hat{L}_{k,1}$ and $\hat{L}_{k,2}$ each has a length of $\delta$ by our construction of $T'$. Observe that the descriptions above imply that $\hat{L}_{k,6} \subset L'_k$ and has length $\varepsilon_k$. Next, we enumerate the sides of parallelogram $P(T, L_k)$ by $\{\hat{l}_{k,\iota}\}_{\iota=1}^{4}$ so that $\hat{l}_{k,\iota}$ is adjacent to $\hat{l}_{k,\iota+1}$ for $1 \leq \iota < 4$. We describe two adjacent sides of $P(T, L_k)$ as
Because $Y \in \text{boundary}$ sides intersect at the corner $c$. Step 1). We subdivide case (I) as follows, recalling the definition of corner $c$ and $\hat{\kappa}$ follows: $\hat{L}_{k,1}$ coincides with $r_k$ and $\hat{L}_{k,2}$ coincides with $L_{k,7}$. Because $P(T, L_k)$ is a parallelogram, $\hat{L}_{k,3} \subset L_k'$ and $\hat{L}_{k,4}$ are isometric and parallel to $\hat{L}_{k,1}$ and $\hat{L}_{k,2}$, respectively. Observe that $\hat{L}_{k,4}$ coincides with the side $\hat{L}_{k+1,3}$ of $Q(T, c_{k+1})$.

The set of polygons $\Omega_Q = \{ Q(T, c_k) \mid T \in S \text{ and } 1 \leq k \leq m_X \}$ where $X \in \mathcal{P}$ such that $T$ is the tiling $\lambda X$} serves as the basis for the corner border tiles which we will define shortly. While defining these tiles, we use the set of parallelograms $\Omega_P = \{ P(T, L_k) \mid T \in S \text{ and } 1 \leq k \leq m_X \}$ where $X \in \mathcal{P}$ such that $T$ is the tiling $\lambda X$} to progressively complete $\mathcal{T}$. We begin with the border tiles associated to a prototile $X \in \mathcal{P}$ and consider the following cases: (I) $B(X) \neq \emptyset$ and (II) $B(X) = \emptyset$. In case (I), we design one corner border tile $t(Y, c)$ for each polygon $Y \in B(X)$ and boundary corner $c$ of $T$ where $T \in S$ such that $T$ is the tiling of $\lambda X$. In case (II) on the other hand, we design one corner border tile $t(X, c)$ for each boundary corner $c$ of $T$. Suppose that $B(X) \neq \emptyset$ so that case (I) holds, and let $Y \in B(X)$. By definition, there exists an isometry $I \in G$ such that $X \cong Y$ via $I$. For case (I), let $Y'$ be the polygon which coincides with $Y$ defined in Step 2, $\hat{T} \in S$ be the tiling which contains $Y$, and $\phi_Y = \varphi_k \circ \mu_\lambda \circ I$. We use the mapping $\phi_Y$ to transfer the markings on $Y'$ to the border tiles which bind to $\alpha_T(0)$ that are associated with $Y$. Note that the isometry $I(Y')$ coincides with $X$ because $Y$ coincides with $Y'$; it follows that $\phi_Y(Y')$ coincides with $\varphi_k(\lambda X)$. Moreover, $\phi_Y(Y) \cong \varphi_k(\lambda X)$ by definition; thus, every corner of $Y$ corresponds to a corner of $\varphi_k(\lambda X)$. If $|\hat{T}| > 1$, then the path in $\overline{G(\hat{T})}$ has at least two vertices; thus, $c(Y)$ is properly defined (see Step 1). We subdivide case (I) as follows, recalling the definition of corner $c(T)$ from Step 1: (A) $|\hat{T}| > 1$ and $\phi_Y(c(Y)) \neq c(T)$; (B) $|\hat{T}| > 1$ and $\phi_Y(c(Y)) = c(T)$; and (C) $|\hat{T}| = 1$.

Before considering the cases described above, we note that border formation always begins with a border tile binding to the boundary sides of $\alpha_T(0)$ which have the bonds $a_X(\bowtie_1)$ and $a_X(\bowtie_2)$. By definition, these boundary sides intersect at the corner $c(T)$. As mentioned previously, we design border tiles so that each $Y \in B(X)$ is associated with a set of border tiles if $B(X) \neq \emptyset$; otherwise, there is just one set of border tiles associated with $X$. In either case, the border tiles associated with $Y \in B(X)$ (X, resp.) will form around $\alpha_T(0)$ in such a way that $t(Y, c(T))$ (or $t(X, c(T))$, resp.) is always the first border tile to bind to $\alpha_T(0)$ and the last border tile to bind will be the one which has $c_k'$ as a boundary corner for some fixed $1 \leq k \leq m_X$. Because $X$ is a polygon, the shape of $\alpha_T(0)$ is a topological disk. Thus, there are at most distinct two paths, in the topological sense, along the boundary of $\bigcup T$ which start at $c(T)$ and end at $c_k$. We use these paths to determine how border tiles bind to $\alpha_T(0)$ and each other; see Figure 4.11 for example. Lastly, we define
the following sets:

\[ \mathbb{L}_1 = \{ |L| \mid L \text{ is a side of some } X' \in \mathcal{P}' \}, \]
\[ \mathbb{L}_2 = \{ \varepsilon_k \mid 1 \leq k \leq m_X \text{ for some } X \in \mathcal{P} \}. \]

Note that both sets \( \mathbb{L}_1 \) and \( \mathbb{L}_2 \) are finite. Because \( \mathcal{R}' \) admits hereditary sides, observe that we could have defined \( \mathbb{L}_1 \) as \( \{ |L| \mid L \text{ is the side of some polygon in the supertile } \sigma_{\mathcal{R}'}^\ell(X') \text{ for some } \ell \geq 0 \text{ and } X' \in \mathcal{P}' \} \).

We use \( \mathbb{L} \) to denote \( \mathbb{L}_1 \cup \mathbb{L}_2 \).

**Figure 4.11.** The idea of border formation around the assembly instance \( \alpha_T(0) \) of the modified Pinwheel substitution rule. We use arrows to denote two paths along the boundary of \( T' \) which start at the corner associated to the red tile and end at the corner associated to the purple tile. By design, side and corner border tiles bind to \( \alpha_T(0) \) so that the red tile is the first to bind and the purple tile is last. We color other corner border tiles yellow and the side border tiles blue for visual contrast.

**Figure 4.12.** Enumeration of the sides of polygon \( Q(T, c_k) \) associated to corner \( c_k \) of \( \lambda X \). As in previous figures, we use the black dashed line to represent \( l_k \), although this line segment is not labeled.

*(Case I.A)* We assume that \( B(X) \neq \emptyset \), \( |\tilde{T}| > 1 \), and \( \phi_Y(c(Y)) \neq c(T) \). Then there are two distinct
(topological) paths, denoted \(f_1\) and \(f_2\), along the boundary of \(\bigcup T\) which start at \(c(T)\) and end at \(\phi_Y(c(Y))\).

We begin by defining the corner border tiles, and note that there exists a corner border tile \(t(Y, c_k) = (Q(T, c_k), g[Y, c_k])\) in \(T\) for each boundary corner \(c_k\) of \(T\). As before, we use \(k + 1\) to mean \((k \mod m_X) + 1\) throughout so that the notation below is well-defined; similarly, we use \(k - 1\) to mean \(((k - 2) \mod m_X) + 1\).

1. Let \(\{\hat{L}_{k,i}\}_{i=1}^7\) denote the sides of \(Q(T, c_k)\) as above for \(1 \leq k \leq m_X\); see Figure 4.12.

First, let \(1 \leq k^* \leq m_X\) be such that \(c_{k^*} = c(T)\). We define the bond mapping \(g[Y, c_{k^*}]\) according to the procedures below.

1. Recall that \(\hat{L}_{k^*,1}\) and \(\hat{L}_{k^*,2}\) coincide with two boundary sides of \(T'\) which we denote by \(\hat{L}_1\) and \(\hat{L}_2\), respectively. Moreover, the bonds \(a_X(\perp_1)\) and \(a_X(\perp_2)\) appear on these two sides in the context of \(\alpha_T(0)\). For \(i = 1, 2\), we define \(g[Y, c_{k^*}]|L_{k^*,i}\) so that it equals the matching, complementary bond associated with \(\hat{L}_i\). For example, if the bond \(a_X(\perp_1)\) appears on \(\hat{L}_1\), then \(g[Y, c_{k^*}]|L_{k^*,1} = -a_X(\perp_1)\).

2. Recall that for each \(L \in S(X)\), there exists a unique bond \(a_X(Y, L)\) in \(\Sigma\). Then \(g[Y, c_{k^*}]|L_{k^*,3} = a_X(Y, L_{k^*,-1})\) and \(g[Y, c_{k^*}]|L_{k^*,7} = a_X(Y, L_{k^*})\).

3. Let \(\tilde{c}\) be the corner of \(Y\) such that \(\phi_Y(\tilde{c}) = c_{k^*}'\). Because \(\tilde{c}\) is also a corner of \(Y'\), let \(\hat{L}_4\) and \(\hat{L}_5\) be sides of \(Y'\) such that \(\tilde{c} \in \hat{L}_4 \cap \hat{L}_5\). \(\phi_Y(\hat{L}_4)\) contains \(\hat{L}_{k^*,4}\), and \(\phi_Y(\hat{L}_5)\) contains \(\hat{L}_{k^*,5}\). Then \(g[Y, c_{k^*}]|L_{k^*,i} = g[Y, \hat{T}]|\hat{L}_i\) for \(i = 4, 5\).

4. Let \(\tilde{L}\) be the side of \(Y\) such that \(\phi_Y(\tilde{L})\) contains \(\hat{L}_{k^*,6}\). If \(\tilde{L}\) is a boundary side of \(\hat{T}\), then \(g[Y, c_{k^*}]|L_{k^*,6} = a(-)\). Otherwise, \(g[Y, c_{k^*}]|L_{k^*,6} = \nu\).

Next, we design the remaining corner border tiles so that \(t(Y, c_{k^*})\) will be the only border tile than can bind directly to \(\alpha_T(0)\). Let for \(1 \leq k \neq k^* \leq m_X\); we define the bond mapping \(g[Y, c_k]\) according to the procedures below.

1. As stated previously, \(\hat{L}_{k,1}\) and \(\hat{L}_{k,2}\) coincide with two boundary sides of \(T'\); the bond \(a(\perp)\) appears on both of these boundary sides of \(T'\) in the context of \(\alpha_T(0)\). If \(c_k = \phi_Y(c(Y))\), then \(g[Y, c_k]|L_{k,i} = \nu\) for \(i = 1, 2\). Otherwise, \(c_k\) is on one path \(f \in \{f_1, f_2\}\) from \(c(T)\) to \(\phi_Y(c(Y))\).

   - If \(f\) visits \(c_{k-1}\) before \(c_k\), then \(g[Y, c_k]|L_{k,1} = -a(\perp)\) and \(g[Y, c_k]|L_{k,2} = \nu\).
   - If \(f\) visits \(c_{k+1}\) before \(c_k\), then \(g[Y, c_k]|L_{k,1} = \nu\) and \(g[Y, c_k]|L_{k,2} = -a(\perp)\).
Recall that $\widehat{L}_{k,1} \subset L_k$ and $\widehat{L}_{k,1} \subset L_{k-1}$. By the conditions above, we assign the empty bond to the first side of $Q(T, c_k)$ which path $f$ visits.

2. By definition, at most one path visits each boundary side of $T$.
   - Let $f$ be the path which visits $L_{k-1}$, and recall that the endpoints of $L_{k-1}$ are $c_{k-1}$ and $c_k$. If $f$ visits $c_{k-1}$ before $c_k$, then $g[Y, c_k](\widehat{L}_{k,3}) = -a_X(Y, L_{k-1})$; otherwise, $g[Y, c_k](\widehat{L}_{k,3}) = a_X(Y, L_{k-1})$.
   - Similarly, let $f'$ be the path which visits $L_k$, and recall that the endpoints of $L_k$ are $c_k$ and $c_{k+1}$. If $f'$ visits $c_k$ before $c_{k+1}$, then $g[Y, c_k](\widehat{L}_{k,7}) = a_X(Y, L_{k})$; otherwise, $g[Y, c_k](\widehat{L}_{k,7}) = -a_X(Y, L_{k})$.

3. We define $g[Y, c_k](\widehat{L}_{k,i})$ for $i = 4, 5, 6$ according to the procedures for $k^*$.

By the definition of the tiles above, we observe that the sum of $\alpha_T(0)$ and $t(Y, c_k)$ is not an assembly instance at temperature $2$ if $c_k \neq c(T)$. Let $1 \leq k \leq k^* \leq m_X$. By our description above, note that at most one side of $t(Y, c_k)$ coincides with a boundary side of $\alpha_T(0)$ and has a matching, complementary bond with latter side. Because $s(a) = 1$ for all non-empty bonds $a \in \Sigma$, our observation follows from the definition of an assembly instance at temperature $\theta$.

Having defined every corner border tile for this case, we turn our attention to the border tiles associated with the set of parallelograms $\{P(T, L_k)\}_{k=1}^{m_X}$. For $1 \leq k \leq m_X$, there exists a border tile $t_{|r_k}|(Y, L_k) = (P(T, L_k), g_{|r_k}|[Y, L_k])$ in $\mathcal{T}$; we explain this notation at the end of this case. We define the bond mapping $g_{|r_k}|[Y, L_k]$ below using $\{\widehat{l}_{k,i}\}_{i=1}^{4}$ to denote the sides of $P(T, L_k)$ as above.

1. Recalling that $\widehat{l}_{k,1}$ coincides with the boundary side $r_k$ of $T'$, we have that $g_{|r_k}|[Y, L_k](\widehat{l}_{k,1}) = -a(-)$. Recall that the bond $a(-)$ is associated with $r_k$ in the context of $\alpha_T(0)$, so $\widehat{l}_{k,1}$ and $r_k$ have matching, complementary bonds.

2. Let $\widehat{L}$ be the side of $Y$ such that $\phi_Y(\widehat{L})$ contains $\widehat{l}_{k,3}$. If $\widehat{L}$ is a boundary side of $\hat{T}$, then $g_{|r_k}|[Y, L_k](\widehat{l}_{k,1}) = a(-)$. Otherwise, $g_{|r_k}|[Y, L_k](\widehat{l}_{k,1}) = \nu$.

3. Recall that $\widehat{l}_{k,2}$ and $\widehat{l}_{k,4}$ are coincident to sides $\widehat{L}_{k,7}$ $\widehat{L}_{k+1,3}$, respectively. With this in mind, we have that $g_{|r_k}|[Y, L_k](\widehat{l}_{k,2}) = -g[Y, c_k](\widehat{L}_{k,7})$ and $g_{|r_k}|[Y, L_k](\widehat{l}_{k,4}) = -g[Y, c_{k+1}](\widehat{L}_{k+1,3})$. Thus, $\widehat{l}_{k,2}$ ($\widehat{l}_{k,4}$, resp.) and $\widehat{L}_{k,7}$ ($\widehat{L}_{k+1,3}$, resp.) have matching, complementary bonds.
By the definition of the tiles above, we observe that the sum of \( t_{|rk|}(Y, L_k) \) and \( \alpha_T(0) \) is not an assembly instance at temperature 2. On the other hand, if corner border tiles \( t(Y, c_k) \) or \( t(Y, c_{k+1}) \) are already bound to \( \alpha_T(0) \), then \( t_{|rk|}(Y, L_k) \) can bind to \( \alpha_T(0) \) as well. Separately, observe that \( g|_{rk} [Y, L_k](\hat{t}_{k,2}) = -g|_{rk}[Y, L_k](\hat{t}_{k,4}) \) because of how the corner tiles \( t(Y, c_k) \) and \( t(Y, c_{k+1}) \) were defined above.

Let \( 1 \leq k \leq m, f \in \{f_1, f_2\} \) be the path that visits \( L_{k-1} \), and \( f' \in \{f_1, f_2\} \) be the path that visits \( L_k \).

By our construction of the border tiles above, observe the following:

- \( g[Y, c_k](\hat{L}_{k,3}) = g|_{rk-1}[Y, L_{k-1}](\hat{t}_{k-1,2}) \in \Sigma^+ \) if \( f \) visits \( c_k \) before \( c_{k-1} \); otherwise \( g[Y, c_k](\hat{L}_{k,3}) = g|_{rk-1}[Y, L_{k-1}](\hat{t}_{k-1,2}) \in \Sigma^- \). In particular, \( g[Y, c_k](\hat{L}_{k,3}) = \pm a_X(Y, L_{k-1}) \).

- \( g[Y, c_k](\hat{L}_{k,7}) = g|_{rk}[Y, L_k](\hat{t}_{k,4}) \in \Sigma^+ \) if \( f' \) visits \( c_k \) before \( c_{k+1} \); otherwise \( g[Y, c_k](\hat{L}_{k,7}) = g|_{rk}[Y, L_k](\hat{t}_{k,4}) \in \Sigma^- \). In particular, \( g[Y, c_k](\hat{L}_{k,7}) = \pm a_X(Y, L_k) \).

As observed previously, only the corner border tile \( t(Y, c(T)) \) can bind with \( \alpha_T(0) \) to form an assembly instance at temperature 2. By the observations above, we conclude that border tiles bind one at a time to the boundary sides of \( \alpha_T(0) \) following paths \( f_1 \) and \( f_2 \). In particular, if corner \( c \) is visited by path \( f \in \{f_1, f_2\} \), then the border tile \( t(Y, c) \) only binds to \( \alpha_T(0) \) once corner and side border tiles which precede \( t(Y, c) \), with respect to \( f \), have bound to \( \alpha_T(0) \) and each other. Thus, the last border tile to bind is \( t(Y, \phi_Y(c(Y))) \) because both paths \( f_1 \) and \( f_2 \) end at \( \phi_Y(c(Y)) \). In other words, \( t(Y, \phi_Y(c(Y))) \) cannot form an assembly instance at temperature 2 with \( \alpha_T(0) \) until every other border tile in the set \( \{t(Y, c_k), t_{|rk|}(Y, L_k)\}_{k=1}^{m_X} \) is already bound to \( \alpha_T(0) \). We use \( \alpha(Y, 1) \) to denote the sum of \( \alpha_T(0) \) and \( \{t(Y, c_k), t_{|rk|}(Y, L_k)\}_{k=1}^{m_X} \), and note that this is an assembly instance at temperature 2.

By construction, the shape of \( \alpha(Y, 1) \) is isometric to \( \varphi_n(\lambda X) \); thus the shape of \( \alpha(Y, 1) \) is similar to \( Y \).

Suppose that \( Y \) has a marking \( \langle x, c \rangle \) for some corner \( c \). By the definition of the tiles in Step 2, \( t(Y) \) has a side \( L \) such that (1) \( |L| = \delta \), (2) \( c \) is an endpoint of \( L \), and (3) the bond \( g[Y](L) \) is associated with the marking \( \langle x, c \rangle \). Observe that \( \alpha(Y, 1) \) has a boundary side \( \tilde{L} \) such that (1) \( |	ilde{L}| = \delta \), (2) \( \phi_Y(c) \) is an endpoint of \( \tilde{L} \), and (3) the bond \( g[Y, \phi_Y(c)](L) \) is associated with the marking \( \langle x, c \rangle \). Hence, we have transferred the bonds on \( t(Y) \) associated with markings from Step 1 to \( \alpha(Y, 1) \) and increased the distance between these bonds proportionally.

Before proceeding with the next case, we use the tiles \( \{t_{|rk|}(Y, L_k)\}_{k=1}^{m_X} \) as a basis for defining more side border tiles. The purpose of defining these new side border tiles is to account for the fact that the supertiles of \( \mathcal{R} \) increase in size proportional to their order. Because the assembly instances associated with
these supertiles have proportionally larger shapes, side border tiles must be able to bind to boundary sides of various lengths. We elaborate on these assembly instances later in the proof once $\Gamma$ is fully defined.

![Figure 4.13](image.png)

**Figure 4.13.** Enumeration of the sides of parallelograms $P(T, L_k)$ and $P(T, k, z)$ for $z \in \mathbb{L} \setminus \{|r_k|\}$.

Let $1 \leq k \leq m_X$ and $z \in \mathbb{L}$ such that $z \neq |r_k|$. We use $P(T, L_k)$ as a basis for defining a parallelogram $P(T, k, z)$; see Figure 4.13. Fix a line segment $l(k, z)_1$ such that $l(k, z)_1$ and $\tilde{l}_{k,1}$ lie on the same line and $|l(k, z)_1| = z$. Let $l(k, z)_2$ be a line segment which is isometric and parallel to $\tilde{l}_{k,2}$. In particular, choose $l(k, z)_2$ such that $l(k, z)_1$ and $l(k, z)_2$ share one endpoint and the angle between these two line segments is the same as the interior angle between $\tilde{l}_{k,1}$ and $\tilde{l}_{k,2}$. Choose line segments $l(k, z)_3$ and $l(k, z)_4$ parallel to $\tilde{l}_{k,3}$ and $\tilde{l}_{k,4}$, respectively, so that $\{l(k, z)_i\}_{i=1}^4$ is the set of sides for a parallelogram; we denote the resulting parallelogram by $P(T, k, z)$. There exists a side border tile $t_z(Y, L_k) = (P(T, k, z), g_z[Y, L_k])$ in $\mathbb{T}$ whose bond mapping $g_z[Y, L_k]$ is defined as follows for $1 \leq i \leq 4$: $g_z[Y, L_k](l(k, z)_i) = g_{|r_k|}[Y, L_k](\tilde{l}_{k,i})$. In essence, $t_z(Y, L_k)$ is a copy of $t_{|r_k|}(Y, L_k)$ with two modified, parallel sides.

![Figure 4.14](image.png)

**Figure 4.14.** Enumeration of the sides of polygons $Q'(T, c_{k^*})$ (top) and $Q''(T, c_{k^*})$ (bottom) associated to the corner $c_{k^*}$ of $\lambda X$ for Case (I.B). While these polygons have coincident sides, we visualize them separately for ease of labeling.

**Case (I.B)** We assume that $B(X) \neq \emptyset$, $|\hat{T}| > 1$, and $\phi_Y(c(Y)) = c(T)$; let $1 \leq k^* \leq m_X$ such that $c_{k^*} = c(T)$. We let $f$ be a (topological) path along the boundary of $\bigcup T$ which starts and ends at $c(T)$ and
visits every boundary side of \( T \) starting with \( L_{k^*} \). We follow the same procedures in Case (I.A) in order to describe most of the border tiles associated to \( Y \) in this case; the notable exception to this is the corner border tile associated to \( c(T) \). Because \( \phi_Y(c(Y)) = c(T) = c_{k^*} \) in this case, we split the polygon \( Q(T, c_{k^*}) \) in half (Figure 4.14) and define two corner border tiles associated with \( c_{k^*} \) instead of one: \( t(Y, c_{k^*})' \) and \( t(Y, c_{k^*})'' \). In particular, the tile \( t(Y, c_{k^*})' \) is adjacent to \( c_k \) while \( t(Y, c_{k^*})'' \) is adjacent to \( c_k' \). The purpose of splitting \( Q(T, c_{k^*}) \) and defining two border tiles is so that (1) the first border tile to bind to \( \alpha_T(0) \) is \( t(Y, c_{k^*})' \) and (2) the last border tile to bind is \( t(Y, c_{k^*})'' \). Note that this mirrors the design process behind Case (I.A).

We begin by defining polygons \( Q(T, c_{k^*})' \) and \( Q(T, c_{k^*})'' \) so that \( Q(T, c_{k^*})' \cup Q(T, c_{k^*})'' \) coincides with \( Q(T, c_{k^*}) \); see Figure 4.14. We use \( \{\tilde{L}_i\}_{i=1}^6 \) to denote the sides of \( Q(T, c_{k^*})' \) and \( \{\tilde{L}_i\}_{i=1}^7 \) to denote the sides of \( Q(T, c_{k^*})'' \). We describe the sides of these polygons as follows:

- For \( i = 1, 2, \tilde{L}_i \) coincides with \( \tilde{L}_{k^*,i} \). Similarly, \( \tilde{L}_i'' \) coincides with \( \tilde{L}_{k^*,i} \) for \( i = 4, 5, 6 \).

- Side \( \tilde{L}_{k^*,3} = \tilde{L}_3 \cup \tilde{L}_3'' \) such that \( |\tilde{L}_3'| = |\tilde{L}_3''| = \frac{1}{2}|\tilde{L}_{k^*,3}| \). Similarly, \( \tilde{L}_{k^*,7} = \tilde{L}_6 \cup \tilde{L}_6'' \) such that \( |\tilde{L}_6'| = |\tilde{L}_6''| = \frac{1}{2}|\tilde{L}_{k^*,7}| \).

- Sides \( \tilde{L}_1'' \) and \( \tilde{L}_2'' \) coincide with \( \tilde{L}_5 '' \) and \( \tilde{L}_4'' \), respectively. Moreover, \( \tilde{L}_2'' \) is parallel to \( \tilde{L}_{k^*,2} \).

Next, we note that there exist two corner border tiles \( t(Y, c_{k^*})' = (Q(T, c_{k^*})', g[Y, c_{k^*}]) \) and \( t(Y, c_{k^*})'' = (Q(T, c_{k^*})'', g[Y, c_{k^*}])'' \) in \( T \). We define bond mappings of these border tiles according to the procedures below; note that these procedures mirror those in Case (I.A) for the corner border tiles corresponding to \( c_{k^*} \) and \( \phi_Y(c(Y)) \).

1. By the definition above, \( \tilde{L}_i \) coincides with \( \tilde{L}_{k^*,i} \) for \( i = 1, 2 \). Let \( \tilde{L}_i \) be the boundary sides of \( T' \) which coincides with \( \tilde{L}_{k^*,i} \) for \( i = 1, 2 \). As noted in Case (I.A), the bonds \( a_X(>01) \) and \( a_X(>02) \) appear on sides \( \tilde{L}_1 \) and \( \tilde{L}_2 \) in the context of \( \alpha_T(0) \). For \( i = 1, 2 \), we define \( g[Y, c_{k^*}](\tilde{L}_i) \) so that it equals the matching, complementary bond associated with \( \tilde{L}_i \).

2. Recall from Step 1 that we defined an additional bond \( a_X(Y) \) not associated with an element of \( S(X) \). We use this bond as follows: \( g[Y, c_{k^*}](\tilde{L}_5') = a_X(Y) \) and \( g[Y, c_{k^*}]''(\tilde{L}_5'') = -a_X(Y) \). Because \( \tilde{L}_5' \) coincides with \( \tilde{L}_5'' \), these two sides have matching, complementary bonds.

3. For \( i = 4, 5, 6 \), we define \( g[Y, c_{k^*}]''(\tilde{L}_i'') \) according to the procedures for \( \tilde{L}_{k^*,i} \) in Case (I.A), recalling that \( \tilde{L}_i'' \) coincides with \( \tilde{L}_{k^*,i} \).
4. Recall that the path \( f \) visits every boundary side of \( T \) starting with \( L_{k^*} \). With this in mind, 
\[
g[Y, c_{k^*}](\hat{L}_b) = a_X(Y, L_{k^*}) \quad \text{and} \quad g[Y, c_{k^*}]^\prime(\hat{L}_b^\prime) = -a_X(Y, L_{k^* - 1}).
\]

5. The sides \( \hat{L}_3, \hat{L}_4, \hat{L}_2', \text{and} \hat{L}_7'' \) are all assigned the bond \( \nu \) by their respective bond mappings.

By the definitions of \( t(Y, c_{k^*})' \) and \( t(Y, c_{k^*})'' \) above, note that the sum of \( \alpha_T(0) \) and \( t(Y, c_{k^*})' \) is an assembly instance at temperature 2. On the other hand, the sum of \( t(Y, c_{k^*})' \) and \( t(Y, c_{k^*})'' \) is not an assembly instance at temperature 2 because these tiles have only one pair of matching, complementary bonds.

Finally, we note that every corner \( c_k \) for \( 1 \leq k \neq k^* \leq m_X \) is associated with a corner border tile \( t(Y, c_k) \). These corner border tiles are defined using the procedures from Case (I.A) with the path \( f \) replacing \( f_1 \) and \( f_2 \); however, we do make two overarching modifications to \( t(Y, c_{k^* + 1}) \) and \( t(Y, c_{k^* - 1}) \) because we split the polygon \( Q(T, c_{k^*}) \) in half:

- We cut the side \( \hat{L}_{k^* + 1,3} \) into two line segments of equal length denoted \( \hat{L}_{k^*+1,3}' \) and \( \hat{L}_{k^*+1,3}'' \). Specifically, \( \hat{L}_{k^*+1,3}' \) intersects the boundary of \( \lambda X \) while \( \hat{L}_{k^*+1,3}'' \) intersects the boundary of \( \varphi_n(\lambda X) \). Leaving the other sides of \( Q(T, c_{k^* + 1}) \) unchanged, we call the resulting polygon \( Q(T, c_{k^* + 1})' \). We then define \( t(Y, c_{k^* + 1}) \) using this polygon and the procedures of Case (I.A) for all unchanged sides. Additionally, \( g[Y, c_{k^* + 1}](\hat{L}_{k^*+1,3}') = -a_X(Y, L_{k^*}) \); we note that this bond would have been assigned to side \( \hat{L}_{k^*+1,3} \) in Case (I.A). On the other hand, \( g[Y, c_{k^* + 1}](\hat{L}_{k^*+1,3}'') = \nu \).

- As above, we cut side \( \hat{L}_{k^* - 1,7} \) into two line segments of equal length denoted \( \hat{L}_{k^*-1,7}' \) and \( \hat{L}_{k^*-1,7}'' \) so that \( \hat{L}_{k^*-1,7}' \) intersects the boundary of \( \lambda X \) while \( \hat{L}_{k^*-1,7}'' \) intersects the boundary of \( \varphi_n(\lambda X) \). Again, we modify the procedures of Case (I.A) when defining \( t(Y, c_{k^* - 1}) \) so that \( g[Y, c_{k^* - 1}](\hat{L}_{k^*-1,7}') = a_X(Y, L_{k^* - 1}) \) and \( g[Y, c_{k^* - 1}](\hat{L}_{k^*-1,7}'') = \nu \).

Likewise, the set of side border tiles \( \{ t_z(Y, L_k) \}_{z \in \mathbb{L}} \) for every \( 1 \leq k \leq m_X \) is defined according the procedures from Case (I.A) with two similar modifications to those above:

- We cut the sides \( \hat{L}_{k^* - 1,2} \) and \( \hat{L}_{k^* - 1,4} \) of \( P(T, L_{k^* - 1}) \) in half. We define \( t_{r_{k^* - 1}}(Y, L_{k^* - 1}) \) according the procedures above and in Case (I.A) so that \( t_{r_{k^* - 1}}(Y, L_{k^* - 1}) \) has two sides which coincide with sides of \( t(Y, c_{k^* - 1}) \) and two sides which coincide with sides of \( t(Y, c_{k^*}). \) In particular, the sides of \( t_{r_{k^* - 1}}(Y, L_{k^* - 1}) \) which coincide with \( \hat{L}_{k^* - 1,7}'' \) and \( \hat{L}_{k^* - 1,7}'' \) have matching, complementary bonds with the latter sides. The other two sides have the empty bond \( \nu \). We modify \( t_z(Y, L_{k^* - 1}) \) similarly for \( z \in \mathbb{L} \setminus \{ r_{k^* - 1} \} \).
• We cut the sides $\tilde{L}_{k^*,2}$ and $\tilde{L}_{k^*,4}$ of $P(T, L_{k^*})$ in half and perform similar modifications to those above.

Note that the modifications above do not change the way that the border associated to $Y$ forms around $\alpha_T(0)$. Rather, the modifications just account for the fact that there are two corner border tiles associated with $c_{k^*} = c(T)$ instead of one. It follows that we can make the similar observations as in Case (I.A):

1. Only $t(Y, c(T))'$ can bind with $\alpha_T(0)$ to form an assembly instance at temperature 2.

2. All border tiles other than $t(Y, c(T))''$ bind one at a time to the boundary sides of $\alpha_T(0)$ following the path $f$. One these border tiles are in place, $t(Y, c(T))''$ can bind to $t(Y, c(T))'$ and $P(T, L_{k^*-1})$. We refer to the resulting assembly instance at temperature 2 by $\alpha(Y, 1)$ as in Case (I.A).

3. By the process above, we have transferred the bonds on $t(Y)$ associated with markings from Step 1 to $\alpha(Y, 1)$ and increased the distance between these bonds proportionally.

![Figure 4.15. Enumeration of the sides of polygons $Q'(T, c_{k^*})$ (top) and $Q''(T, c_{k^*})$ (bottom) associated to the corner $c_{k^*}$ of $\lambda X$ for Case (I.C). While these polygons have coincident sides, we visualize them separately for ease of labeling.](image)

Case (I.C) We assume that $B(X) \neq \emptyset$ and $|\hat{T}| = 1$; let $1 \leq k^* \leq m_X$ such that $c_{k^*} = c(T)$. We let $f$ be as defined in Case (I.B). Again, we follow the same procedures in Case (I.A) in order to describe most of the border tiles associated to $Y$ except for two corner border tiles associated to $c_{k^*}$, which we define below. As in Case (I.B), we use path $f$ instead of paths $f_1$ and $f_2$ where appropriate.

Let $\hat{X} \in \mathcal{P}$ so that $\hat{T}$ is the tiling of $\lambda \hat{X}$. Because $|\hat{T}| = 1$, we note that $t(Y)$ has two sides adjacent to $c(\hat{T})$ which have each been assigned either $a_{\hat{X}}(\triangledown_1)$ or $a_{\hat{X}}(\triangleleft_2)$. By the Step 1 marking process, observe that $\phi_Y(c(\hat{T})) = c_{k^*}$. If we define a corner border tile $t$ for $c_{k^*}$ as in Case (I.A) or (I.B), then the tiles belonging
to tile type $[t]$ would be able to bind wherever the tiles in $[t(Y)]$ can bind via the two bonds $a_X(\infty_1)$ and $a_X(\infty_2)$. To prevent this, we split the polygon $Q(T, c_{k^*})$ as shown in Figure 4.15.

First, we define $Q(T, c_{k^*})'$ and $Q(T, c_{k^*})''$ below so that $Q(T, c_{k^*})' \cup Q(T, c_{k^*})''$ coincides with $Q(T, c_{k^*})$. We use $\{\hat{L}_i\}_{i=1}^8$ to denote the sides of $Q(T, c_{k^*})'$ and $\{\hat{L}_i''\}_{i=1}^4$ to denote the sides of parallelogram $Q(T, c_{k^*})''$. We describe the sides of these polygons as follows:

- For $i = 1, 2, \hat{L}_i'$ coincides with $\hat{L}_{k^*,i}$. On the other hand, $\hat{L}_i'$ coincides with $\hat{L}_{k^*,i-1}$ for $i = 6, 7, 8$.
  Similarly, $\hat{L}_i''$ coincides with $\hat{L}_{k^*,i}$.

- Side $\hat{L}_{k^*,3} = \hat{L}_3' \cup \hat{L}_3''$ such that $|\hat{L}_3'| = |\hat{L}_3''| = \frac{1}{2}|\hat{L}_{k^*,3}|$.

- Sides $\hat{L}_4'$ and $\hat{L}_5'$ coincide with $\hat{L}_2'$ and $\hat{L}_1''$, respectively. Moreover, $\hat{L}_4'$ is parallel and isometric to $\hat{L}_2$.

By the above, note that $|\hat{L}_1'| = |\hat{L}_1''| = \frac{1}{2}|L_1|$. Next, we note that there exist two corner border tiles $t(Y, c_{k^*})' = (Q(T, c_{k^*}), g[Y, c_{k^*}]')$ and $t(Y, c_{k^*})'' = (Q(T, c_{k^*}), g[Y, c_{k^*}]'')$ in $T$. We define bond mappings of these border tiles according to the procedures below. As in Case (I.B), these procedures mirror those in Case (I.A) for the corner border tiles corresponding to $c_{k^*}$ and $\phi_Y(c(Y))$.

1. We use the bond $a_X(Y)$ as follows: $g[Y, c_{k^*}]'(\hat{L}_1') = a_X(Y)$ and $g[Y, c_{k^*}]''(\hat{L}_2'') = a_X(Y)$. Because $\hat{L}_1'$ coincides with $\hat{L}_2''$, these two sides have matching, complementary bonds.

2. For $i = 6, 7, 8$, we define $g[Y, c_{k^*}]'(\hat{L}_i')$ according to the procedures for $\hat{L}_{k^*,i-1}$ in Case (I.A), recalling that $\hat{L}_i'$ coincides with $\hat{L}_{k^*,i-1}$. Similarly, we define $g[Y, c_{k^*}]''(\hat{L}_i'')$ according to the procedures for $\hat{L}_{k^*,i}$ in Case (I.A).

3. Note that the sides $\hat{L}_1', \hat{L}_2'$, and $\hat{L}_3''$ are defined in the same manner in Case (I.B). We define the bonds assigned to these sides by their respective bond mappings according to the procedures in Case (I.B).

4. The sides $\hat{L}_3'$, $\hat{L}_5'$, and $\hat{L}_4''$ are all assigned the bond $\nu$ by their respective bond mappings.

As in Case (I.B), note that the sum of $\alpha_T(0)$ and $t(Y, c_{k^*})'$ is an assembly instance at temperature 2. On the other hand, the sum of $t(Y, c_{k^*})'$ and $t(Y, c_{k^*})''$ is not an assembly instance at temperature 2 because these tiles have only one pair of matching, complementary bonds. For the remaining border tiles, we follow the procedures of Case (I.A) and modify the corner border tile $t(Y, c_{k^*-1})$ and the set of side border tiles $\{t_z(Y, L_{k^*-1})\}_{z \in \mathbb{L}}$ according the corresponding procedures in Case (I.B). We conclude this case by adopting
the same notation for $\alpha(Y,1)$ as in Case (I.B) and noting that all of the observations from Cases (I.A) and (I.B) also hold for this case.

**Case (II)** We assume that $B(X) = \emptyset$, and let $f$ be as defined in Case (I.B). As was the case with tile $t(X) \in \mathbb{T}$ in Step 2, the assembly instance resulting from a border forming around $\alpha_T(0)$ will not participate in the simulation process associated with $\Gamma$. We define all of the border tiles in this case as in Case (I.A), using path $f$ in place of $f_1$ and $f_2$. However, we modify the notation by replacing $Y$ with $X$ when the former occurs. We also modify the bond mappings rather than the polygons associated to the border tiles according to the condition below for a side $L$ of a border tile $t = (P,g)$ defined in Case (I.A).

\((\ast)\) If $g(L)$ would be equal to $a(-)$, $a(\perp)$, or a bond associated to a Step 1 marking (excluding $-a_X(\triangleleft_1)$ and $-a_X(\triangledown_1)$ but not their complementary bonds), then $g(L) = \nu$.

Note that the modifications above do not prevent the border tiles from binding to $\alpha_T(0)$ one at a time. While $t(X,c(T))$ is still the first border tile to bind to $\alpha_T(0)$, border formation does not necessarily follow the path $f$. In fact, there is no unique last border tile which binds to $\alpha_T(0)$. However, the resulting sum $\alpha(X,1)$ is an assembly instance at temperature 2 such that every boundary side of $\alpha(X,1)$ is assigned the empty bond $\nu$. In this way, $\alpha(X,1)$ helps satisfy condition (1) of Definition 2.3.3 but does not participate in the simulation process after it is formed.

Observe that the border tiles defined in the cases above were always defined with respect to a finite collection of finite sets. Thus, $\mathbb{T}$ is finite as desired. We let $\mathcal{T}_0 = \{[t] \mid t \in \mathbb{T}\}$ as mentioned in Step 2.

**Claim:** The TAS $\Gamma = (\mathcal{T}_0, 2)$ which we constructed in Steps 1–3 simulates $R$ with border.

**Proof of Claim.** We begin by defining the assembly blocks $B_\ell$ which form the substitution chain associated to $\Gamma$. Along the way, we show that $\Gamma$ satisfies condition (1) of Definition 2.3.3. We begin by formally defining the set $B_0(X)$ for each $X \in \mathcal{P}$:

$$B_0(X) = \begin{cases} 
\{[t(Y)] \mid Y \in B(X)\} & \text{if } B(X) \neq \emptyset \\
\{[t(X)]\} & \text{otherwise.} 
\end{cases}$$

We let $B_0 = \bigcup_{X \in \mathcal{P}} B_0(X)$ and note that the set of border tile types $\mathcal{T}_B$ is $\mathcal{T}_0 \setminus B_0$.

Let $T \in \mathcal{S}$ and $X \in \mathcal{P}$ such that $T$ is the tiling of $\lambda X$. In Step 2, we showed that the sum $\alpha_T(0)$ of $\{t(Y)\}_{Y \in T}$ is an assembly instance at temperature 2; note that $[\alpha_T(0)]$ is a producible assembly of $\Gamma$ accordingly. In Step 3 we showed that the following hold:
If \( B(X) = \emptyset \), then there exists an assembly instance \( \alpha(X,1) \) which is the sum of \( \alpha_T(0) \) and a set of border tiles. Furthermore, the shape of \( \alpha(X,1) \) is isometric to \( \kappa(\lambda X) \) by construction and \( [\alpha(X,1)] \) is a producible assembly of \( \Gamma \). In this situation, we let \( B_1(X) = \{[\alpha(X,1)]\} \).

If \( B(X) \neq \emptyset \), then there exists an assembly instance \( \alpha(Y,1) \) for each \( Y \in B(X) \) which is the sum of \( \alpha_T(0) \) and a set of border tiles. Furthermore, the shape of each \( \alpha(Y,1) \) is isometric to \( \kappa(\lambda X) \) by construction and each \( [\alpha(Y,1)] \) is a producible assembly of \( \Gamma \). In this situation, we let \( B_1(X) = \{[\alpha(Y,1)]\} \). Let \( B_1 = \bigcup_{X \in \mathcal{P}} B_1(X) \). Note that there exist assembly sequences of \( \Gamma \) from \( B_0 \) to \( B_1 \) for each assembly in \( B_1 \) as required by the definition of an assembly chain.

By the definition of the border tiles in Step 3, each \( \alpha(Y,1) \) inherited the bonds associated to Step 1 markings from the tile \( t(Y) \). Moreover, recall that each the set of tiles \( \{t(Y)\}_{Y \in T} \) formed an assembly instance \( \alpha_T(0) \) using only the bonds associated to Step 1 markings. Choose \( \alpha(Y,1) \in [\alpha(Y,1)] \) for each \( Y \in T \) such that the shape of \( \alpha(Y,1) \) coincides with \( \kappa \cdot \lambda Y \). It follows that the sum of \( \{\alpha(Y,1)\}_{Y \in T} \) is an assembly instance at temperature 2 whose shape is isometric to \( \kappa \cdot \lambda^2 X \). Our choice of \( \{\alpha(Y,1)\}_{Y \in T} \) guarantees that the bonds associated with Step 1 markings on the boundary sides of each \( \alpha(Y,1) \) will be coincident to boundary sides which have matching, complementary bonds. We can repeat the observations about \( \alpha_T(0) \) in Step 2 for this sum of assembly instances, which we denote by \( \alpha_T(1) \). Thus, \( [\alpha_T(1)] \) is also a producible assembly of \( \Gamma \).

Before continuing, let \( \alpha(Y_1,1)' \) and \( \alpha(Y_2,1)' \) be assembly instances which have overlapping boundary sides. We remark that several of these boundary sides may not be coincident by our definition of the border tiles in Step 3. However, the adjacent corner border tiles of \( \alpha(Y_1,1)' \) and \( \alpha(Y_2,1)' \) will always have coincident sides of length \( \delta \) because of how the differences in lengths between sides of \( \lambda X \) and those of \( \varphi(\lambda X) \) were incorporated into the corner border tiles in Step 3.

Note that \( \alpha_T(1) \) has two adjacent boundary sides of length \( \delta \) with bonds \( a_X(\gg_1) \) and \( a_X(\gg_2) \) because the assembly instances \( \{\alpha(Y,1)\}_{Y \in T} \) inherited all Step 1 markings. By our definition of the corner border tiles in Step 3, note that the following hold.

- If \( B(X) = \emptyset \), then there exists a tile in \([t(X,c(T))]) \) which can bind to \( \alpha_T(1) \) to form an assembly instance at temperature 2.

- If \( B(X) \neq \emptyset \), then there exists a tile in \([t(Y,c(T))]) \) for each \( Y \in B(X) \) which can bind to \( \alpha_T(1) \) to
form an assembly instance at temperature 2.

Observe that a border can form starting from each of the border tiles above in the same manner that borders formed according to the cases in Step 3. This observation holds primarily because we added side border tiles \( t_z(X, L) \) or \( t_z(Y, L) \), respectively, for each \( z \in \mathbb{L} \) (and for each \( Y \in B(X) \) if this set is nonempty). The set \( \mathbb{L} \) captures all possible lengths which can appear on the boundary sides of \( \alpha_T(1) \). Furthermore, we can use the previous statement and the fact that \( \{\alpha(Y, 1)\}_{Y \in T} \) inherited the boundary bonds from the tiles \( \{t(Y)\}_{Y \in T} \) to repeat the same observations as in the cases in Step 3. We define an assembly instance \( \alpha(X, 2) \) if \( B(X) = \emptyset \) such that \( \alpha(X, 2) \) is the sum of \( \alpha_T(1) \) and a collection of border tiles associated to \( X \); in this situation, we note that \( [\alpha(X, 2)] \) is a producible assembly of \( \Gamma \). Likewise, we define assembly instances \( \{\alpha(Y, 2)\} \) if \( B(Y) \neq \emptyset \) such that each \( \alpha(Y, 2) \) is the sum of \( \alpha_T(1) \) and a collection of border tiles associated to \( Y \); in this situation, we note that each \( [\alpha(Y, 2)] \) is a producible assembly of \( \Gamma \).

Next, we consider the shape of assembly instance \( \alpha(X, 2) \) assuming that \( B(X) = \emptyset \). Recall that the lengths of the line segments used to define the border tiles in Step 3 were either constant (i.e. equal to \( \delta \)) or could be determined from the boundary corners of \( T \) and the dilation \( \varphi_\kappa \). Moreover, the shape of \( \alpha_T(1) \) is similar to \( X \) by the construction above; specifically, it was isometric to \( \kappa \cdot \lambda^2 X \). Let \( z \) be the point in \( \kappa \cdot \lambda^2 X \) which corresponds to the center of dilation for \( \varphi_\kappa \). It follows that when the border forms around \( \alpha_T(1) \) to form \( \alpha(X, 2) \), the shape of \( \alpha(X, 2) \) is coincident to a dilation of \( \kappa \cdot \lambda^2 X \) centered at \( z \) by some factor \( \kappa_2 > 1 \). This factor can be calculated from the lengths of the sides of \( \kappa \cdot \lambda^2 X \) and the lengths associated to the border tiles which bind to \( \alpha_T(1) \). The same observations hold for each assembly instance in \( \{\alpha(Y, 2)\}_{Y \in T} \) if \( B(Y) \neq \emptyset \). In particular, we note that the factor \( \kappa_2 > 1 \) is constant because the shape of each assembly instance in \( \{\alpha_T(1)\}_{T \in \mathcal{S}} \) is a similar to its corresponding polygon \( X \in \mathcal{P} \) via the same factor \( \kappa \cdot \lambda^2 \).

We can continue the process above recursively to define the substitution chain \( \mathcal{A} = \{B_t\}_{t=0}^\infty \) of \( \Gamma \). Just as we can calculate the dilation factor \( \kappa_2 > 1 \), every subsequent dilation factor \( \kappa_t \) associated with assembly block \( B_t \) can be calculated from the shape of an instance of an element in \( B_t \). Hence, we conclude that \( \Gamma \) satisfies condition (1) of Definition 2.3.3.

To show that condition (2) of Definition 2.3.3 holds, we consider the assembly sequences from \( B_0 \) to \( B_1 \). Let \( T \in \mathcal{S} \) and \( X \in \mathcal{P} \) such that \( T \) is the tiling of \( \lambda X \). Moreover, let \( x_1 \neq x_2 \) be in \( T \) such that \( x_1 \) and \( x_2 \) are marked with \( \langle \tau, c \rangle \in \mathcal{M}_T \); specifically, recall that \( x_1 \in \pi(p) \) and \( x_2 = \tau(p) = v_{|T| - 1} \). Denote \( x_1 = v_{i^*} \) for some \( 0 \leq i^* < |T| - 1 \); because \( x_1 \in \pi(p) \), there exists \( r > i^* \) such that \( p \) is robust up to
Alternatively, if \( \alpha \) is the sum of \( t(v_{i_j}) \) and some subset of \( \{t(v)\}_{v \in T} \) which does not contain both \( t(v_{i_{j - 1}}) \) and \( t(v_k) \), then \( \alpha \) is not an assembly instance at temperature 2. We extend the previous argument to observe that the following also holds for each \( 1 \leq j \leq m \):

ii. If \( \alpha \) is an assembly instance at temperature 2 and \( \alpha \) is the sum of \( t(v_{i_j}) \) and a subset \( W \subseteq \{t(v)\}_{v \in T} \setminus \{t(v_{i_j})\} \), then \( \{t(v_{i_j})\}_{i = 0}^{j - 1} \subseteq W \).

We make a final observation based on the fact that \( x_1 \in \pi(p) \) and \( x_2 = \tau(p) = v_{|T| - 1} \):

iii. If \( \alpha \) is an assembly instance at temperature 2 and \( \alpha \) is the sum of \( t(x_1), t(x_2) \), and a subset \( W \subseteq \{t(v)\}_{v \in T} \setminus \{t(x_1), t(x_2)\} \), then \( W = \{t(v)\}_{v \in T} \setminus \{t(x_1), t(x_2)\} \).

In other words, if \( \alpha \) is an assembly instance at temperature 2 and \( t(x_1), t(x_2) \in \text{dom } \alpha \), then \( \{t(v)\}_{v \in T} \subseteq \text{dom } \alpha \).

Second, suppose that \( \alpha \) is the sum of a set of tiles \( W \) such that for every \( t \in W \), \( [t] \in B_0 \). If \( \alpha \) is an assembly instance at temperature 2, then observe that \( \{[t] \mid t \in W\} \subset B_0(X) \) for some \( X \in \mathcal{P} \). That is to say, only tiles whose tile types belong to the same set \( B_0(X) \) can bind to one another. Furthermore, the shape \( \alpha \) is isometric to some subset \( Z \) of \( T \in \mathcal{S} \) which is the tiling of \( \lambda X \). The two observations above hold because of how we defined the markings in Step 1 and how we defined the tiles in Step 2 using the bonds associated to the aforementioned markings. If \( \alpha' \) is the sum of \( \alpha \) and some border tile, then observe that \( \alpha \in [\alpha_T(0)] \) for some \( T \in \mathcal{S} \). This observation follows from the previous paragraph and our definition of the border tiles in Step 3.

From the previous two paragraphs, we conclude that conditions (2)(a)-(c) hold for an assembly sequence \( \{[\alpha_j]\}_{i=0}^{m} \) which starts at \( B_0 \) and ends at \( B_1 \). By the manner in which we designed border formation in Step 3, we also note that condition (2)(e) must hold. To observe that condition (2)(d) holds for \( \{[\alpha_j]\}_{i=0}^{m} \), we note that the unbordered assembly of \( \{[\alpha_j]\}_{i=0}^{m} \) must be of the form \( [\alpha_T(0)] \) for some \( T \in \mathcal{S} \) by the last observation in the previous paragraph. Recall that the boundary sides of \( \alpha_T(0) \) are all assigned a bond
in \( \{a(-), a(\perp), a_X(\triangleright\triangleleft_1), a_X(\triangleright\triangleleft_2)\} \) by our construction in Step 2. Once the first border tile \( t \) binds to the unique pair of bonds \( a_X(\triangleright\triangleleft_1) \) and \( a_X(\triangleright\triangleleft_2) \) on two boundary sides of \( \alpha_T(0) \), only an assembly instance \( \beta \) which has at least two matching, complementary bonds to \( a(-), a(\perp) \), or the bonds on the sides of \( t \) can bind to the sum of \( \alpha_T(0) \) and \( t \). By the way the we assigned bonds in Steps 2 and 3, we observe that \( \beta \) must be a border tile. Continuing in this way, we observe that condition (2)(d) holds as well.

We conclude the proof of our claim and our proof overall by noting that condition (3) of Definition 2.3.3 holds from the work above. Indeed, the bonds in \( \Sigma \) were assigned to tiles in Steps 2 and 3 so that each was given a specific purpose in the overall assembly process. While elements in each assembly block \( B_\ell \) for \( \ell \geq 0 \) use the bonds associated to the markings from Step 1 to bind to one another, these bonds are assigned to boundary sides that are separated from one another by distances proportional to \( \ell \). Therefore, assemblies in \( B_{\ell_1} \) cannot bind to those in \( B_{\ell_2} \) when \( \ell_1 \neq \ell_2 \).

Before proceeding with our main result, we note that the border formation associated with the construction in Theorem 4.2.3 is implicitly non-deterministic at the start. By this we mean that there are usually multiple border tiles which can bind to the same pair of bonds \( (a_X(\triangleright\triangleleft_1), a_X(\triangleright\triangleleft_2)) \) for some \( X \in \mathcal{P} \) of an assembly instance \( \alpha \). One of these border tiles is non-deterministically “chosen” to initiate border formation by binding to \( \alpha \). By construction, this first border tile not only determines which other border tiles can subsequently bind to \( \alpha \) but how the resulting assembly instance can bind to other assembly instances. The previous statement informally implies that the tiles within the domain of \( \alpha \) do not carry this binding information. We observe that the non-determinism discussed above is also crucial in allowing the set of tiles \( \mathcal{T} \) to be finite. Non-determinism has been extensively studied in the context of tile assembly models \([3,5,7,8,26]\) and other self-assembly models \([21,28]\). In general, it has been found that some degree of non-determinism is required for complex computation and the efficient assembly of target shapes.

**Corollary 4.2.4.** Let \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) be a substitution rule which admits hereditary and sibling sides such that every \( X \in \mathcal{P} \) is star-shaped. If every tiling \( T \in \mathcal{S} \) is backtrack constructible, then there exists a TAS \( \Gamma = (\mathcal{T}_0, 2) \) which simulates \( \mathcal{R} \) with border.

**Proof.** Let \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) be as given. The construction process for designing the TAS \( \Gamma = (\mathcal{T}_0, 2) \) which simulates \( \mathcal{R} \) with border is nearly identical to the process described in the proof of Theorem 4.2.3. After modifying the marking process below, Steps 2 and 3 remain unchanged from the aforementioned proof.

We describe the changes to the marking process in Step 1 in the proof of Theorem 4.2.3 below for a
given tiling $T$ which is backtrack constructible. By definition, this means that $\overline{G}(T)$ is $G(T)$-backtrack constructible at stage $\eta \geq 0$ via $(\Lambda, \rho)$. First, we follow the procedures of Step 1 to mark the vertices (i.e. polygons) in the stage 1 backtrack components of $\overline{G}(T)$ within the hierarchy of $(\Lambda, \rho)$. Then for $0 < i \leq \eta$, we use $(\simeq^i)$ to mark the corners of vertices in $\overline{G}(T)$ according the edges in stage $i$ routes connecting stage $i$ components of $\overline{G}(T)$. By Definition 4.1.6, recall that these edges are all in $\overline{G}(T)$ so that the corners which we mark are associated to side adjacent polygons which have at least one pair of coincident sides. The only time that we need to be careful when choosing the corners to mark with $(\simeq^i)$ is when a backtrack component $\hat{V} \subset T$ is a singleton. By Definition 4.1.6, the stage $i$ predecessors of $\hat{V}$ satisfy a minor backtrack connected requirement (see condition (2)(a) in this definition). We use the first claim in the proof of Theorem 4.2.3 to choose a corner in the single polygon in $\hat{V}$ as done with the markings $(\odot)$ and $(\oplus)$. Once every edge in $\epsilon^\eta(\Lambda, \rho)$ has been associated to a marking in $T$, we use the condition (2) of Definition 4.1.7 to assign the marking $(\blacktriangleleft)$ as in the proof of Theorem 4.2.3. We give an example of this modified marking process in Section C.3.

We account for the additional markings described above when defining $\Sigma$. However, Steps 2 and 3 proceed as in the proof of Theorem 4.2.3, since the set of markings $\mathcal{M}_T$ for a given tiling $T$ has already been adjusted above. We also note that the observations presented in Steps 1–3 and final claim of the aforementioned proof transfer over directly into this context because of Definition 4.1.6 generalizes backtrack paths into backtrack routes.
Chapter 5

Conclusion

In this work, we formalized the idea of simulating substitution rules from the perspective of tile self-assembly and then provided results associated to our notions of simulation. Motivated by similar approaches in other tile assembly models [24,31], we defined and focused on bordered simulation wherein the formation of a border is incorporated into the simulation process. Once a border is formed, the tiles associated with this border then coordinate how the resulting assembly instance binds to tiles and other assembly instances. Thus, the formation of a border can be seen as an external mechanism which coordinates how intermediary structures interact during a self-assembly process.

We provided several necessary conditions for bordered simulation in Chapter 3, concluding that tile assembly systems with a temperature parameter of 1 cannot simulate a substitution rule with border (Theorem 3.1.4). On the other hand, we provided a sufficient condition in Chapter 4 for bordered simulation based on backtrack constructible graphs. In the proof of Theorem 4.2.3, we constructed a tile assembly system which simulates a given substitution rule $R$ with border if every tiling of $R$ is backtrack constructible at stage 0 (i.e. backtrack connected); this tile assembly system has a temperature parameter of 2. Our main result (Corollary 4.2.4) generalizes this construction to account for tilings which are backtrack constructible at stage $\eta \geq 0$; however, the resulting tile assembly system still has a temperature parameter of 2. Considering Theorem 3.1.4, we note that the aforementioned tile assembly system is minimal with respect to temperature.

As mentioned in Section 1.1, we considered a collection of over one hundred substitution rules [12–14, 18–20,43] in an attempt to capture all known substitution rules adhering to our definition in Section 2.1. We observed that every substitution rule in this collection either (1) satisfies the conditions of our main result (Corollary 4.2.4) and admits bordered simulation accordingly or (2) can be shown to not admit bordered simulation (see Section 3.2). In this way, we provide evidence that the sufficient condition presented in Corollary 4.2.4 may also be a necessary condition. If it is not, we conjecture that a necessary and sufficient
condition for bordered simulation may be found by replacing backtrack paths and routes with partial orders on trees.

In addition to border simulation, we also defined strict simulation in Section 2.3; this notion of simulating a substitution rule follows the supertiles of the substitution rule directly. However, we are not aware of any substitution rule which admits strict simulation. Preliminary work shows that there do exist several substitution rules which admit bordered simulation but not strict simulation. However, this work has been done on a case by case basis considering specific substitution rules. To this end, we pose the following questions: Does there exist any substitution rule which admits strict simulation? If so, what conditions characterize such substitution rules? We note that our approach of using adjacency graphs may provide some insight into the second question above if there do exist substitution rules which admit strict simulation. On the other hand, if there exist no such substitution rules, then the distinction between strict and bordered simulation could provide insight into hierarchical growth in general. Suppose that border formation is necessary for simulating the hierarchical growth of substitution rules. In a general setting, this requirement could imply that an external mechanism is necessary in order for intermediary structures to identify and interact with each other.

We conclude by considering some generalizations associated to our work. First, we note that there are some tile assembly models which incorporate signaling [30, 39]. By this, we mean that a tile \( t \) is defined with signals which then determine whether the bonds of \( t \) are available for binding. There exist several results [23, 30–32, 34, 39, 41] which give evidence to the strength of adding signals to tiles. Notably, [23] considers a model based on 2HAM (see Section 1.2) which incorporates signals and allows tiles and assembly instances to detach from one another. The signaling in this model is based on a strand displacement mechanism studied in the context of DNA tile self-assembly [40]. Given a “discrete, self-similar” fractal, [23] provides constructions for tile assembly systems which produce the given fractal while following a hierarchical assembly process. In particular, small assembly instances are used as external tools to modify the growing fractal structure. After accomplishing their purpose, these small assembly instance then detach and no longer participate in the self-assembly process. In a generalization of p-2HAM which incorporates signaling, a similar approach could enable the strict simulation of substitution rules by allowing a border to modify the bonds of an assembly instance before detaching. Note that this gives further evidence for the idea that hierarchical growth may require an external mechanism in order for intermediary structures to interact and bind with one another.
Next, recall from Section 1.1 that there are several ways to generalize our definition of substitution rules. One such generalization modifies the way that the tilings of a substitution rule $\mathcal{R}$ are associated with the prototiles of $\mathcal{R}$. This modification can be informally described as follows using our notation for a substitution rule $\mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S})$: a tiling $T$ in $\mathcal{S}$ is associated to a prototile $X$ in $\mathcal{P}$ if $T$ intersects $\lambda X$ in such a way that supertiles of $\mathcal{R}$ are well-defined tilings [12, 13]. Note that the sets $T \setminus \lambda X$ and $\lambda X \setminus T$ may both be non-empty in this setting; see Figure 5.01. It is likely that some our results about simulation extend to substitution rules adhering to this more general definition. Most of our results deal with the adjacency graphs of a tiling and thus do not depend on the shape of the tiling. However, we would need to be careful when defining simulation in this general setting because of how tilings can be associated to prototiles.

Figure 5.01. The Penrose Kite and Dart substitution rule [13] and some of its supertiles. The blue prototile is called a kite and the red prototile is called a dart. Top: A tiling $T$ is associated to the kite (left) and the dart (right). We use dashed lines to indicate the outline of $\lambda X$ within the associated tiling $T$ for each prototile $X$. Middle: The supertiles of order 2 for the kite (left) and the dart (right). As before, we use dashed lines to indicate the outline of $\lambda^2 X$ for each prototile $X$. Bottom: The supertile of order 3 for the dart.
References


Appendix A
Sample of Substitution Rules and Associated Graphs

Here we collect and add to the substitution rules presented throughout our work. Most of the substitution rules below have been adapted from the Tiling Encyclopedia, [13]. For each substitution rule, we indicate whether the associated tiling(s) is (are, resp.) backtrack constructible at stage \( \eta \geq 0 \), abbreviated “b.c. at stage \( \eta \)”. Let \( \mathcal{R} = (\mathcal{P}, \lambda, \mathcal{S}) \) be one of the substitution rules below. If a tiling \( T \in \mathcal{S} \) is backtrack constructible at stage 0, then the polygons in \( T \) are enumerated in ascending order in accordance with the associated stage 0 route. Similarly, if a tiling \( T \in \mathcal{S} \) is backtrack constructible at stage 1, then the polygons in \( T \) are grouped according to the associated stage 1 backtrack partition. In the latter case, the polygons in each element \( V' \) of the partition are also enumerated in accordance with the backtrack path associated to \( V' \).

**Figure A.01.** Sphinx substitution rule [13]; b.c. at stage 0.

**Figure A.02.** Chair substitution rule [13]; b.c. at stage 0.
Figure A.03. Pinwheel substitution rule [13]; b.c. at stage 0.

Figure A.04. Pentiamond AC Factor 2 substitution rule [13]; both b.c. at stage 0.

Figure A.05. T2000 substitution rule [13]; b.c. at stage 0.
Figure A.06. Square substitution rule; both b.c. at stage 0.

Figure A.07. Domino Variant substitution rule [13]; not b.c. at any stage $\eta$.

Figure A.08. Triangle substitution rule; not b.c. at any stage $\eta$.

Figure A.09. Trapezotriangular substitution rule [13]; not b.c. at any stage $\eta$ despite both tilings having backtrack paths.
Figure A.10. Extended Armchair substitution rule; b.c. at stage 1. Note that there are three mutually disjoint choke-hold pairs in the graph. We infer from Remark 4.1.2 that the associated tiling is not b.c. at stage 0. The sets in stage 1 backtrack partition for this substitution rule are \{1, 2, 3, 4, 5, 6\}, \{7, 8\}, and \{9, 10, 11, 12, 13, 14, 15, 16\}. 
Figure A.11. Pentiamond AC Factor 3 substitution rule [13]; top is b.c. at stage 1 and bottom is b.c. at stage 0. Note that there are three mutually disjoint choke-hold pairs in the top graph. We infer from Remark 4.1.2 that the top tiling is not b.c. at stage 0. The sets in stage 1 backtrack partition for the top tiling are \{1, 2, 3, 4, 5\}, \{6, 7, 8\}, and \{9\}. 
Figure A.12. Tetris T substitution rule; b.c. at stage 1. Note that there are three mutually disjoint chokehold pairs in the graph. We infer from Remark 4.1.2 that the associated tiling is not b.c. at stage 0. The sets in stage 1 backtrack partition for this substitution rule are \{1, 2, 3, 4, 5, 6\}, \{7, 8, 9, 10, 11, 12\}, and \{13, 14, 15, 16\}.
Appendix B

Square Substitution Tile Assembly System

We present the set of tile types $T_0$ for the tile assembly system $\Gamma = (T_0, 2)$ discussed in Example 2.3.6. In particular, we define a set of tiles $T$ which are distinct up to equivalence and then let $T_0 = \{ [t] \mid t \in T \}$. The set of bonds $\Sigma$ for $T$ is denoted as follows: $\{ \nu, \pm a_\perp, \pm a_\perp \} \cup \{ \pm a_j, \pm \hat{b}_j, \pm \hat{c}_j, \ldots, \pm \hat{e}_j \}_{j=1}^8$. Recalling that $s(a) = 1$ for every $a \in \Sigma$ such that $a \neq \nu$, where $s : \Sigma \to \{0, 1\}$ is the strength function for $\Gamma$. We begin by reproducing Figure 2.21 in Figure B.01 in order to define the only four non-border tiles in $T$. 

![Figure B.01. The four non-border tiles for the TAS $\Gamma$, labeled $t(Y_i)$ for $1 \leq i \leq 4$. As in Chapter 2, any side without a bond is assigned the empty bond.](image)

Next, we present four polygons in Figures B.02–B.04 with labeled sides. We refer to these polygons in
Tables B.01–B.03 when defining the bond mapping $g$ of a specific border tile $t = (P, g)$. Please refer to Figures 2.18 and 2.25 for the relative lengths of the sides of the polygons in Figures B.02–B.04. The naming scheme for the border tiles is based on the labeling scheme in Figure B.05 of the boundary corners and sides of the tiling of the Square substitution rule.

![Figure B.02. L-shaped polygon $P_1$ used to define border tiles.](image)

Table B.01 Border tiles defined with the L-shaped polygon from Figure B.02.

<table>
<thead>
<tr>
<th>Tile $t = (P_1, g)$</th>
<th>$g(l_1)$</th>
<th>$g(l_2)$</th>
<th>$g(l_3)$</th>
<th>$g(l_4)$</th>
<th>$g(l_5)$</th>
<th>$g(l_6)$</th>
<th>$g(l_7)$</th>
<th>$g(l_8)$</th>
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<tr>
<td>$t(Y_1, c_2)$</td>
<td>$b_2$</td>
<td>$a_-$</td>
<td>$a_\perp$</td>
<td>$a_-$</td>
<td>$-\dot{b}_1$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
<td></td>
</tr>
<tr>
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<td>$b_4$</td>
<td>$\nu$</td>
<td>$a_2$</td>
<td>$a_\perp$</td>
<td>$a_-$</td>
<td>$-\dot{b}_3$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
</tr>
<tr>
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<td>$\nu$</td>
<td>$a_5$</td>
<td>$a_1$</td>
<td>$\nu$</td>
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<td>$\nu$</td>
<td>$\nu$</td>
</tr>
<tr>
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<td>$a_-$</td>
<td>$a_8$</td>
<td>$\nu$</td>
<td>$\nu$</td>
<td>$\dot{b}_7$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
</tr>
<tr>
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<td>$\dot{c}_2$</td>
<td>$a_-$</td>
<td>$a_\perp$</td>
<td>$-a_2$</td>
<td>$\nu$</td>
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<td>$a_-$</td>
<td>$a_\perp$</td>
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<tr>
<td>$t(Y_3, c_8)$</td>
<td>$-\dot{d}_8$</td>
<td>$\nu$</td>
<td>$a_6$</td>
<td>$a_\perp$</td>
<td>$a_-$</td>
<td>$\dot{d}_7$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_4, c_2)$</td>
<td>$\dot{e}_2$</td>
<td>$\nu$</td>
<td>$\nu$</td>
<td>$a_7$</td>
<td>$a_-$</td>
<td>$-\dot{e}_1$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
</tr>
<tr>
<td>$t(Y_4, c_4)$</td>
<td>$-\dot{e}_4$</td>
<td>$\nu$</td>
<td>$-a_5$</td>
<td>$\nu$</td>
<td>$-\dot{e}_3$</td>
<td>$\nu$</td>
<td>$\nu$</td>
<td></td>
</tr>
<tr>
<td>$t(Y_4, c_6)$</td>
<td>$-\dot{e}_6$</td>
<td>$a_-$</td>
<td>$a_\perp$</td>
<td>$-a_6$</td>
<td>$\nu$</td>
<td>$\dot{e}_5$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_4, c_8)$</td>
<td>$-\dot{e}_8$</td>
<td>$a_-$</td>
<td>$a_\perp$</td>
<td>$a_-$</td>
<td>$\dot{e}_7$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
<td></td>
</tr>
</tbody>
</table>
Figure B.03. Modified rectangle $P_2$ used to define border tiles.

Table B.02 Border tiles defined with the rectangle from Figure B.03.

<table>
<thead>
<tr>
<th>Tile $t = (P_2, g)$</th>
<th>$g(l_1)$</th>
<th>$g(l_2)$</th>
<th>$g(l_3)$</th>
<th>$g(l_4)$</th>
<th>$g(l_5)$</th>
<th>$g(l_6)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t(Y_1, c_1)$</td>
<td>$a_-$</td>
<td>$\dot{b}_8$</td>
<td>$-a_7$</td>
<td>$-a_8$</td>
<td>$b_1$</td>
<td>$a_-$</td>
</tr>
<tr>
<td>$t(Y_1, c_3)$</td>
<td>$a_-$</td>
<td>$-\dot{b}_2$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
<td>$b_3$</td>
<td>$a_-$</td>
</tr>
<tr>
<td>$t(Y_1, c_5)$</td>
<td>$\nu$</td>
<td>$-\dot{b}_4$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
<td>$b_5$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_1, c_7)$</td>
<td>$\nu$</td>
<td>$\dot{b}_6$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
<td>$-\dot{b}_7$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_2, c_1)$</td>
<td>$\nu$</td>
<td>$\dot{c}_8$</td>
<td>$-a_7$</td>
<td>$-a_8$</td>
<td>$\dot{c}_1$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_2, c_3)$</td>
<td>$a_-$</td>
<td>$-\dot{b}_2$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
<td>$b_3$</td>
<td>$a_-$</td>
</tr>
<tr>
<td>$t(Y_2, c_5)$</td>
<td>$a_-$</td>
<td>$-\dot{b}_4$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
<td>$b_5$</td>
<td>$a_-$</td>
</tr>
<tr>
<td>$t(Y_2, c_7)$</td>
<td>$\nu$</td>
<td>$-\dot{b}_6$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
<td>$b_7$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_3, c_1)$</td>
<td>$\nu$</td>
<td>$\dot{d}_8$</td>
<td>$-a_7$</td>
<td>$-a_8$</td>
<td>$\dot{d}_1$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_3, c_3)$</td>
<td>$\nu$</td>
<td>$\dot{d}_2$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
<td>$-\dot{d}_3$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_3, c_5)$</td>
<td>$a_-$</td>
<td>$\dot{d}_4$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
<td>$-\dot{d}_5$</td>
<td>$a_-$</td>
</tr>
<tr>
<td>$t(Y_3, c_7)$</td>
<td>$a_-$</td>
<td>$\dot{d}_6$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
<td>$-\dot{d}_7$</td>
<td>$a_-$</td>
</tr>
<tr>
<td>$t(Y_4, c_1)$</td>
<td>$a_-$</td>
<td>$\dot{e}_8$</td>
<td>$-a_7$</td>
<td>$-a_8$</td>
<td>$\dot{e}_1$</td>
<td>$a_-$</td>
</tr>
<tr>
<td>$t(Y_4, c_3)$</td>
<td>$\nu$</td>
<td>$-\dot{e}_2$</td>
<td>$\nu$</td>
<td>$-a_\perp$</td>
<td>$\dot{e}_3$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_4, c_5)$</td>
<td>$\nu$</td>
<td>$\dot{e}_4$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
<td>$-\dot{e}_5$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$t(Y_4, c_7)$</td>
<td>$a_-$</td>
<td>$\dot{e}_6$</td>
<td>$-a_\perp$</td>
<td>$\nu$</td>
<td>$-\dot{e}_7$</td>
<td>$a_-$</td>
</tr>
</tbody>
</table>
Table B.03 Border tiles defined with the rectangle and square from Figure B.04. We note that $1 \leq i \leq 8$ for the tiles above; accordingly, we have defined 64 tiles in this table.

<table>
<thead>
<tr>
<th>Tile $t = (P_3 \text{ or } P_4, g)$</th>
<th>$g(l_1)$</th>
<th>$g(l_2)$</th>
<th>$g(l_3)$</th>
<th>$g(l_4)$</th>
<th>$g(l'_1)$</th>
<th>$g(l'_2)$</th>
<th>$g(l'_3)$</th>
<th>$g(l'_4)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t(Y_1, L_i,</td>
<td>l_1</td>
<td>)$</td>
<td>$a_-$</td>
<td>$-b_i$</td>
<td>$-a_-$</td>
<td>$b_i$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$t(Y_1, L_i,</td>
<td>l'_1</td>
<td>)$</td>
<td>$-</td>
<td>$-</td>
<td>$-</td>
<td>$a_-$</td>
<td>$-b_i$</td>
<td>$-a_-$</td>
</tr>
<tr>
<td>$t(Y_2, L_i,</td>
<td>l_1</td>
<td>)$</td>
<td>$a_-$</td>
<td>$-c_i$</td>
<td>$-a_-$</td>
<td>$c_i$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$t(Y_2, L_i,</td>
<td>l'_1</td>
<td>)$</td>
<td>$-</td>
<td>$-</td>
<td>$-</td>
<td>$a_-$</td>
<td>$-c_i$</td>
<td>$-a_-$</td>
</tr>
<tr>
<td>$t(Y_3, L_i,</td>
<td>l_1</td>
<td>)$</td>
<td>$a_-$</td>
<td>$-d_i$</td>
<td>$-a_-$</td>
<td>$d_i$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$t(Y_3, L_i,</td>
<td>l'_1</td>
<td>)$</td>
<td>$-</td>
<td>$-</td>
<td>$-</td>
<td>$a_-$</td>
<td>$-d_i$</td>
<td>$-a_-$</td>
</tr>
<tr>
<td>$t(Y_4, L_i,</td>
<td>l_1</td>
<td>)$</td>
<td>$a_-$</td>
<td>$-e_i$</td>
<td>$-a_-$</td>
<td>$e_i$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$t(Y_4, L_i,</td>
<td>l'_1</td>
<td>)$</td>
<td>$-</td>
<td>$-</td>
<td>$-</td>
<td>$a_-$</td>
<td>$-e_i$</td>
<td>$-a_-$</td>
</tr>
</tbody>
</table>

Figure B.05. An enumeration of the boundary sides and corners of the tiling of the Square substitution rule.
Appendix C

Tile Assembly Systems for Selected Substitution Rules

In the following sections, we give an overview of the construction processes of Theorem 4.2.3 and Corollary 4.2.4 applied to selected substitution rules.

C.1 Square Substitution Rule

Recall the TAS $\Gamma = (T_0, 2)$ from Example 2.3.6 which we described to simulate the Square substitution rule with border. The design of this TAS follows the construction process of Theorem 4.2.3 with a minor modification which we detail later in this section. We refer the reader to Appendix B for a description of $T_0$ as necessary. We begin with the marking process for the squares in the only tiling $T$ of the Square substitution rule; see Figure C.02. Let $p = Y_1Y_2Y_3Y_4$, and note that $p$ is a $G(T)$-backtrack path in $G(T)$.

Moreover $p$ is robust up to $Y_4$ because this square is adjacent to $Y_1$ in $G(T)$.

Following Step 1 of Theorem 4.2.3, we first mark $Y_3$ and $Y_2$ with $(\oplus_3, c_9)$ and mark $Y_2$ and $Y_1$ with $(\ominus_3, c_9)$ by condition A of the marking process. We mark these polygons as stated because $Y_1$, $Y_2$, and $Y_3$ share corner $c_9$ which meets the criteria of the first claim in the proof of Theorem 4.2.3. Second, we mark $Y_1$ and $Y_4$ with $(\odot_4, c_9)$ by condition B; we mark these polygons as stated because they have a pair of sides which coincide. Third, we mark $Y_1$ and $Y_2$ with $(\bullet_2, c_3)$, mark $Y_2$ and $Y_3$ with $(\bullet_3, c_5)$, and mark $Y_3$ and
We mark $Y_4$ with $(\bullet_4, c_7)$; all of these markings are done following condition D. Finally, we mark $Y_1$ and $Y_4$ with $(\blacktriangleleft, c_1)$. The markings we describe in this paragraph are summarized in Table C.01.

![Diagram of a 2x2 square with corners labeled c1, c3, c5, and c7.](image)

**Figure C.02.** A partial enumeration of the corners of squares in the tiling of the Square substitution rule. We base this enumeration on the one presented in Figure B.05.

<table>
<thead>
<tr>
<th>Polygon</th>
<th>Associated Markings</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_1$</td>
<td>$(\blacktriangleleft, c_1), (\bullet_2, c_3), (\ominus_3, c_9), (\odot_4, c_9)$</td>
</tr>
<tr>
<td>$Y_2$</td>
<td>$(\bullet_2, c_3), (\bullet_3, c_5), (\ominus_3, c_9), (\oplus_3, c_9)$</td>
</tr>
<tr>
<td>$Y_3$</td>
<td>$(\bullet_3, c_5), (\bullet_4, c_7), (\ominus_3, c_9)$</td>
</tr>
<tr>
<td>$Y_4$</td>
<td>$(\blacktriangleleft, c_1), (\bullet_4, c_7), (\odot_4, c_9)$</td>
</tr>
</tbody>
</table>

**Table C.01** Markings for the Square substitution rule.

Having marked the polygons in $T$, we then define the set of bonds for $\Gamma$. However, this set $\Sigma$ has already been defined in Appendix B. So instead we provide a conversion table (Table C.02) for converting the bonds discussed in Example 2.3.6 to bonds adhering to the notation from Step 1. We note that we exclude bonds of the form $a_X(Y_j)$ for $1 \leq j \leq 4$ because these are not used in any tile. Refer to Figure B.05 for an enumeration of the boundary sides of $T$. We chose $\delta = \frac{1}{4}|L_1|$ because this satisfies the requirements in Step 2. Using $\delta$, we then define $T'$ and the polygons for the non-border tiles in $T$ according to the procedures in Step 2. However, we have already done this in Appendix B; see Figure B.01. Recall that $T'$ is the tiling of $2X$ which coincides with $T$ but has the polygons modified to incorporate sides of length $\delta$. For Step 3, we choose $\kappa_1 = \frac{5}{4}$ in order to define the corner and side border tiles in $T$. Using the notation in Step 3, note that $\varepsilon_i = \delta$ for $1 \leq i \leq 8$. See Figure C.03(a) for a visual reference of $T'$ within $\varphi_{\kappa_1}(2X)$.

We slightly deviate the procedures in Step 3 when incorporating $\varepsilon_i$ into the polygon $Q(T, c_i)$ associated with corner $c_i$ (for $1 \leq i \leq 8$). For $2 \leq 2i \leq 8$, we incorporate $\varepsilon_{2i}$ and $\varepsilon_{2i-1}$ in the polygon $Q(T, c_{2i})$. 

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instead of just $\varepsilon_{2i}$. This produces the $L$-shaped polygons and the rectangles in Figures B.01 and B.02, respectively. We deviate from the procedures in Step 3 in order to simplify the definition of the border tiles in Appendix B. More importantly, we note that the definition of the corner border tiles $t(Y_j, c_i)$ for $1 \leq j \leq 4$ and $1 \leq i \leq 8$ in Appendix B fundamentally follow the same procedures as in Step 3 for defining corner and side border tiles, including the notation used. See Figure C.03 as a visual reference for these differences.

**Table C.02** Conversion table for the bonds of $\Gamma$ to the notation of Step 1. We note that $1 \leq i \leq 8$ in the right portion of the table.

<table>
<thead>
<tr>
<th>Bond in $\Sigma$</th>
<th>Step 1 Notation</th>
<th>Bond in $\Sigma$</th>
<th>Step 1 Notation</th>
<th>Bond in $\Sigma$</th>
<th>Step 1 Notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$</td>
<td>$\nu$</td>
<td>$a_-$</td>
<td>$a(-)$</td>
<td>$a_-$</td>
<td>$a(\bot)$</td>
</tr>
<tr>
<td>$a_X(\ominus 3)$</td>
<td>$a_1$</td>
<td>$a_X(\ominus 4)$</td>
<td>$a_5$</td>
<td>$\hat{b}_i$</td>
<td>$a_X(Y_1, L_i)$</td>
</tr>
<tr>
<td>$a_X(\bullet_2)$</td>
<td>$a_2$</td>
<td>$a_X(\bullet_4)$</td>
<td>$a_6$</td>
<td>$\hat{c}_i$</td>
<td>$a_X(Y_2, L_i)$</td>
</tr>
<tr>
<td>$a_X(\oplus 3)$</td>
<td>$a_3$</td>
<td>$a_X(\approx 1)$</td>
<td>$a_7$</td>
<td>$\hat{d}_i$</td>
<td>$a_X(Y_3, L_i)$</td>
</tr>
<tr>
<td>$a_X(\bullet_3)$</td>
<td>$a_4$</td>
<td>$a_X(\approx 2)$</td>
<td>$a_8$</td>
<td>$\hat{e}_i$</td>
<td>$a_X(Y_4, L_i)$</td>
</tr>
</tbody>
</table>

**C.2 Pinwheel Substitution Rule**

In this section, we complete the construction overview from Section 4.2 for the Pinwheel substitution rule. Recall that we modified the Pinwheel substitution rule (see Figure 4.05) so that the resulting substitution rule admits hereditary and sibling sides. We note that the TAS constructed via Theorem 4.2.3 which simulates this modified substitution rule with border also simulates the Pinwheel substitution rule with border. As with the Square substitution rule in Section C.1, we begin with the marking process from Step 1 of Theorem 4.2.3. We present the markings in Table C.03, using Figure C.05 as a visual reference. Note that we use the modified tiling from Figure 4.05.

Next, we complete Step 1 of Theorem 4.2.3 by defining the set of bonds $\Sigma$ as we did with the Square substitution rule (Section C.1). Rather than defining these explicitly, we mention that there are 11 bonds associated with the markings (2 for the $\approx$ marking) and 48 bonds for border formation: $a_X(Y_j, L_i)$ and $a_X(Y_j)$ for $1 \leq j \leq 5$ and $1 \leq i \leq 8$. We note that $\{L_i\}_{i=1}^{8}$ is an enumeration of the boundary sides of the tiling in Figure C.05. Additionally, only $a_X(Y_2)$ out of $\{a_X(Y_j)\}_{j=1}^{8}$ is used for defining border tiles; we
Figure C.03. Visualizations of the tiling $T'$ within $\varphi_{\kappa_1}(2X)$. Left: Outline of the polygons for the corner and side border tiles according to the procedures in Step 3 of Theorem 4.2.3. Right: Outline of the polygons for the corner and side border tiles according to the description of Example 2.3.6. Recall from the proof of Theorem 4.2.3 that $c'_i = \varphi_{\kappa_1}(c_i)$ for $1 \leq i \leq 8$, which we have indicated above; we also indicate $\varepsilon_i$.

Figure C.04. Pinwheel substitution rule [13] and its associated adjacency graphs. Let $T$ be the tiling of this substitution rule. The edges colored in red indicate a $G(T)$-backtrack path in $\overline{G(T)}$ from $Y_1$ to $Y_5$.

elaborate on this later.

Recall that we already chose $\delta > 0$ in Section 4.2 for this substitution rule and defined the adjusted tiling $T'$ by introducing additional sides of length $\delta$; see Figure 4.07. As with the Square substitution rule, we define the five non-border tiles in the set of distinct tiles $T$ using the triangles in the tiling $T'$. For brevity, we omit a visual representation of the definition of these tiles.

We conclude this example by giving a general, visual description of the construction the corner and side border tiles in $T$ following Step 3 of Theorem 4.2.3. As with Step 2, we have already defined $\kappa > 1$ and
Figure C.05. A partial enumeration of the corners of triangles in the tiling of the (modified) Pinwheel substitution rule and an enumeration of the boundary sides of this tiling.

Table C.03 Markings for the Pinwheel substitution rule.

<table>
<thead>
<tr>
<th>Polygon</th>
<th>Associated Markings</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_1$</td>
<td>$(\bullet_2, c_1), (\circ_2, c_2), (\bigcirc_3, c_3), (\oplus_4, c_3), (\triangleleft, c_3)$</td>
</tr>
<tr>
<td>$Y_2$</td>
<td>$(\bullet_2, c_1), (\circ_2, c_2), (\bullet_3, c_4)$</td>
</tr>
<tr>
<td>$Y_3$</td>
<td>$(\bigcirc_3, c_3), (\bigcirc_4, c_3), (\oplus_4, c_3), (\bigotimes_5, c_3), (\bullet_3, c_4)$</td>
</tr>
<tr>
<td>$Y_4$</td>
<td>$(\oplus_4, c_3), (\bigotimes_5, c_3), (\oplus_5, c_3), (\bullet_3, c_4), (\bullet_5, c_5)$</td>
</tr>
<tr>
<td>$Y_5$</td>
<td>$(\oplus_5, c_3), (\triangleleft, c_3), (\bullet_5, c_5)$</td>
</tr>
</tbody>
</table>

provided the dilation used to define the border tiles; see Figure 4.08. We visualize the polygons for the corner border tiles associated with each triangle in $T$ in Figure C.06. This visualization also provides the basis for defining the side border tiles and gives the direction(s) of border formation associated with triangle $Y_2$ through $Y_5$. Note that we do not include triangle $Y_1$ because the visualization associated with this triangle is already provided in Figure 4.11. By design, red tiles in Figures 4.11 and C.06 bind before other border tiles and initiate border formation; note that every red tile binds to the same two triangle tiles. As discussed in Section 4.2, this observation illustrates the non-determinism associated with border formation which is essential to the bordered simulation of $\mathcal{R}$.  

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Figure C.06. Visualization of border formation and border tiles for triangles (top) $Y_2$, (middle) $Y_3$, and (bottom) $Y_4 - Y_5$. As in Figure 4.11, we use arrows to denote the path(s) along the boundary of $T'$ associated with each triangle. Each path starts at the corner associated to the red tile and ends at the corner associated to the purple tile. In each case, the side and corner border tiles bind such that the red tile is the first to bind and the purple tile is last. We color other corner border tiles yellow and the side border tiles blue for visual contrast.

C.3 Extended Armchair Substitution Rule

Before discussing bordered simulation, we modify the Extended Armchair substitution rule so that it admits hereditary and sibling sides. This modification is straightforward: we cut the sides of prototile $X$ so
Figure C.07. Extended Armchair substitution rule and its associated adjacency graphs. Let \( T \) be the tiling of this substitution rule. The edges colored in red indicate three \( G(T) \)-backtrack paths in \( \overline{G}(T) \): \( p_1 = Y_1 \cdots Y_6 \), \( p_2 = Y_7Y_8 \), and \( p_3 = Y_9 \cdots Y_{16} \). The edges colored in blue indicate the clumps at stage 1 for the stage 1 route \( \rho = C_1^1C_2^2, C_1^1 = \{\{Y_5, Y_8\}, \{Y_6, Y_7\}\} \) and \( C_1^1 = \{\{Y_7, Y_{15}\}, \{Y_6, Y_{16}\}\} \).

that it becomes a polygon with 10 sides, all of which have equal lengths. We also modify the tiling \( T \) of this substitution rule accordingly; see Figure C.08. As with the Pinwheel substitution rule in Section C.2, the TAS constructed via Corollary 4.2.4 which simulates the modified Extended Armchair substitution rule with border also simulates the Extended Armchair substitution rule with border. For simplicity, we imply this modification when discussing the corners of the tiling \( T \) below instead of showing it visually.

Rather than describe the full TAS which simulates the Extended Armchair substitution rule, we focus on the modification in the proof of Corollary 4.2.4 to the construction associated with Theorem 4.2.3. Let \( T \) be the tiling of this substitution rule. Recall that this modification is made to Step 1, the marking procedure. We begin by explicitly defining the stage 1 backtrack partition of \( T \): \( V_1 = \{Y_1, \ldots, Y_6\}, V_2 = \{Y_7, Y_8\}, \) and \( V_3 = \{Y_9, \ldots, Y_{16}\}\). For \( 1 \leq k \leq 3 \), there is a \( G(T) \)-backtrack path \( p_k \) in \( \overline{G}(T) \) which visits every polygon (vertex) in \( V_i \). These three paths follow the enumeration given for \( T \). We show that \( \overline{G}(T) \) is \( G(T) \)-backtrack constructible at stage 1 by defining the associated stage 1 route \( \rho = C_1^1C_2^2 \) where \( C_1^1 = \{\{Y_5, Y_8\}, \{Y_6, Y_7\}\} \) and \( C_1^1 = \{\{Y_7, Y_{15}\}, \{Y_6, Y_{16}\}\} \).

Following the marking procedures of Corollary 4.2.4, we first mark the polygons in each of the paths \( p_1, p_2, \) and \( p_3 \) according to the procedures in Step 1 of Theorem 4.2.3; see Table C.04. Then, we mark
Figure C.08. Modified Extended Armchair substitution rule. Note that this substitution rule admits hereditary and sibling sides.

the four polygons associated with the clumps $C_1^1$ with ($\succsim 1$) and mark the four associated with $C_2^1$ with ($\succsim 2$), respectively. Finally, we assign the marking ($\succsim$) to two polygons ($Y_6$ and $Y_10$) following Step 1 of Theorem 4.2.3. See Table C.05 for the latter markings and Figure C.09 for visual reference. As noted in the proof of Corollary 4.2.4, the definition of the set of bonds $\Sigma$ naturally extends the procedures as in Step 1 of the proof of Theorem 4.2.3 to include the markings ($\succeq$). We can follow similar processes as in Sections C.1 and C.2 to define the set of tile types for the TAS $\Gamma$ which simulates the Extended Armchair substitution rule with border.
Figure C.09. A partial enumeration of the corners of polygons in the tiling of the Extended Armchair substitution rule. We enumerate the polygons as well and label them in bold for ease of visibility.
**Table C.04** Markings for the Extended Armchair substitution rule associated to backtrack paths.

<table>
<thead>
<tr>
<th>$V_1$</th>
<th>$V_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polygon</td>
<td>Associated Markings</td>
</tr>
<tr>
<td>$Y_1$</td>
<td>$(\circ_2, c_1), (\bullet_2, c_2), (\circ_3, c_3)$, $(\circ_4, c_5), (\circ_5, c_7), (\circ_6, c_9)$</td>
</tr>
<tr>
<td></td>
<td>$Y_2$</td>
</tr>
<tr>
<td>$Y_3$</td>
<td>$(\circ_3, c_3), (\bullet_3, c_4), (\bullet_4, c_6)$</td>
</tr>
<tr>
<td>$Y_4$</td>
<td>$(\circ_4, c_5), (\bullet_4, c_6), (\bullet_5, c_8)$</td>
</tr>
<tr>
<td>$Y_5$</td>
<td>$(\circ_5, c_7), (\bullet_5, c_8), (\bullet_6, c_{10})$</td>
</tr>
<tr>
<td>$Y_6$</td>
<td>$(\circ_6, c_9), (\bullet_6, c_{10})$</td>
</tr>
<tr>
<td></td>
<td>$Y_7$</td>
</tr>
<tr>
<td>$Y_8$</td>
<td>$(\bullet_8, c_{11}), (\circ_8, c_{12})$</td>
</tr>
</tbody>
</table>

**Table C.05** Remaining markings for the Extended Armchair substitution rule.

<table>
<thead>
<tr>
<th>$C_1^1$</th>
<th>$C_2^1$</th>
<th>$(\triangleright_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polygon</td>
<td>Marking</td>
<td>Polygon</td>
</tr>
<tr>
<td>$Y_5$</td>
<td>$(\succ_1, c_{27})$</td>
<td>$Y_7$</td>
</tr>
<tr>
<td>$Y_8$</td>
<td>$(\succ_1^1, c_{27})$</td>
<td>$Y_{15}$</td>
</tr>
<tr>
<td>$Y_6$</td>
<td>$(\succ_1^1, c_{28})$</td>
<td>$Y_6$</td>
</tr>
<tr>
<td>$Y_7$</td>
<td>$(\succ_1^1, c_{28})$</td>
<td>$Y_{16}$</td>
</tr>
</tbody>
</table>
Appendix D

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About the Author

Daniel Alejandro Cruz Ortega was born Quito, Ecuador in 1990. After immigrating to the United States with his parents and brother in 1997, he became a recipient of the Deferred Action for Childhood Arrivals (DACA) program in 2013. He received a Bachelor of Arts in Mathematics in 2012 from the University of South Florida. His current research interests include self-assembly, discrete geometry, formal languages, and cellular automata. His hobbies include rock climbing, building Lego sets, playing board games, and taking pictures of his cat Bittle with his wife Angela.