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Counter machines and crystallographic structures

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Abstract

One way to depict a crystallographic structure is by a periodic (di)graph, i.e., a graph whose group of automorphisms has a translational subgroup of finite index acting freely on the structure. We establish a relationship between periodic graphs representing crystallographic structures and an infinite hierarchy of intersection languages $\mathscr{DCL}_d$, $d = 0, 1, 2, \ldots$, within the intersection classes of deterministic context-free languages. We introduce a class of counter machines that accept these languages, where the machines with d counters recognize the class $\mathscr{DCL}_d$ An intersection of d languages in $\mathscr{DCL}_1$ defines $\mathscr{DCL}_d$. We prove that there is a one-to-one correspondence between sets of walks starting and ending in the same unit of a d-dimensional periodic (di)graph and the class of languages in $\mathscr{DCL}_d$. The proof uses the following result: given a digraph and a group G, there is a unique digraph Γ such that G Aut Γ, G acts freely on the structure, and $\Gamma/G \cong$.

Keywords

Counter machines; Crystallographic structures; Context-free languages; Periodic digraphs

1 Introduction

We consider periodic digraphs that are often associated with periodic (or crystallographic) nano structures such that vertices of the digraph correspond to the molecular (or atomic) arrangement in the structure, and the arcs represent their bonds. Although the development of X-ray diffraction analysis of crystals (Glusker 1990; Moore 1990) enabled physicists and chemists to develop graphical representations of crystals ("crystal nets") found in nature, or obtained in the lab, the "de novo" generation of crystal nets appear to have begun in earnest in the 1970s and 1980s, especially with the cataloguing work of Wells (1977) (see also O'Keeffe and Hyde 1996). A variety of crystallographic structures have been obtained by allowing self-assembly of chemical building blocks, from DNA (Zheng et al. 2009) to metal-organic frameworks (Wang et al. 2013). Recently, even structures that seem to violate chemistry textbook rules have been assembled through pressurizing the environment (Zhang et al. 2013). However, a systematic theoretical study and analysis of self-assembled nanostructures seems to be lagging behind. Even the notion of a periodic structure seems to have different meanings in different contexts (see for example Delgado-Friedrichs 2005; Eon

2005; Klee 2004 as well as Sect. 3 herein). With this paper we suggest an approach to study periodic structures through formal language theory.

Given two (crystallographic) nano structures, how can they be distinguished? One way to answer this question is by considering walks in the underlying (periodic) (di)-graphs. We label the edges of the graphs with appropriate labels indicating the distinct bonds within the structure. The set of labels of all such walks represents a language over the alphabet of bonds. In Jonoska and McColm (2006, 2009) the computational power of molecular bondings without geometric constraints imposed by their spacial embedding was considered, and it was shown that there is a hierarchy of complexity classes of computable languages that can be associated with these constructions. In this paper we address periodic nano structures only, and examine the set of languages associated with cyclic walks in periodic digraphs, thereby considering also the spacial embedding of the structures. We show that these languages are closely related to nested families of deterministic context-free languages.

It is known that context-free languages (CFLs) lie at the base of an intersection hierarchy of languages (see Liu and Weiner 1973 or Kintala 1978). If we let $\mathcal{CFL}_n$($\mathcal{DCFL}_n$) be the class of languages that are intersections of n CFLs (n deterministic CFLs, respectively) then for each n, $\mathcal{CFL}_n \subsetneq \mathcal{CFL}_{n+1}$ and $\mathcal{DCFL}_n \subsetneq \mathcal{DCFL}_{n+1}$ Liu and Weiner (1973) showed that for each n, there is a language $L_{n+1} \in \mathcal{DCFL}_{n+1} - \mathcal{CFL}_n$, which, together with the fact that $\mathcal{DCFL}_n \subseteq \mathcal{CFL}_n$ for each n (to our knowledge, proper containment has not been established for the entire hierarchy), results in two hierarchies, one embedded in the other.

In this paper, we consider a class of languages, starting with a proper subclass of $\mathcal{DCFL}$, recognized by machines with counters that can be closely associated with periodic digraphs. Ibarra (1978), Ibarra and Yen (2011) introduced PDA-like *multi-counter machines* with counters instead of stacks. As it is known that a two-counter machine has computational power equivalent to a universal Turing machine, the authors in Ibarra (1978) restricted the number of permitted "reversals" in the counters for each computation (i.e., the number of counter changes from incremental to decremental and vice versa was restricted). In this paper we bar communication between the counters, there are no ε -moves, and the machine accepts only if all counters are at zero at the termination of the computation. As a result, if $\mathcal{DCL}_n$ is the class of languages accepted by such deterministic counter machines with n counters, then a language in $\mathcal{DCL}_n$ is the intersection of n languages in $\mathcal{DCL}_1$. The counter automata we consider are also known as $\mathbb{Z}^d$-automata (Cleary et al. 2006; Elder et al. 2008; Kambites 2009), and have been used to study word problems in groups. In particular, in Elder et al. (2008) it was shown that a group is virtually free abelian if and only if its word problem can be recognized by a $\mathbb{Z}^d$-automaton.

We show that $\mathcal{DCL}_1 \subsetneq \mathcal{DCFL}_1$ (Sect. 2.2), and thus $\mathcal{DCL}_n \subseteq \mathcal{DCFL}_n$ for each n. We conjecture that these inclusions are proper. Further, we show that Liu and Weiner's language L_n is in $\mathcal{DCL}_n$ for all n 1, and hence $\mathcal{DCL}_n \subsetneq \mathcal{DCL}_{n+1}$ for all n 1, suggesting Fig. 1. We also observe that $\mathcal{DCFL}_1$ contains a language that is not in $\mathcal{DCL}_n$ for any n (Proposition 2.4) and further that $\mathcal{DCL}_1 \subsetneq \mathcal{DCL}_2 \cap \mathcal{DCFL}_1$ (Proposition 2.5), conjecturing that such inequality holds for all $n > 1$ as well.

Our interest in the deterministic counter language (DCL) hierarchy arises from their prominent role in understanding cyclic walks in periodic digraphs.

Intuitively, a periodic graph is a graph that is, or can be, embedded in the Euclidean space so that it is periodic in the requisite number of axial directions. Thus, the space that a Euclidean graph is embedded in can be regarded as being partitioned into *unit cells*, with the subgraph of each unit cell isomorphic to the subgraph of any other unit cell. The corresponding intuition applies also to a periodic digraph. Periodic digraphs capture the $\mathscr{DCL}$ hierarchy in the following way (Theorem 4.1):

- For any $\mathscr{DCL}_n$ language $L \subseteq \Sigma^*$, there is a periodic digraph that can be embedded in n-dimensional Euclidean space, with a distinguished vertex v and arcs labeled by letters in Σ, such that the words of L correspond precisely to labels of paths from v back to an appropriate vertex in v's unit cell.

- For any labeled periodic digraph that can be embedded in n-dimensional Euclidean space with a distinguished vertex v, there exists a $\mathscr{DCL}_n$ language whose words correspond precisely to labels of paths from v back to v's unit cell.

We start by introducing "deterministic counter machines" and their languages, denoted DCLs (Sect. 2.1). Because of the requirement that the counters have no ε-moves and the computation terminates with all counters at value 0, it follows that the DCLs form a proper subset of the DCFLs (Proposition 2.1). We consider the DCL hierarchy: we verify that it is of the same (infinite) "height" if not the same "width," as the DCFL and CFL hierarchies (Sect. 2.2).

We provide algebraic background on group actions on graphs and fundamental transversals in Sect. 3.2, and in Sect. 3.3, we review the extant notions of a periodic graph. Two of these notions are equivalent for directed graphs (Proposition 3.2) and those become the notion that we use in the rest of the paper. In order to establish the relationship between counter machines and periodic graphs, we show how to construct a periodic graph that has as quotient a given finite weakly connected digraph (Sect. 3.4). We observe that class of regular languages coincides with a set of walks in a labeled periodic graphs. Section 4 contains the main theorems verifying that the cyclic walks in (appropriately labeled) periodic digraphs capture the DCL hierarchy. We end with a few concluding remarks. A preliminary extended abstract of this paper appeared in Jonoska et al. (2014).

2 Counter machines

We presume familiarity with the notion of a regular language – a language accepted by some deterministic finite automaton (DFA) – and the notion of a context-free language (CFL) – a language accepted by some (nondeterministic) pushdown automaton (PDA). For background on these notions we refer the reader to Autebert et al. (1997), Hopcroft and Ullman (1979).

We consider a variant of the multicounter (one-way) machines introduced in Ibarra (1978), Ibarra and Yen (2011) where a family of pushdown-automaton-like machines with counters

rather than stacks was proposed. At the beginning of the computation, a counter (or counters) is initialized at 0, and during the subsequent computation it could be incremented or decremented by 1. These automata are a special case of so-called G-automata, where G is a finitely generated group (Cleary et al. 2006; Elder et al. 2008), or more generally a monoid (Kambites 2009); in our case G is the free abelian $\mathbb{Z}^d$. It is known that an unrestricted two-counter machine can simulate a Turing machine and therefore has universal computational power (Minsky 1967). The multi-counter machines in Ibarra (1978), Ibarra and Yen (2011) have restrictions that the counters cannot get a negative value, and the number of "reversals" (an increment of the counter followed by a decrement, or vice versa) is bounded. These machines have more restricted computational power and recognize subclasses of context-free languages. Here we consider other changes in the counter machines such that negative as well as nonnegative integers on the counters are permitted, there is no limitation on the number of reversals, and the communication between counters is not permitted. Furthermore, we require that the machine accepts if and only if all counters have value 0. These changes provide another sub-hierarchy of deterministic context-free languages that are closely related to the set of cyclic walks in periodic digraphs.

Given an alphabet Σ, the set of all words over Σ is denoted Σ^*, and the set of all words of positive length is Σ^+. For a word $w = a_1 \cdots a_k \in \Sigma^*$, $k = |w|$ is the length of w, and $(w)_j = a_j$ so that the last symbol a_k is $(w)_{|w|}$. Similarly, if S is a set, $|S|$ is the cardinality of S.

2.1 Limited access counter machines

We introduce a variant of the standard counter machines (Ibarra 1978; Ibarra and Yen 2011) with the following.

Definition 2.1—A *deterministic d-counter machine* (d-DCM) is a tuple

$$M = (Q, \Sigma, \delta, q_0, F)$$

where Q is a finite set of *states*, Σ is a finite set of *symbols*, called the *alphabet*, $\delta: Q \times \Sigma \rightarrow Q \times \mathbb{Z}^d$ *transition function*, $q_0 \in Q$ is an *initial state*, while $F \subseteq Q$ is a set of *accepting states*.

We follow the standard approach of defining a computation as a sequence of configurations of the machine. The computation is analogous to that of a pushdown automaton except there are d counters instead of a stack, the content of the counters is not consulted for making a transition, and the counters must all be zero in order to accept.

Definition 2.2—Let $M = (Q, \Sigma, \delta, q_0, F)$ be a d-DCM. A *configuration* for a given state $q \in Q$ and word w is a triple $(q, w, \mathbf{z}) \in Q \times \Sigma^* \times \mathbb{Z}^d$.

A configuration $(q_0, w, (0, \ldots, 0))$ is *initial on input* w, and a configuration $(q, \varepsilon, \mathbf{z})$ for some $\mathbf{z} \in \mathbb{Z}^d$, where ε is the empty word, is *terminal*. A terminal configuration $(q, \varepsilon, \mathbf{z})$ is *accepting* if $q \in F$ and $\mathbf{z} = (0, \ldots, 0)$

For two configurations $C = (q, aw, \mathbf{z})$ and $C' = (q', >w, \mathbf{z}')$ we say C' *follows* C if $\delta(q, a) = q', \mathbf{z}' - \mathbf{z}$). A *computation* of a d-DCM on an input $w = s_1 s_2 \cdots s_n$ is a sequence of

configurations $C_0, \ldots, C_n$ such that C_0 is initial on input w, C_{i+1} follows C_i for $i = 0, \ldots, n - 1$, and C_n is terminal. The computation is *accepting* if C_n is accepting; it is *rejecting* otherwise.

A word w is accepted by a d-DCM if there is an accepting computation on input w. The set of all words accepted by a d-DCM M is called the language recognized by M, and is denoted $L(M)$.

A *deterministic finite state automaton* is a 0-DCM. This coincides with a standard definition of a finite state automaton (Hopcroft and Ullman 1979), which in our case is a DCM with no counters.

Definition 2.3—For any integer $d \geq 0$, a *deterministic d-counter language* is a language accepted by a d-DCM. The class of deterministic d-counter languages is denoted $\mathscr{DCL}_d$.

Thus, the class of regular languages is precisely the class $\mathscr{DCL}_0$. In the case of DCMs with one counter, we observe that they recognize deterministic context-free languages. This follows because one can construct a deterministic PDA (DPDA) from a given 1-DCM by removing and adding symbols to the stack according to the increments and decrements of the counter. We formalize this observation with the following proposition.

Proposition 2.1—All $\mathscr{DCL}_1$ languages are deterministic context-free.

<u>Proof:</u> Given a 1-DCM $M = (Q, \Sigma, \delta, q_0, F)$, we construct a deterministic PDA M' that recognizes $L(M)$. Since the domain $Q \times \Sigma$ of δ is finite, there exists an integer $m > 0$ such that for each $(q, a) \in Q \times \Sigma$, $\delta(q, a) \in Q \times [-m, m]$.

Let $M' = (Q \cup Q_m, \Sigma, X, \delta', q_0, F)$ be a PDA where $Q_m = Q \times [-m, m]$, $X = \{\mu, \nu, \#\}$ is a stack alphabet (with $\#$ the distinguished "end of the stack" symbol), and δ' is a transition function

$$\delta' : (Q \cup Q_m) \times (\Sigma \cup \{\varepsilon\}) \times (X \cup \{\varepsilon\}) \to (Q \cup Q_m) \times X^*$$

defined as follows. We set μ and ν as complementary symbols that simulate the positive and negative steps of the counter transitions, respectively. The PDA accepts a string if the computation ends in a terminal state and the stack is empty. For each transition $\delta(q, a) = (q', t)$ in the 1-DCM M we define the following transitions in M':

$$\delta'(q, a, s) = ((q', t), s), \text{ for } s \in X$$
$$[\text{move to the states that count symbols}]$$

and if $t > 0$, define a sequence of transitions in the PDA M' for $i = t, t - 1, \ldots, 1$

$$\delta'((q, i), \varepsilon, s) = ((q, i - 1), \mu s), \text{ for } s = \mu, \#$$
$$[\text{add a positive symbol to the stack}]$$

$$\delta'\left(\left(q,i\right),\varepsilon,v\right)=\left(\left(q,i-1\right),\varepsilon\right),$$
[remove a complementary symbol from the stack.]

if $t < 0$, define a sequence of transitions in the PDA M' for i = t, t + 1, …, −1

$$\delta'\left(\left(q,i\right),\varepsilon,s\right)=\left(\left(q,i+1\right),vs\right),\text{ for s}=v,\#$$
[add a negative symbol to the stack]

$$\delta'\left(\left(q,i\right),\varepsilon,\mu\right)=\left(\left(q,i+1\right),\varepsilon\right).$$
[remove a complementary symbol from the stack.]

Finally, let

$$\delta'\left(\left(q,0\right),\varepsilon,s\right)=\left(q',s\right),\text{ for s}\in\mathrm{X}.$$
[move back to the next state of the counter machine]

By construction, M' is deterministic (if δ' $((q, i), \varepsilon, s)$ Ø then δ' $((q, i), a, s)$= Ø for all a ∈ Σ) The symbols μ and v count the positive and the negative steps of the counter machine, hence at each instance the stack contains only μ's or only v's (except for the # at the bottom of the stack). If the counter machine has a positive step, followed by a negative step (or vice versa) the symbols are popped from the stack until the end of stack is reached, and then appropriate symbols are added. Notice that whenever we have a configuration (q, w, z) in the 1-DCM where $z \in \mathbb{Z}$ we have $|z|$ number of μ's or v's on the stack depending whether z is positive or negative, respectively. Thus, $L(M) = L(M')$. □

In Sect. 3 we define periodic weakly-connected digraphs and their corresponding quotient graphs. Our main results (Sect. 4) show that walks in d-periodic weakly-connected digraphs that start on a fixed vertex and terminate at a vertex in the same unit correspond precisely to the class of d-DCM languages. First we observe that classes $\mathscr{DCL}_d$ define an intersection hierarchy of context-free languages.

2.2 The intersection hierarchies

Given a class of languages $\mathcal{L}$, an *intersection hierarchy for $\mathcal{L}$* is the sequence of classes

$$\mathscr{L}_d=\left\{\bigcap_{k=1}^{d} L_k : L_k\in\mathscr{L}, k=1,\ldots,d\right\}.$$

This hierarchy *collapses* if, for some N, $\mathcal{L}_{N+1} = \mathcal{L}_N$; otherwise $\mathcal{L}_1 \subsetneq \mathcal{L}_2 \subsetneq \cdots$. By definition, $\mathcal{L}_1 = \mathcal{L}$ and frequently one adds some natural subclass $\mathcal{L}_0$ of $\mathcal{L}$. If $\mathcal{L}$ is closed under intersection, then the hierarchy collapses at $N = 1$.

One of the non-collapsing intersection hierarchies is the context-free language hierarchy. For each $d > 0$, let $\mathscr{CFL}_d$ be the class of intersections of d context free languages, and let $\mathscr{DC}$

$\mathscr{FL}_d$ be the class of intersections of d deterministic context free languages. Let $\mathscr{CFL}_0 = \mathscr{DC}$ $\mathscr{FL}_0$ be the class of regular languages. Liu and Weiner (1973), (see also Kintala 1978) proved that for each $d > 0$, the language

$$L_d = \{a_1^{k_1} a_2^{k_2} \cdots a_d^{k_d} b_1^{k_1} b_2^{k_2} \cdots b_d^{k_d} : k_1, k_2, \cdots, k_d \geq 0\}$$
$$\subseteq \{a_1, a_2, \cdots, a_d, b_1, b_2, \cdots, b_d\}^*$$

satisfies $L_{d+1} \notin \mathscr{CFL}_d$. But as $L_d = \cap_{i=1}^d L_{d,i}$ where

$$L_{d,i} = \{a_1^{k_1} a_2^{k_2} \cdots a_d^{k_d} b_1^{l_1} b_2^{l_2} \cdots b_d^{l_d} : k_1, k_2, \ldots, k_d, l_1, l_2, \ldots, l_d \geq 0 \& k_i = l_i\},$$

and $L_{d,i}$ is a DCFL for each i, we have $L_{d+1} \in \mathscr{DCFL}_{d+1} - \mathscr{CFL}_d$ for each d. As $\mathscr{DCFL}_d$ $\subseteq \mathscr{CFL}_d$ (we do not know if it has been determined whether this inclusion is strict for each d), we have a non-collapsing DCFL intersection hierarchy within a non-collapsing CFL intersection hierarchy.

In this subsection, we consider the intersection hierarchy of deterministic d-counter languages for $d = 0, 1, \ldots$ The following proposition is a special case of Kambites (2009, Theorem 4); we include a proof for the reader's convenience.

Proposition 2.2—For each d, $\mathscr{DCL}_d$ is the set of languages that are intersections of d languages in $\mathscr{DCL}_1$.

<u>Proof:</u> Let L be accepted by a d-DCM $M = (Q, \Sigma, \delta, q_0, F)$. We construct d 1-counter DCMs $M_1, \ldots, M_d$, whose languages $L_1, \ldots, L_d$ satisfy $L = \cap_{k=1}^d L_k$. For each k, let $M_k = (Q, \Sigma, \delta_k, q_0, F)$, where for each $q \in Q$, $s \in \Sigma$ with $\delta(q, s) = (q', (z_1, \ldots, z_d))$ in M, and let $\delta_k(q, s) = (q', z_k)$. We claim that $L = \cap_{k=1}^d L_k$.

Let $w = s_1 \cdots s_n \in \Sigma^*$. Starting at q_0, the computation of M with input w gives a sequence of states $q_1, q_2, \ldots, q_n$ such that $\delta(q_{t-1}, s_t) = (q_t, (z_{1,t}, \ldots, z_{d,t}))$ for $t = 1, \ldots, n$. By definition, in M_k we have a transition $\delta_k(q_{t-1}, s_t) = (q_t, z_{k,t})$ for each k. The final states of M coincide with the final states of M_k for each k. Further, all counters of M are at 0 if and only if each counter in M_k is at 0. So M accepts w if and only if each M_k accepts w.

Conversely, let $L = \cap_{k=1}^d L_k$ where each L_k is accepted by a 1-DCM $M_k = \left(Q_k, \Sigma, \delta_k, q_k^0, F_k\right)$. Consider a d-DCM $M = (Q, \Sigma, \delta, q_0, F)$ where

$Q = \prod_{k=1}^d Q_k, q_0 = \left(q_1^0, \ldots, q_k^0\right), F = \prod_{k=1}^d F_k$, and for each $s \in \Sigma$ define

$$\delta\left((q_1, \ldots, q_d), s\right) = \left(\left(q_1', \ldots, q_d'\right), (z_1, \ldots, z_d)\right) \text{ if and only if } \delta_k(q_k, s) = \left(q_k', z_k\right) \text{ for all } k = 1, \ldots, d.$$

Let $w = s_1 \cdots s_n \in \Sigma^*$. For each k, the computation of M_k starts at q_k^0 so the computation of M starts at q_0. Then for each k, M_k reads the tth symbol of w through transition $\delta_k(q_{k,t-1}, s_t) = (q_{k,t}, Z_{k,t})$ if and only if M reads the tth symbol of w with transition $\delta((q_{1,t-1}, \ldots, q_{d,t-1}),$

$s_t) = ((q_{1,t}, ..., q_{d,t}), (z_{1,t}, ..., z_{d,t}))$. Also, $(q_{1,n}, ..., q_{d,n}) \in F$ if and only if $q_{k,n} \in F_k$ for each k, and all the counters of M are zeroed out if and only if for each k, the counter of M_k is zeroed out. Thus M accepts if and only if each M_k accepts. $\square$

Proposition 2.3—The language L_d is in $\mathscr{DCL}_d$

Proof: Because $L_d = \cap_{i=1}^{d} L_{d,i}$, the statement follows from Proposition 2.2 and the following observation that $L_{d,i} \in \mathscr{DCL}_1$. For each i there is a deterministic one-counter machine M that recognizes $L_{d,i}$ with $2d$ states. The first d states are used to read the a-symbols and the next d states are used to read the b-symbols such that the first encounter of symbol a_j ($j = 1, ..., d$) changes the state of the machine to q_j where it remains until a different symbol is read. Similarly the first encounter of b_j changes the machine to state q_{d+j} where it remains until a different symbol is read. If a_j (or b_j) is followed by a_k (resp. b_k) with $k < j$, then machine rejects. Also, if any a's are encountered after a b (states $q_{d+1}, ..., q_{2d}$) then the machine rejects. If a symbol read is not a_i nor b_i, the counter is left unchanged. With each reading of a symbol a_i (moving to, or remaining at a state q_i) the counter is increased by 1, and with each reading of symbol b_i (moving to, or remaining at a state q_{d+i}) the counter is decreased by 1. Then a word w in $\{a_1, ..., a_d, b_1, ..., b_d\}^*$ is accepted if and only if the indexes of the a-symbols and the indexes of the b-symbols in w appear in ascending order and also $w = a_1^{k_1} a_2^{k_2} \cdots a_d^{k_d} b_1^{l_1} b_2^{l_2} \cdots b_d^{l_d}$ where $k_j, l_j \geq 0$ and $k_i = l_i$.

Corollary 2.1—For every $d \geq 0$, $\mathscr{DCL}_d$ is a proper subset of $\mathscr{DCL}_{d+1}$.

Proof: By Proposition 2.1, for each $\mathscr{DCL}_d \subseteq \mathscr{DCFL}_d$. By Proposition 2.3, the language $\mathcal{L}_{d+1} \in \mathscr{DCL}_{d+1} \setminus \mathscr{DCL}_d$. $\square$

In the case of Cayley graphs, it was shown in Cleary et al. (2006) that if the word problem of $\mathbb{Z}^d$ is an n-counter language, then $n \geq d$. This, as well as the above Proposition 2.3 and Corollary 2.1 follow from the Liu and Weiner's construction of language L_d. In Elder et al. (2008) it was shown the following.

Corollary 2.2—(Elder et al. 2008) The word problem of a finitely generated group G is in $\mathscr{DCL}_d$ for some d $\geq$ 1 if and only if G is virtually free abelian.

By Proposition 2.1, all DCLs are DCFLs, from which it follows that for each d, $\mathscr{DCL}_d \subseteq \mathscr{DCFL}_d$. Liu Weiner's results for languages L_d show that for each d, $\mathscr{DCL}_{d+1} \setminus \mathscr{CFL}_d$ is nonempty, suggesting that something like Fig. 1 holds. This figure suggests a lot of details to fill in, and we conclude with two of those. In both cases we use Pumping Lemma-type arguments. Let $\mathscr{DCL}_\infty = \cup_{k=0}^{\infty} \mathscr{DCL}_k$.

Proposition 2.4—There exists a language in $\mathscr{DCFL}_1$ that is not in $\mathscr{DCL}_\infty$.

Proof: Consider the language $L = \{0^m 1^n : m > n \geq 0\}$. This language is accepted by a Deterministic PDA that adds to its stack for each 0 encountered, then subtracts from the stack each time a 1 is encountered, making sure that the input is a substring of 0s followed

by a substring of 1s, and accepting if and only if the stack is nonempty when the string ends (Autebert et al. 1997).

To prove the inequality, suppose that $L \subseteq \cap_{k=1}^{d} L_k$ for DCLs $L_1, \ldots, L_d$, where for each k, L_k accepted by a 1-DCM M_k of at most N states. We show that L is always a proper subset of such intersection. Since every M_k accepts each $0^{N+2}1^n$ for $n < N + 2$, and because M_k is deterministic, each M_k must have its counter zeroed out for all transitions after scanning 0^{N+2}. In particular, M_k must have had its counter zeroed out for the last $N + 1$ transitions on input $0^{N+2}1^{N+1}$. Because M_k has at most N states, during the last $N + 1$ transitions it must have encountered some (final) state twice. For some i, j $(i < j)$ the $(N + 2 + i)$th and $(N + 2 + j)$th configurations have the same state and the counter has the same zero increment, staying at 0. But then, given $0^{N+2}1^{N+2}$ and any t ≥ 0, the $(N + 2 + j + t)$th state must be the same as the $(N + 2 + i + t)$th state, so in particular the $(2N+4)$th state is the same as the $(2N + 4 - j + i)$th state, the latter of which has a final state and zeroed counter and is thus accepting. Because the counter after $0^{N+2}1^{N+2-j+i}$ stayed at 0, the counter after $0^{N+2}1^{N+2}$ also stays at 0, by determinism. Thus M_k accepts $0^{N+2}1^{N+2}$ for each k, hence $0^{N+2}1^{N+2} \in \cap_k L_k \setminus L$.

Seki (2013) showed that an n-DCM can be simulated by a nondeterministic 1-reversal counter machine as in Ibarra (1978) with $2n$ counters. Hence, the construction in Chiniforooshan et al. (2012) showing that there exists a language in $\mathscr{DCFL}_1$ that cannot be accepted by any nondeterministic 1-reversal counter machine can be also used to show Proposition 2.4. We conclude by taking out our microscope.

Proposition 2.5—$\mathscr{DCL}_1$ is a proper subset of $\mathscr{DCL}_2$ intersect $\mathscr{DCFL}_1$.

Proof: Consider the language $L = \{0^n1^m0^m1^n: m, n > 0\}$. This is in $\mathscr{DCFL}_1$: it is accepted by a deterministic push down machine that on its stack pushes 0s as it encounters 0s, then pushes 1s as it encounters 1s, and then it removes (pops) 1s as it encounters 0s, and removes 0s as it encounters 1s; it accepts if the input consists of 0s followed by 1s, followed by 0s, followed by 1s, and if the stack is empty at the end of the string.

The language L is also in $\mathscr{DCL}_2$. Consider two languages $L_1 = \{0^n1^m0^k1^n: k, m, n > 0\}$ and $L_2 = \{0^n1^m0^k1^n: k, m, n > 0\}$ Both are in $\mathscr{DCL}_1$: the 1-DCM accepting L_1 adds to the counter during the first substring of 0s, remains unchanged during the first substring of 1s and the second substring of 0s, and subtracts from the counter during the second substring of 1s. The DCM accepting L_2 does not change the counter during the first substring of 0s, adds to the counter during the first substring of 1s, subtracts from the counter during the second substring of 0s, and leaves the counter unchanged during the last substring of 1s. We have $L = L_1 \cap L_2$.

But L is not in $\mathscr{DCL}_1$. We show that if L is a subset of a language in $\mathscr{DCL}_1$ then L must be a strict subset of that language. Suppose that $M = (Q, \Sigma, \delta, q_0, F)$ is a 1-counter DCM that accepts a language containing L

Let

$$Z \geq 2 + \max \left\{ |z| : \delta(q, a) = (q', z), \text{for } q, q' \in Q, a \in \Sigma \right\}.$$

Suppose that $Z \cdot |Q|^2 < n, m$. For each string $0^n 1^m 0^m 1^n \in L$, let 0^n be the "first block" of the word, 1^m be the "second block", 0^m be the "third block", and 1^n the "fourth block". Because $2 \cdot |Q| < n, m$, during the computation of the word, the machine has to repeat some state at least 2 times while scanning any one of the blocks. There are two possibilities:

1.   for some configuration when the states are repeated within the same block, the content of the counter is the same, or

2.   for all configurations when the states are repeated while scanning a single block, the counter has different content.

For Case 1, suppose that there exists $q \in Q$ such that for some j and k ($j < k$), the configurations $(q, 0^{n-j} 1^m 0^m 1^n, z)$ and $(q, 0^{n-k} 1^m 0^m 1^n, z)$ both occur in the computation. We claim that the string $0^{n+k-j} 1^m 0^m 1^n$ is not in L but it is accepted by M. When after the first j steps the computation of $0^{n+k-j} 1^m 0^m 1^n$ reaches the configuration $(q, 0^{n+k-2j} 1^m 0^m 1^n, z)$, the next $k - j$ transitions, due to determinism, recapitulate the transitions for the configurations $(q, 0^{n-j} 1^m 0^m 1^n, z)$ to $(q, 0^{n-k} 1^m 0^m 1^n, z)$ and M reaches the configuration $(q, 0^{n-j} 1^m 0^m 1^n, z)$. After recapitulating again the next $k - j$ transitions, M reaches $(q, 0^{n-k} 1^m 0^m 1^n, z)$. The rest of the computation is the same as the one for $0^n 1^m 0^m 1^n$. Hence, because M accepts $0^n 1^m 0^m 1^n$, it also accepts $0^{n+k-j} 1^m 0^m 1^n$. But the latter word is not in L, i.e., L is a proper subset of the language of M.

The case when the state and the counter content repeats while scanning any of the other blocks can be proven similarly.

For the second case, by the choice of m and n, for each block b ($b = 1, 2, 3, 4$) there is a state q_b appearing in two configurations while scanning block b, but with distinct counter content. As the counter content is not repeated in any of those four pairs of configurations, let δ_b ($\delta_b \neq 0$) be the difference of the counter content of the second minus the first counter content in the two configurations containing q_b for block b. Because the computation terminates when the counter is 0, we prove that at least one of the δ_b's is positive and at least one of the δ_b's is negative. Consider the scan of one of the blocks b. Since the machine is deterministic and the block consists of a single symbol, the portion of M's transition diagram that scans the block consists of a sequence of states (path) followed up with a cycle of states. Let q_0^b be the state from which the scanning of the block starts, let q_b be the first state encountered in the cycle and let q_f be a state on the cycle that is the last state entered by M after finishing with the scan of the block. Let the net difference of the counter between the first configuration containing the state q_0^b and the first configuration containing the state q_b be d_1. Let the difference of the counter going through the cycle, from state q_b to state q_b be δ_b ($\delta_b \neq 0$) and let the difference of the counter by going from state q_b to q_f be d_2. Then we have $|d_1| + |d_2| < Z \cdot |Q|$ and $|\delta_b| \geq 1$. Since both m and n are larger than $Z \cdot |Q|^2$, the machine M must encounter $|Q|^2 + 1$ states while scanning the block, and hence go through the cycle at least $|Q|$ times. Thus the counter difference from the start of the scan of the block at state q_0^b till the

end of the scan of the block q_f is at least $d_1 + d_2 + Z \cdot |Q|_b$, which is positive (negative) if and only if $_b$ is positive (resp. negative). Because the counter must be 0 to accept the word, there must at least one block b such that $_b > 0$ and at least one block b' such that $_{b'} < 0$. Moreover, one such pair of blocks b and b' is among the pairs 1, 2, or 1, 3 or 2, 4.

Without loss of generality, we choose $_1 > 0$ and $_2 < 0$. Let c_1 and c_2 be the lengths of the words scanned between the two occurrences of q_1 and the two occurrences of q_2, respectively. Consider the string $_w = 0^m 0^{|\Delta_2|c_1} 1^n 1^{\Delta_1 c_2} 0^n 1^m$. By determinism of the machine, and similarly as in case 1, after scanning the first block of 0's of w the counter is increased by $_1 \cdot |_2|$ and after scanning the second block consisting of 1's it is decreased by the same amount. Hence the configuration of the machine after reading

$_w = 0^m 0^{|\Delta_2|c_1} 1^n 1^{\Delta_1 c_2}$ is the same as the configuration of the machine after reading the string $0^m 1^n$. Therefore, $_w 0^n 1^m = 0^{n+|\Delta_2|c_1} 1^{n+|\Delta_1|c_2} 0^n 1^m \notin L$ is accepted by the machine. $\square$

3 Periodic digraphs

3.1 Preliminaries and nomenclature

A function $f \colon X \to Y$ is *partial* if its domain is a proper subset of X; it is *total* if X is its domain. A *digraph structure* is a tuple $\Gamma = \langle V, A, \tau, \iota \rangle$, where V is the set of *vertices*, A is the set of *arcs*, $\iota \colon A \to V$ is a (possibly partial) function assigning *initial vertices* to arcs and $\tau \colon A \to V$ is a (possibly partial) function assigning *terminal vertices* to arcs. For each $a \in A$, let $\{\iota(a), \tau(a)\}$ denote the set of the two endpoints of a. We write a^{-1} for an arc $a \in A$ to indicate an arc with opposite orientation of a, that is, $\tau(a) = \iota(a^{-1})$ and $\iota(a) = \tau(a^{-1})$. The set of all arcs with opposite orientations is A^{-1}. Call Γ a *digraph* if ι and τ are total.

Let $\Gamma = \langle V, A, \tau, \iota \rangle$, be a digraph structure. A *digraph substructure* of Γ is a structure $\langle V', A', \iota', \tau' \rangle$, where $V' \subseteq V$, $A' \subseteq A$, and for each arc $a \in A'$, $\iota(a) \in V' \Rightarrow \iota'(a) = \iota(a)$ and $\tau(a) \in V' \Rightarrow \tau'(a) = \tau(a)$. Notice that a digraph substructure of a digraph need not have total initial and terminal functions, hence a digraph substructure need not be a digraph.

Given a digraph $\Gamma = \langle V, A, \tau, \iota \rangle$, a *walk* in Γ is a string of arcs $a_1 a_2 \cdots a_n$ such that for each i, $\tau(a_i) = \iota(a_{i+1})$; $\iota(a_1)$ is the *initial vertex* of the walk while $\tau(a_n)$ is the *terminal vertex* of the walk. The number of arcs, n, is the length of the walk $a_1 a_2 \cdots a_n$. The walk is *trivial* if its length is zero, i.e., it starts and ends at the same vertex and has no edges. There is one trivial walk for each vertex v. A *path* is a walk in which no vertex occurs twice (i.e., there is no distinct i, j such that $\iota(a_i) = \iota(a_j)$) except possibly for the initial and terminal vertices, which may be equal. We say that a path or walk is a path or walk *from* its initial vertex *to* its terminal vertex. A walk or path in which the initial and terminal vertices are the same is *cyclic*.

A *semi-walk* in Γ is a string of arcs $a_1 a_2 \cdots a_n$ such that there is a substring $a_{i_1} \cdots a_{i_k}$ and a walk $a_1^{\varepsilon_1} \cdots a_n^{\varepsilon_n}$ where

$$\varepsilon_j = \begin{cases} 1 & \text{if } j \neq i_s \text{ for all } s = 1, \dots k \\ -1 & \text{if } j = i_s \text{ for some } s = 1, \dots k \end{cases}$$

for each $j = 1, \ldots, n$. We write $a_1^{\varepsilon_1} a_2^{\varepsilon_2} \cdots a_n^{\varepsilon_n}$ for the semi-walk where the negative exponent for an arc indicates walking across the arc in an opposite direction. A semi-walk is *from u to v* if $u = \iota\left(a_1^{\varepsilon_1}\right)$ and $v = \tau\left(a_n^{\varepsilon_n}\right)$. A digraph structure Γ is *weakly connected* if, for any vertices u, v, there is a semi-walk from u to v.

An *automorphism* of Γ is a bijection $f: V \to V: A \to A$ such that for any $a \in A$, $f(\iota(a)) = \iota(f(a))$ and $f(\tau(a)) = \tau(f(a))$. Let Aut Γ denote the group of automorphisms of Γ. Given any subgroup G Aut Γ, and any $v \in V$, the *G-orbit of v* is the set of vertices $G(v) = \{g(v): g \in G\}$; similarly, given any arc $a \in A$, the *G-orbit of a* is the set of arcs $G(a) = \{g(a): g \in G\}$. If $V' \subseteq V$, let $G\left(V'\right) = \cup_{v \in V'} G(v)$, and similarly if $A' \subseteq A$, let $G\left(A'\right) = \cup_{a \in A'} G(a)$. We use e to denote a group identity.

Given a set X and a function $f: X \to X$, a *fixed point of f* is an element $x \in X$ such that $f(x) = x$. We say that *f acts on X*, and if f has no fixed points, we say that *f acts freely on X*. Given a digraph Γ; *f acts freely on Γ* if f acts freely on the set of vertices of Γ. Thus f acts freely on Γ even if f fixes some arcs of Γ – but notice that if it does so, f must reverse the orientation of all arcs it fixes. For a group $G \subseteq$ Aut Γ we say that *G acts freely on Γ* if all non-identity elements of G act freely on (the vertices of) Γ.

There are several definitions of "periodic graphs" in literature. In this section, we give a short overview of several such definitions providing examples where they differ. As we are interested in digraphs, we show that two notions of periodicity, called here "concretely periodic" and "abstractly periodic", coincide in the case of weekly connected digraphs. We observe that the regular languages are precisely those representing walks on periodic digraphs. First, we develop some of the machinery that we need for the next sections.

3.2 Fundamental transversals

Let $\Gamma = \langle V, A, \iota, \tau \rangle$ be a digraph and let G Aut Γ.

Definition 3.1—Let Γ be a weakly connected digraph, and let G Aut Γ. A *fundamental G-transversal* is a weakly connected digraph substructure of Γ that intersects each orbit exactly once.

The following definition of a fundamental G-transversal is adapted from McColm (2012), Meier (2008). We follow the nomenclature from Dicks and Dunwoody (1989).

Example 3.1: Consider the digraph in Fig. 2. Let G be the group of automorphisms generated by the two translations α and β (depicted). Vertices depicted with squares belong to one orbit and those depicted by circles belong to another: no group element can map a circle to a square or vice versa. Under the automorphism group itself, the arcs whose both endpoints are squares belong to a single orbit. The other two orbits of arcs are those going to, and from, circles. A fundamental G-transversal consists of a black square with four arcs either terminating or starting at the square vertex and, adjacent to it (with both arcs coming in and going out), a circular vertex (in purple). There are 16 isomorphism classes of such fundamental G-transversals (as each of the four arcs that are missing an endpoint can be either coming in or going out of the square), but only one whose arcs are all outwards.

The following could be considered as part of the lore. For graphs, Proposition 3.1 is proven in Dicks and Dunwoody (1989), Meier (2008). We adapt the same idea for weakly connected digraphs for the convenience of the reader. We note that the proposition holds also for infinite number of G-orbits, where the proof would presume the Axiom of Choice (Meier 2008).

Proposition 3.1—For every weakly connected digraph Γ and every $G \leq \text{Aut } \Gamma$ such that there are finitely many G-orbits, there exists a fundamental G-transversal for Γ.

<u>Proof:</u> Let $\Gamma = \langle V, A, \iota, \tau \rangle$ be weakly connected, and let $G \leq \text{Aut } \Gamma$. Let $v_0 \in V$. We construct a fundamental G-transversal recursively with inductive basis being $\Gamma_0 = \langle V_0, A_0, \iota_0, \tau_0 \rangle$, where $V_0 = \{v_0\}$, $A_0 = \varnothing$, and ι_0, τ_0 have empty domains. In each odd step of the construction we add new arcs and in each even step we add new vertices, until all orbits are exhausted.

For $n \geq 0$, given $\Gamma_{2n} = \langle V_{2n}, A_{2n}, \iota_{2n}, \tau_{2n} \rangle$, construct $\Gamma_{2n+1} = \langle V_{2n+1}, A_{2n+1}, \iota_{2n+1}, \tau_{2n+1} \rangle$ as follows.

Let $V_{2n+1} = V_{2n}$. For each $v \in V_{2n}$, let

$$A_v = \{a \in A : v \in \{\iota(a), \tau(a)\} \ \& \ a \notin G(A_{2n})\}$$

and let $A'_{2n+1} = A_{2n} \cup \bigcup_{v \in V_{2n}} A_v$ We define A_{2n+1} to be a subset of A'_{2n+1} containing A_{2n} that intersects each orbit represented in A'_{2n+1} exactly once. Extend ι_{2n} and τ_{2n} to ι_{2n+1} and τ_{2n+1} on domain A_{2n+1}, respectively, but so that if $\iota(a) \notin V_{2n}$ or $\tau(a) \notin V_{2n}$, then $\iota_{2n+1}(a)$ or $\tau_{2n+1}(a)$ is undefined, respectively.

For $n \geq 1$, given $\Gamma_{2n-1} = \langle V_{2n-1}, A_{2n-1}, \iota_{2n-1}, \tau_{2n-1} \rangle$, construct $\Gamma_{2n} = \langle V_{2n}, A_{2n}, \iota_{2n}, \tau_{2n} \rangle$ as follows. Let A' be the set of all $a \in A_{2n-1} - A_{2n-2}$ such that $\{\iota(a), \tau(a)\} \nsubseteq V_{2n-1}$; note that for each $a \in A'$, exactly one of $\iota(a)$ and $\tau(a)$ is not in V_{2n-1}, so call that vertex v_a. Let $V' \supseteq V_{2n-1}$ intersect each orbit $G(v_a)$, $a \in A_{2n-1}$, exactly once, and let $V_{2n} = V_{2n-1} \cup V'$ and $A_{2n} = A_{2n-1}$. Extend ι_{2n-1} to ι_{2n} and τ_{2n-1} to τ_{2n}, respectively.

As there are finitely many orbits, there exists N such that $V_N = \bigcup_n V_n$, $A_N = \bigcup_n A_n$. Let $\Gamma_G = \Gamma_N$ We claim that Γ_G is a fundamental G-transversal, i.e., it is weakly connected and intersects each G-orbit exactly once.

By construction, for each n, for each vertex $v \in V_n$, there is a semi-walk from the initial vertex v_0 to v. As this holds also for $n = N$, Γ_G is weakly connected. In addition, by construction, Γ_G intersects each G-orbit at most once.

We now observe that Γ_G intersects each G-orbit at least once. For $v \in V$, we show that Γ_G contains some $v' \in G(v)$. Let $a_1^{\varepsilon_1} a_2^{\varepsilon_2} \cdots a_m^{\varepsilon_m}$ be a semi-walk from v_0 to $v \in \{\iota(a_m), \tau(a_m)\}$ in which no vertex appears twice. For each k, let v_k be the vertex shared by $a_k^{\varepsilon_k}$ and $a_{k+1}^{\varepsilon_{k+1}}$. We have $v_0 \in V_N = V(\Gamma_G)$ and inductively for all $k > 0$, if $G(v_{k-1}) \cap V_N \neq 0$ then for some

$v'_{k-1} \in G(v_{k-1}), v'_{k-1} \in V_{2n}$ for some n. Since $v_{k-1} \in \{\iota(a_k), \tau(a_k)\}$, there is $a'_k \in A_{2n+1}$ with $a'_k \in G(a_k)$ and $v'_{k-1} \in \left\{\iota\left(a'_k\right), \tau\left(a'_k\right)\right\}$. So for some $v'_k \in G(v_k), v'_k \in V_{2n+2}$. Repeating this construction, there is $v' = v'_m \in G(v) \cap V_N$. The argument that A_N intersects all orbits of arcs is similar. $\square$

3.3 Notions of periodicity

We review four notions of periodicity that appear in literature. Beukemann and Klee (1992), extended the notion of a "polyhedral net" (i.e., a graph whose vertices are corners of a polyhedron and whose edges are edges of that polyhedron) to the notion of a "periodic" net. Such a periodic net is preserved under a set of translations. This notion of periodicity includes nets like those called *rods* and *layers* in the chemical literature (see, e.g., Delgado-Friedrichs et al. 2007): these are 1-periodic (Fig. 3) and 2-periodic nets, respectively, that do not lie in any plane in $\mathbb{R}^3$. We tighten this notion of periodicity to a notion of "concrete" periodicity for digraphs. The same notion, under name "periodic", appears in Cohen and Megiddo (1991).

Given a digraph Γ with vertices V and arcs A, an injective map $\pi: V \to \mathbb{R}^d$ is *uniformly discrete* if there exist $\delta > 0$ such that for any $\mathbf{u}, \mathbf{v} \in \pi[\mathbf{V}]$, $\|\mathbf{v} - \mathbf{u}\| > \delta$.

Definition 3.2—A digraph $\langle V, A, \iota, \tau \rangle$ is *concretely d-periodic* if there exists an injection $\pi: V \to \mathbb{R}^d$ and a basis $\{\mathbf{v}_1, \ldots, \mathbf{v}_d\}$ of $\mathbb{R}^d$ such that the image $\pi[\mathbf{V}]$ is uniformly discrete, and the translations corresponding to the basis vectors induce automorphisms of the digraph.

Following the periodicity notion of Beukemann and Klee, several definitions of periodicity have appeared in the literature, including the three below. In order to distinguish between these notions we propose the following nomenclature. We recall that a group G is said to be a *d-dimensional crystallographic group* if it is a subgroup of isometries of $\mathbb{R}^d$ whose intersection with the group of translations $\mathbb{R}^d$ is an abelian group isomorphic to $\mathbb{Z}^d$ (Schwarzenberger 1980).

Definition 3.3—Let $\Gamma = \langle V, A, \iota, \tau \rangle$ be a digraph.

- Γ is *abstractly d-periodic* if there is a subgroup G Aut Γ of the group of automorphisms of Γ that is isomorphic to the free abelian group of d generators and satisfies the following two conditions: (a) G acts freely on V and (b) there are finitely many orbits of vertices and edges under G (Delgado-Friedrichs 2005).

- Γ is *d-crystallographic* if its automorphism group is a d-dimensional crystallographic group (Eon 2005; Klee 2004).

- Suppose Γ is *concretely d-periodic*. An embedding $\pi: V \to \mathbb{R}^d$ such that for each $v \in V$,

$$\sum_{u \in V:(u,v) \in A \text{ or } (v,u) \in A} (\pi(u) - \pi(v)) = \mathbf{0}$$

is called an *equilibrium embedding*. The digraph Γ is *d-barycentrizable* if it admits an equilibrium embedding (Delgado-Friedrichs 2005).

We need an additional notion.

Definition 3.4—If a digraph is embedded in $\mathbb{R}^d$, then its *symmetry group* is the group of automorphisms of the digraph that are induced by isometries of $\mathbb{R}^d$.

Although closely related, the three notions in Definition 3.3 are distinct. For example, the *d*-barycentrizable digraphs form a proper subset of the *d*-crystallographic digraphs. In Delgado-Friedrichs (2005), it is proven that for any *d*-barycentrizable digraph Γ, the automorphism group of Γ is the symmetry group of the graph that is the image of the equilibrium embedding. As that symmetry group is *d*-crystallographic, it follows that any *d*-barycentrizable digraph is *d*-crystallographic. In Delgado-Friedrichs (2012) the authors observe that the converse is not true, even if we restrict attention to graphs. Figure 4a depicts a variant of an example from Delgado-Friedrichs (2012) that is a 2-crystallographic graph but is not 2-barycentrizable. This graph has no equilibrium embedding, and is not 2-barycentrizable. Nevertheless, the graph's automorphism group is isomorphic to the 2-dimensional crystallographic group whose Hermann-Mauguin (or IUC) symbol is **p4g** (Radaelli 2011), and hence it is 2-crystallographic.

On the other hand the *d*-crystallographic digraphs form a proper subset of the abstractly *d*-periodic digraphs, as we see from Fig. 4b, which may be folklore, and c from Delgado-Friedrichs (2005). The automorphism group of the graph in Fig. 4b is generated by two translations, horizontal and vertical, and has a dihedral subgroup $\mathbf{D}_5$. Actually this group is isomorphic to $\mathbb{Z}^2 \times \mathbf{D}_5$, which is not 2-crystallographic. Although it has a subgroup isomorphic to $\mathbb{Z}^2$, it also has an element of order five, thus violating the "crystallographic restriction" which allows only order 2, 3, 4 and 6 fold rotations in the plane (Yale 1968). The graph of Fig. 4c has "twin vertices", i.e., pairs of vertices who share the same (graph theoretic) neighborhoods, and thus could be switched by an automorphism that fixes the rest of the graph. This graph has a distinct automorphism for each of the uncountably many sets of twins, and hence its automorphism group is uncountable and so not crystallographic. All three graphs in Fig. 4 are 2-abstractly periodic.

In this paper we consider the most general class, the abstractly *d*-periodic graphs. We observe that for digraphs the notion of concretely *d*-periodic coincides with the notion of abstractly *d*-periodic. The following proposition is probably lore, although we do not know if it has already appeared in print.

Proposition 3.2—Let Γ be a weakly connected digraph. For any d, Γ is concretely *d*-periodic if and only if it is abstractly *d*-periodic.

Proof: Fix a positive integer *d*. Suppose that $\Gamma = \langle V, A, \iota, \tau \rangle$ is concretely *d*-periodic, witnessed by an injection $\pi: V \to \mathbb{R}^d$ such that $\pi[V]$. is uniformly discrete in $\mathbb{R}^d$. We claim that Γ is also abstractly *d*-periodic, that is, its group of automorphisms has a subgroup isomorphic to the free abelian group of rank *d* that acts freely, and has a finite fundamental transversal (i.e., it has a finite set of orbits). Without loss of generality, suppose that $V \subseteq \mathbb{R}^d$.

Then there exists a basis $\{\mathbf{b}_1, \ldots, \mathbf{b}_d\}$ of $\mathbb{R}^d$ such that the corresponding translations P_k: $\mathbb{R}^d \rightarrow \mathbb{R}^d$: $\mathbf{x} \rightarrow \mathbf{x} + \mathbf{b}_k$ for $k=1, \ldots, d$ induce automorphisms on Γ. Let G denote this group of translations. As a group of translations, G acts freely on Γ. We observe that any fundamental transversal Γ_G of Γ is finite.

Suppose Γ_G has one of its vertices at the origin and is infinite. If Γ_G is bounded then it lies within a compact subset of $\mathbb{R}^d$, in which case its vertices together with all of the end-points of the arcs in Γ_G (which may not necessarily be in Γ_G) contain an infinite sequence of points within a compact set. This infinite sequence must contain a convergent subsequence, hence for all $\delta > 0$ there are vertices in V whose distance is less than δ, violating the condition for uniformly discrete embedding of V. If Γ_G is not bounded, let $\hat{\Gamma}_G$ be the weakly connected digraph obtained from Γ_G by the addition of all end-points of the arcs in Γ_G. Let $\mathbf{z}_i$, $i \in I$, be the set of vectors, each an integer linear combination of $\mathbf{b}_1, \ldots, \mathbf{b}_d$, such that the d-dimensional box $B_i \subseteq \mathbb{R}^d$ with vertices $\mathbf{z}_i$, $\mathbf{z}_i + \mathbf{b}_j$ ($j = 1, \ldots, d$) has a non-empty intersection with vertices in $\hat{\Gamma}_G$. Consider a vertex $v_i \in V\left(\hat{\Gamma}_G\right) \cap B_i$. Then a translation for $-\mathbf{z}_i$ of vertex v_i falls in the d-dimensional box $B \subseteq \mathbb{R}^d$ with vertices $(0, \ldots, 0)$, $\mathbf{b}_1, \ldots, \mathbf{b}_d$. Since $\hat{\Gamma}_G$ is infinite, there are infinite number of vertices (points) of V in the box B, which is bounded. Then similarly as in the case when Γ_G is bounded, the embedding of V in $\mathbb{R}^d$ fails to be uniformly discrete.

Hence Γ_G is finite, and the group G generated by the translations $\{P_1, \ldots, P_d\}$ is isomorphic to the free abelian group of d generators, acts freely on Γ, and this action has a finite number of orbits.

Conversely, suppose that $\Gamma = \langle V, A, \iota, \tau \rangle$ is abstractly d-periodic: we claim that Γ is also concretely d-periodic. As a free abelian group G of d generators acts freely on Γ, there exists a weakly connected fundamental G-transversal $\Gamma_G = \langle V_G, A_G, \iota_G, \tau_G \rangle$.

Let $v_0 \in V_G$, and denote the generators of G by $g_1, \ldots, g_d$. For each $v \in V$, let $\kappa(v)$ be the unique vertex in V_G intersecting $G(v)$, and let $g_v \in G$ be the unique group element in G such that $g_v(\kappa(v)) = v$ (the uniqueness of g_v follows from the fact that G acts freely on the digraph). We embed Γ in $\mathbb{R}^d$ by defining a one-to-one function p: $V \rightarrow \mathbb{R}^d$ as follows.

- Set $p(v_0) = \mathbf{0} \in \mathbb{R}^d$ and define p on V_G as an injective map from $V_G - \{v_0\}$ into the open unit cube $(0, 1)^d$. Let $\varepsilon > 0$ be the minimum distance from any $p(v)$, $v \in V_G \backslash \{v_0\}$, to the boundary of $[0, 1]^d$.

- For each $v \in V$, if $g_v = g_1^{k_1} \cdots g_d^{k_d}$, let $p(v) = p(\kappa(v)) + \sum_{i=1}^{d} k_i \mathbf{e}_i$, where $\{\mathbf{e}_1, \ldots, \mathbf{e}_d\}$ is the standard basis of $\mathbb{R}^d$.

And for each $a \in A$, let $p(a)$ be an arc from $p(\iota(a))$ to $p(\tau(a))$, and define $\iota_p(p(a)) = p(\iota(a))$ and $\tau_p(p(a)) = p(\tau(a))$

Then p is one-to-one: if $p(v) = p(v')$, then $p(\kappa(v)) + \mathbf{c} = p(\kappa(v')) + \mathbf{c}'$ for some integer vectors $\mathbf{c}$ and $\mathbf{c}'$. Because both $p(\kappa(v))$ and $p(\kappa(v'))$ are in $[0,1)^d$ we have $p(\kappa(v)) = p(\kappa(v'))$ and $\mathbf{c} = \mathbf{c}'$. Hence $g_v = g_{v'}$, forcing $v = v'$. By construction, Γ is isomorphic to $\langle p[V], p[A],$

$\iota_p,\ \tau_p\rangle$. We observe that $p[V]$ is uniformly discrete by taking

$\delta < min\left(\varepsilon,\ \left\{\|\mathbf{u}-\mathbf{v}\|\ |\mathbf{u},\mathbf{v}\in p[\hat{V}_G]\right\}\right)$ where $\hat{V}_G$ is the set of all endpoints of the arcs A_G.

$\square$

In view of Proposition 3.2, for the remainder of this article we refer to an abstractly or concretely periodic graph as *periodic*.

3.4 Quotient graphs and *G*-labeling

Like finite state machines, one can consider the counter machines as labeled directed graphs where each arc corresponds to a transition in the machine and the set of vertices is the set of states. In order to associate a periodic graph to a given determinist counter language which is given by a corresponding counter machine, we develop a construction that provides an appropriate periodic digraph from a given finite weakly connected digraph. In particular, the finite weakly connected graph is a quotient graph modulo the translation group acting on the periodic graph. This construction generalizes the result announced in Chung et al. (1984).

Let Σ be a finite set (which we treat as an alphabet). A *labeled digraph* is a pair $(\Gamma,\ \xi)$ where $\xi\colon A\to\Sigma$ is the *labeling function*. We extend arc labels to labels on walks naturally through concatenation of symbols. When Σ is a group G we say that Γ is *G-labeled*; such a labeled graph is sometimes called a *voltage graph* (Gross 1974; Gross and Tucker 1977) (see Gross and Yellen 2003) or a *gain graph* (Zaslavsky 1989, 1991) (see Zaslavsky 1999). In this case we extend the labeling function to semi-walks $p=a_1^{\varepsilon_1}a_2^{\varepsilon_2}\cdots a_n^{\varepsilon_n}$ with $\xi(p)=\xi(a_n)^{\varepsilon_n}\xi(a_{n-1})^{\varepsilon_{n-1}}\cdots\xi(a_1)^{\varepsilon_1}$. Notice that ξ is anti-morphic.

Definition 3.5—Let Γ be a weakly connected digraph and let $G\ \leq\ $Aut Γ act freely on Γ. We say that a *G*-labeling ξ of Γ *is consistent with G* (or *G-consistent*) if, for every pair of vertices v and v' such that $v'\in G(v)$, if p is a semi-walk from v to v', then $\xi(p)(v)=v'$.

Here is one important consequence of consistency.

Lemma 3.1—Let Γ be a weakly connected digraph and let $G\ \leq\ $Aut Γ act freely on Γ. Let ξ be a *G*-consistent labeling. For any $g\in G$ and any arcs $a,\ a'\in A$, if $g(a)=a'$ with $g(\iota(a))=\iota(a')$ (and thus $g(\tau(a))=\tau(a')$), then $\xi(a')=g\,\xi(a)g^{-1}$.

<u>Proof:</u> Let g be as above, and let p be any semi-walk from $\iota(a)$ to $\iota(a')$, and $\xi(p)(\iota(a))=\iota(a')$ by consistency. As G acts freely on the vertices of Γ, $\xi(p)$ is the only map in G sending $\iota(a)$ to $\iota(a')$, so $\xi(p)=g$. Thus $\xi(p)(\tau(a))=\tau(a')$. By consistency, $\xi(a^{-1}pa')(\tau(a))=\tau(a')$, so as G acts freely on Γ, $\xi(a^{-1}pa')(\tau(a))=g$, i.e., $\xi(a')\xi(p)\xi(a)^{-1}=g$, i.e., $\xi(a')g\xi(a)^{-1}=g$ giving us $\xi(a')=g\xi(a)g^{-1}$. $\square$

Directly from Lemma 3.1 we have that in a *G*-consistent labeling, when *G* is abelian, arcs in the same orbit have the same labels.

The notion of a quotient subgraph below is related to the fundamental transversal and it is a helpful tool to link periodic digraphs with counter machines.

Definition 3.6—Let $\Gamma = \langle V, A, \iota, \tau \rangle$ be a digraph and let G Aut Γ. The *quotient digraph* Γ/G is the digraph $\langle V/G, A/G, \iota/G, \tau/G \rangle$ defined as follows.

- The vertices and edges of Γ/G are the sets of orbits $V/G = \{G(v): v \in V\}$ and $A/G = \{G(a): a \in A\}$.

- For each $a \in A$, let $(\iota/G)(G(a)) = G(\iota(a))$ and $(\tau/G)(G(a)) = G(\tau(a))$.

For a semi-walk $p = a_1^{\varepsilon_1}, \cdots a_k^{\varepsilon_k}$ in Γ we write $G(p)$ for the semi-walk $G(a_1^{\varepsilon_1}), \cdots, G(a_k^{\varepsilon_k})$ in Γ/G.

Let G Aut Γ, ξ be a G-consistent labeling of Γ and $\xi_{\Gamma/G}: A/G \rightarrow G$ be a G-labeling for Γ/G. We say that ξ *honors* $\xi_{\Gamma/G}$ with respect to a reference vertex v_0 in Γ if the following holds. There is a fundamental transversal Γ_G containing v_0 for Γ such that $\xi(a^e) = \xi_{\Gamma/G}(G(a))^e$ for every arc a^e that starts at v_0. Furthermore, if a is an arc in Γ with $a_1^{\varepsilon_1} a_2^{\varepsilon_2} \ldots a_k^{\varepsilon_k}$ being a semi-walk from v_0 whose last arc a_k is a, then $\xi(a) = g\xi_{\Gamma/G}(G(a))g^{-1}$ where g is the label of the semi-walk $a_1^{\varepsilon_1} a_2^{\varepsilon_2} \ldots a_{k-1}^{\varepsilon_{k-1}}$. The situation when ξ honors $\xi_{\Gamma/G}$ is depicted in Fig. 5 where $h = \xi_{\Gamma/G}(a)$.

Example 3.2: Let Γ be the digraph depicted in Fig. 2 where G is the group generated by the translations α and β. The quotient graph Γ/G is the one shown to the right in Fig. 6. Notice that as G acts freely on Γ, ξ is well-defined, and by construction, ξ is G-consistent. The labeling $\xi_{\Gamma/G}$ is also honored by ξ.

Given *any* group G, the theorem below starts with a G-labeling of a digraph , builds a digraph Γ with a G-labeling such that the quotient of Γ over G is isomorphic to . The theorem is a generalization of a result announced in Chung et al. (1984), where G is considered to be a finitely generated free abelian group. Here we extend the result to arbitrary groups.

Theorem 3.1—Let G be a group, and let (, ξ) be a G-labeled weakly connected digraph. There exists a unique (up to isomorphism) digraph Γ with G-consistent labeling ξ such that G Aut Γ acts freely on Γ, and there is an isomorphism $\lambda: \Gamma/G \rightarrow$ with G-labeling $\xi_{\Gamma/G} = \xi \lambda$ such that ξ honors $\xi_{\Gamma/G}$.

Compare with Gross and Tucker (1977, Theorem 2).

Proof: Let $= (V, A, \iota, \tau)$ be weakly connected and ξ be a G-labeling of . Define $\Gamma = \langle V, A, \iota, \tau \rangle$ where $V = V \times G$, $A = A \times G$, and for each $a \in A$ and $g \in G$, let $\iota(a, g) = (\iota(a), g)$ and $\tau(a, g) = (\tau(a), g\xi(a))$. (From the point of view of voltage graphs, Γ is the *derived graph* from the *base graph* .)

We show that Aut Γ contains a subgroup isomorphic to G, acting freely on Γ. For each $g \in G$, let $\pi_g: V \rightarrow V$, $A \rightarrow A$ be defined by $\pi_g(v, h) = (v, gh)$ and $\pi_g(a, h) = (a, gh)$. Let $\pi[G] = \{\pi_g: g \in G\}$. We verify that $\pi[G]$ is a group of automorphisms acting freely on Γ, isomorphic to G. For each $g \in G$, π_g is one-to-one on V because $\pi_g(v, h) = \pi_g(w, k)$ implies $(v, gh) = (w, gk)$, so $v = w$ and $gh = gk$, and hence $h = k$; similarly π_g is one-to-one on A. For each g, π_g is onto V because for any $(v, h) \in V$, $\pi_g(v, g^{-1}h) = (v, h)$; similarly π_g is onto

A. For each *g*, π_g is a digraph homomorphism preserving the initial and terminal vertices of arcs: for any $g \in G$ and $(a, h) \in A$, $\iota(\pi_g(a, h)) = \iota(a, gh) = (\iota\,(a), gh) = \pi_g(\iota\,(a), h) = \pi_g(\iota(a, h))$ while $\tau(\pi_g(a, h)) = \tau(a, gh) = (\tau\,(a), gh\xi\,(a)) = \pi_g(\tau\,(a), h\xi\,(a)) = \pi_g(\tau(a, h))$.

The automorphisms of $\pi[G]$ act freely on Γ: observe that as $\pi_e(v, h) = (v, h)$ and $\pi_e(a, h) = (a, h)$, π_e is the identity on Γ. For any $g \in G$, $(v, h) \in V$, if $\pi_g(v, h) = (v, h) = (v, gh)$, we have $g = e$ and hence $\pi_g = \pi_e$.

Further, $G \cong \pi[G]$ as follows. The map $g \mapsto \pi_g$ is one-to-one (notice that it is clearly onto): if $\pi_g = \pi_h$, then for every $k \in G$ and every $v \in V$, $(v, gk) = \pi_g(v, k) = \pi_h(v, k) = (v, hk)$, and hence $gk = hk$, so $g = h$. To prove isomorphism, we start with the observation that π_e is the identity in $\pi[G]$. For any $g, h \in G$, as $\pi_g\pi_h(v, k) = \pi_g(\pi_h(v, k)) = \pi_g(v, hk) = (v, ghk) = \pi_{gh}(v, k)$ and similarly for the arcs, hence we have $\pi_{gh} = \pi_g\pi_h$. Similarly, from the definitions it follows that $\pi_g^{-1} = \pi_{g^{-1}}$. In the following, we identify G with $\pi[G]$.

We now define a G-labeling ξ of Γ honoring $\xi_{\Gamma/G}$. Given ξ we define a G-labeling on Γ: $\xi(a, e) = \xi\,(a)$ and $\xi(a, g) = g\xi(a, e)g^{-1} = g\xi\,(a)g^{-1}$.

Consider the quotient graph Γ/G with labeling $\xi_{\Gamma/G}$ defined by $\xi_{\Gamma/G}(G(a, e)) = \xi\,(a)$: we claim that $\Gamma/G \cong$. Then ξ honors $\xi_{\Gamma/G}$ with respect to any vertex (v, e) by definition. Define $\lambda : \Gamma/G \to$ by $\lambda: G(v, e) \mapsto v$ and $\lambda : G(a, e) \mapsto a$. The map λ is bijective by definition and it also preserves the initial and the terminal vertices, e.g.,

$$\lambda\left(\iota_{\Gamma/G}\left(G\left(a, e\right)\right)\right) = \lambda\left(G\left(\iota_\Delta\left(a\right), e\right)\right) = \iota_\Delta\left(a\right)$$

and similarly for τ. For the labels, we have: $\xi_{\Gamma/G} = \xi\,\lambda$ (the diagram to the left in Fig. 7 commutes).

We conclude the proof by proving uniqueness of Γ (up to isomorphism).

Let $\Gamma^* = \langle V^*, A^*, \iota^*, \tau^* \rangle$ satisfy the properties listed in the theorem. Let $\gamma^*: \Gamma^* \to \Gamma^*/G$ be the quotient map and let $\lambda^*: \Gamma^*/G \to$ be the isomorphism from the theorem [see Fig. 7(right)]. Let v_0^* be the vertex in Γ^* such that ξ^* honors $\xi_{\Gamma^*/G}$ with respect to v_0^*. Let $v_0 \in V$ be a vertex in such that $\lambda^*\left(G\left(v_0^*\right)\right) = v_0$. Let $'$ be a spanning substructure of , i.e., it is a minimal weakly connected substructure of such that $V = V'$. For any $w_0 \in V$, there is a unique semi-path (i.e, a semi-walk with no repeated arcs or vertices) $p_{w_0} = a_1^{\varepsilon_1}, \ldots, a_k^{\varepsilon_k}$ from v_0 to w_0 in . Given $w_0 \in V$, let $w_0^* \in V^*$ be the terminal vertex of a semi-walk $p_{w_0}^* = \left(a_1^{\varepsilon_1}\right)^*, \ldots, \left(a_k^{\varepsilon_k}\right)^*$ starting at v_0^* such that $a_i = \lambda^*\gamma^*\left(a_i^*\right)$ for $i = 1, \ldots, k$. Then $\cup_{w_0 \in \Delta} G\left(w_0^*\right) = V^*$.

We define an isomorphism $F: V^* \to V$, $A^* \to A$ with $F\left(v_0^*\right) = (v_0, e)$ and for each $w^* \in G\left(w_0^*\right)$ with $g\left(w_0^*\right) = w^*$ we set $F(w^*) = (w_0, g\xi^*(p_{w_0}^*))$. This is well-defined since G acts freely on Γ^* and ξ^* honors $\xi_{\Gamma^*/G}$. For each $a^* \in A^*$, if $v \in V$ and $g \in G$ satisfies $F(\iota^*(a^*)) = (v, g)$, set $F(a^*) = (\gamma^*(a^*), g)$ and observe that $F(\tau^*(a^*)) = (\gamma^*(\tau^*(a^*)), g\xi\,(\gamma^*(a^*)))$.

Observe that F is an isomorphism: F is surjective by definition. Because p_{w_0} is unique for w_0, F is injective on the vertices, and because ξ^* honors $\xi_{\Gamma*/G}$, it is injective on the arcs. Further, if $F(a^*) = (a, g)$, then $\iota(F(a^*)) = \iota(a, g) = (\iota(a), g) = (\gamma^*(\iota^*(a^*)), g) = F(\iota^*(a^*))$, and similarly $\tau(F(a^*)) = F(\tau^*(a^*))$. □

Example 3.3—Consider the digraph depicted to the left in Fig. 8 containing $\mathbb{Z}$-labeling. The construction in Theorem 3.1 gives a graph Γ (to the right) where each vertex in A appears in $\mathbb{Z}$ copies, as labeled. The arcs are obtained such that each arc a from vertex v to vertex v' in corresponds to an orbit of the set of arcs in Γ consisting of arcs that start at vertices (v, z) ($z \in \mathbb{Z}$) and terminate at vertices $(v', \xi(a) + z)$. The labels of the arcs are indicated in red. Clearly, Γ is 1-periodic.

4 Periodicity and the language hierarchies

We conclude by establishing a connection between languages of the DCL hierarchy and the walks on periodic digraphs. We consider periodic digraphs and we define "regular" labeling. Then we observe that the class of regular languages coincides with the sets of walks in a regularly labeled periodic digraph. Finally, we establish a correspondence between the class $\mathscr{DCL}_d$ and certain sets of labels of walks in regularly labeled d-periodic weakly connected digraphs.

If Γ is periodic with translation group G, then analogously with crystallographic nomenclature a fundamental G-transversal is called a *G-unit;* we call it simply a *unit* when G is understood. Units of periodic graphs and digraphs are not unique, as one can see from Fig. 9.

Lemma 4.1

The vertices and arcs of a d-periodic digraph can be partitioned into isomorphic units.

Proof—Given $\Gamma = \langle V, A, \iota, \tau \rangle$ of translational subgroup P, choose a unit $\Gamma' = \langle V', A', \iota', \tau' \rangle$, and suppose that P is generated by $p_1, p_2, \ldots, p_d \in P$. For each $\mathbf{z} = (z_1, \ldots, z_d) \in \mathbb{Z}^d$, let

$$V'_{\mathbf{z}} = \{ p_1^{z_1} \cdots p_d^{z_d}(v) : v \in V' \},$$
$$A'_{\mathbf{z}} = \{ p_1^{z_1} \cdots p_d^{z_d}(a) : a \in A' \},$$
$$\Gamma'_{\mathbf{z}} = \langle V'_{\mathbf{z}}, A'_{\mathbf{z}}, \iota'_{\mathbf{z}}, \tau'_{\mathbf{z}} \rangle .$$

where $\iota'_{\mathbf{z}}\left(p_1^{z_1} \cdots p_d^{z_d}(a)\right) = p_1^{z_1} \cdots p_d^{z_d}(\iota'(a))$, and $\tau'_{\mathbf{z}}\left(p_1^{z_1} \cdots p_d^{z_d}(a)\right) = p_1^{z_1} \cdots p_d^{z_d}\left(\tau'(a)\right)$. Then each $\Gamma'_{\mathbf{z}}$ must be a unit because it intersects each P-orbit exactly once. Furthermore, $\Gamma'_{\mathbf{z}} \cong \Gamma'$ We verify that this is a partition of the graph.

First we observe that distinct units are disjoint. Suppose $\mathbf{z} \neq \mathbf{z}'$ and $u \in V'_{\mathbf{z}} \cap V'_{\mathbf{z}'}$. Then there are $v, v' \in V'$ such that $u = p_1^{z_1} \cdots p_d^{z_d}(v) = p_1^{z'_1} \cdots p_d^{z'_d}(v')$. But then

$p_1^{z_1 - z'_1} \cdots p_d^{z_d - z'_d}(v) = v'$, so that v and v' belong to the same P-orbit, and as they are in the same unit, $\mathbf{z} = \mathbf{z}'$, a contradiction. Similarly, no two units may share an edge.

Second, the units cover the graph. For any $v \in V$, $v = p(u)$ for some $u \in V'$ and $p \in P$ as V' intersects each orbit of vertices. As $p_1, \ldots, p_d$ freely generate the abelian group P, there exist $\mathbf{z} = (z_1, \ldots, z_d) \in \mathbb{Z}^d$ such that $p = p_1^{z_1} \cdots p_d^{z_d}$, and hence $v \in V_{\mathbf{z}}$. Similarly, every arc is in one of these units. $\square$

Example 4.1—The edges of the graph depicted in Fig. 9 correspond to pairs of oppositely oriented arcs of the digraphs in Fig. 2. This 2-periodic (Euclidean) graph has four types of units, shown in red, blue, yellow, and green. Each unit has exactly one vertex from each orbit of vertices under the translational group generated by the vectors of Fig. 2, and also one edge from each orbit of edges. Figure 9 (right) shows how this periodic graph may be partitioned by units as described in Lemma 4.1.

4.1 Periodic digraphs and regular languages

We show a connection between periodic graphs and regular languages. In a weakly connected digraph, call a vertex v_0 *initial* if for every vertex v there is a walk from v_0 to v. Recall that regular languages are those accepted by Deterministic Counter Machines (Definition 2.1) without counters, also known as deterministic finite state automata. In the following, Σ is a set of symbols.

Definition 4.1—Given a d-DCM $M = (Q, \Sigma, \delta, q_0, F)$, its *transition diagram* is a pair (Γ_M, ζ) where $\Gamma_M = \langle Q, A, \iota, \tau \rangle$ is a digraph having arcs $A \subseteq Q \times \Sigma$ with $\iota(q, s) = q$, $\delta(q, s) = (\tau(q, s), \mathbf{z})$ for some $\mathbf{z}$, and $\zeta: A \rightarrow \Sigma$ is an arc-labeling $\zeta(q, s) = s$.

Notice that in such a transition diagram, for each $q \in Q$ and $s \in \Sigma$, there exists at most one $a \in A$ such that $\iota(a) = q$ and $\zeta(a) = s$. Also, the vertex q_0 is initial in the transition diagram whenever the automaton is trimmed to contain only essential states (i.e., states that lie on a walk from q_0 to a state in F). In the following we consider only trimmed automata.

Let $\Gamma = \langle V, A, \iota, \tau \rangle$ and let $G \leq \text{Aut } \Gamma$. A labeling $\zeta: A \rightarrow \Sigma$ is *G-invariant* if, for each $a_1, a_2 \in A$, $a_1 \in G(a_2)$ implies $\zeta(a_1) = \zeta(a_2)$. In addition, a set $F \subseteq V$ is *G-invariant* if it is a union of G-orbits of vertices.

If $F_\Gamma \subseteq V$ is a set of vertices in a G-invariantly labeled Γ, the language that consists of labels of walks in Γ that start at a vertex v_0 and terminate in F_Γ is denoted with $L(\Gamma, F_\Gamma, \zeta, v_0)$.

Proposition 4.1—A language $L \subseteq \Sigma^*$ is regular if and only if there is a weakly connected periodic digraph Γ with translational group G, G-invariant labeling ζ, G-invariant subset of vertices F_Γ, and a vertex v_0 such that $L = L(\Gamma, F_\Gamma, \zeta, v_0)$.

<u>Proof:</u> Let $M = (Q, \Sigma, \delta, q_0, F)$ be a 0-DCM (a finite state automaton) accepting a regular language L, and let (Γ_M, ζ_M) be the transition diagram for M. Choose a subset $A' \subseteq A$ such that $\langle Q, A', \iota, \tau \rangle$ is a spanning subdigraph of Γ_M. Define a labeling ξ_M on Γ_M such that for any $a' \in A'$, $\xi_M(a') = e$ and arbitrary symbols $\xi_M(a)$ for $a \in A \setminus A'$. Let G be a free

abelian group generated by $\{\xi_M(a): a \in A\}$ such that e is the identity. By Theorem 3.1, there exists a digraph Γ with vertices $Q \times G$ and arcs $A \times G$ whose quotient graph is isomorphic to $_M$. We define a regular labeling $\zeta: A \times G \to \Sigma$ on Γ with $\zeta(a, g) = \zeta_M(a)$ for each $a \in A$, $g \in G$. Then ζ is G-invariant (by definition) and there is a unit that contains $v_0 = (q_0, e)$ as initial vertex. Hence, if a string $w = s_1 s_2 \cdots s_n \in \Sigma^*$ is a label of a path $(a_1, g_1), \ldots, (a_n, g_n)$ from (q_0, e), then $s_k = \zeta(a_k, g_k) = \zeta_M(a_k)$ for each k. This path corresponds to a path of arcs $a_1, \ldots, a_n$ in $_M$ starting at q_0. And if $F_\Gamma = \{(q, g): q \in F, g \in G\}$, then F_Γ is G-invariant and $w \in L$ iff $w \in L(\Gamma, F_\Gamma, \zeta, (q_0, e))$.

Conversely, given Γ as in the theorem, notice that the natural homomorphism from Γ onto Γ/G preserves ζ labels of arcs and hence strings of labels encoding walks. In addition, the quotient graph Γ/G is a transition diagram of a 0-DCM that recognizes the language L consisting of the strings of labels encoding walks on Γ from v_0/G to F_Γ/G. Thus L is regular.

4.2 Periodicity and counter machines

The main theorem says that for every language L recognized by a d-counter machine there is a d-periodic regularly labeled digraph that contains a unit with a vertex vo such that the words in L are precisely those that are labels of walks in the digraph that start at vo and terminate in the same unit, i.e., walks that make "cycles" on the d-grid of unit partitions of the digraph.

Theorem 4.1—A language L is in $\mathscr{DCL}_d$ if and only if there exists a d-periodic digraph Γ with a translation group $\mathbb{Z}^d$, a $\mathbb{Z}^d$-invariant labeling ζ and a set of vertices F_0 in a $\mathbb{Z}^d$-unit containing a vertex v_0 such that $L = L(\Gamma, F_0, \zeta, v_0)$.

<u>Proof:</u> Suppose that L is in $\mathscr{DCL}_d$ and let $M = (Q, \Sigma, \delta, q_0, F)$ be a d-DCM with $L(M) = L$. Consider the transition diagram $(_M, \zeta_M)$ of M with vertices Q and arcs $A_M \subseteq Q \times \Sigma$. Let $\xi: A_M \to \mathbb{Z}^d$ be defined by $\xi(q, s) = \mathbf{z}$ for $\delta(q, s) = (q', \mathbf{z})$, where vector $\mathbf{z}$ changes the counters. By Theorem 3.1, there exists a digraph $\Gamma = \langle Q \times \mathbb{Z}^d, A_M \times \mathbb{Z}^d, \iota, \tau \rangle)$ with $\Gamma/\mathbb{Z}^d$ isomorphic to $_M$ and labeling $\xi: A_M \times \mathbb{Z}^d \to \mathbb{Z}^d$ honoring ξ. As $A = A_M \times \mathbb{Z}^d \subseteq Q \times \Sigma \times \mathbb{Z}^d$ is the set of arcs of Γ, we define $\zeta((a, \mathbf{z})) = \zeta_M(a)$ s for each arc $a = (q, s)$ in $_M$. Then $\zeta: A_M \times \mathbb{Z}^d \to \Sigma$ is $\mathbb{Z}^d$-invariant by definition. The natural homomorphism $\Gamma \to \Gamma/\mathbb{Z}^d \cong _M$ preserves the labels. Furthermore, $F \times \mathbb{Z}^d$ is a union of $\mathbb{Z}^d$-orbits. Consider the $\mathbb{Z}^d$-unit $\Gamma_0 = \langle V_0, A_0, \iota_0, \tau_0 \rangle$ with vertices $V_0 = Q \times \{\mathbf{0}\}$, arcs $A_0 = A_M \times \{\mathbf{0}\}$ and $v_0 = (q_0, \mathbf{0}) \in V_0$. We set $F_0 = F \times \{\mathbf{0}\}$.

If M accepts $w = S_1 \cdots s_n = \zeta_M(a_1) \cdots \zeta_M(a_n) \in \Sigma^*$, then there is a walk $a_1 \cdots a_n$ in $_M$ from the initial vertex $q_0 = \iota(a_1)$ to a terminal vertex $\tau(a_n) \in F$ that zeros out the counters. Then there is a walk $\alpha = (a_1, \mathbf{x}_1)(a_2, \mathbf{x}_2) \cdots (a_n, \mathbf{x}_n)$ with $\mathbf{x}_1 = \mathbf{0}$ in Γ starting at $(q_0, \mathbf{0})$. By definition, $\zeta(\alpha) = w$. By construction in Theorem 3.1, the terminal vertex of $(a_1, \mathbf{0})$ is $\delta(q_0, s_1) = (\tau(q_0, s_1), \zeta(a_1))$ and the terminal vertex of $(a_k, \mathbf{x}_k)$ is $(\tau(q_{k-1}, s_k), \mathbf{X}_k + \zeta(a_k))$ and so $\mathbf{x}_{k+1} = \mathbf{x}_k + \zeta(a_k)$ for each $k = 1, \ldots, n-1$. Hence $\mathbf{x}_n + \xi_\Delta(a_n) = \sum_{i=1}^{n-1} \xi_\Delta(a_i) + \xi_\Delta(a_n) = 0$ as $\xi(a_i)$'s are precisely the counter changes of the transitions of the a_i's. Thus the terminal vertex of α is in Γ_0, and because the terminal vertex of a_n is in F, the terminal vertex of α is in F_0. On the other hand, given a walk $(a_1, \mathbf{x}_1) \cdots (a_n, \mathbf{x}_n)$ in Γ from $(q_0, \mathbf{0})$, $a_1 \cdots a$ is clearly

a walk in $_M$ from q_0 with the same labels; further, the terminal vertex of $(a_n, \mathbf{x}_n)$ is $(\tau(a_n), \mathbf{x}_n + \xi(a_n))$ is in F_0 iff $\tau(a_n) \in F$ and $\mathbf{x}_n + \xi(a_n) = \mathbf{0}$.

Conversely, suppose $L = L(\Gamma, F_0, \zeta, v_0)$ as stated in the theorem. Let $\Gamma_0 = \langle V_0, A_0, \iota_0, \tau_0 \rangle$ be a $\mathbb{Z}^d$-unit containing v_0 and F_0. Consider $\Gamma/\mathbb{Z}^d$. Let $Q = V/\mathbb{Z}^d$ and we set $q_0 = \mathbb{Z}^d(v_0)$. Since ζ is $\mathbb{Z}^d$-invariant labeling on the arcs of Γ, all arcs in the same orbit have the same label, hence we set $\zeta' : A/\mathbb{Z}^d \to \Sigma$ with $\zeta'(\mathbb{Z}^d(a)) = \zeta(a)$. For each $a \in A_0$, let

$$\xi(\mathbb{Z}^d(a)) = \begin{cases} (0, \dots, 0) \\ \quad \text{if } \iota(a), \tau_0(a) \in V_0 \\ \mathbf{z} = (i_1, \dots, i_d) \\ \quad \text{if } \tau(a) \notin V_0 \text{ and for some } v \in V_0, \tau(a) = \mathbf{z}(v) \\ -\mathbf{z} = -(i_1, \dots, i_d) \\ \quad \text{if } \iota(a) \notin V_0 \text{ and for some } v \in V_0, \iota(a) = \mathbf{z}(v). \end{cases}$$

Observe that by Lemma 4.1, ξ is well-defined. If $a \in A_0$, let $\delta(\mathbb{Z}^d(\iota_0(a)), \zeta(a)) = (\tau(a), \zeta(\mathbb{Z}^d(a)))$. We set $F = \{\mathbb{Z}^d(v) : v \in F_0\}$. We claim that $M = (Q, \Sigma, \delta, q_0, F)$ is the desired DCM.

From the definition, a word is a ζ-label of a walk in Γ if and only it is a ζ-label of a walk in M. Also walks in Γ starting at v_0 and terminating in F_0 *are* walks in M starting at $q_0 = \mathbb{Z}^d(V_0)$ and terminating at F. We only need to check that the counters in M zero out if and only if the walks in Γ start at v_0 and terminate in F_0. This follows directly from the fact that starting at a $\mathbb{Z}^d$-unit and following an arc with label $\mathbf{z}$ we land in a $\mathbb{Z}^d$-unit in Γ that is a $\mathbf{z}$ translate of the original. Let $a_1, \dots, a_n$ be a walk in Γ with $\tau(a_i) = v_i$ for $i = 1, \dots, n$. Let $v'_k \in P(v_k) \cap V_0$ and $a'_k \in P(a_k) \cap A_0$ for each k. Then $v_1 = \xi(\mathbb{Z}^d(a_1))(v'_1)$ and $v_2 = \left[\xi(\mathbb{Z}^d(a_1)) + \xi(\mathbb{Z}^d(a_2))\right](v'_2), \dots, v_n = \left[\sum_{k=1}^{n} \xi(\mathbb{Z}^d(a_k))\right](v'_n)$ So $v_n \in V_0$, i.e., $v_n = v'_n$ if and only if $\xi(a_1 \cdots a_n) = \mathbf{0}$, meaning M terminates with 0s in all its counters. So $a_1 \cdots a_n$ is a walk terminating in F_0 if and only if M accepts w. $\square$

<u>Example 4.2:</u> Observe that in Fig. 8, the digraph to the left is the transition diagram of a 1-counter DCM (with say vertex a as initial and vertex b as terminal). The 1-periodic digraph at right corresponds to the periodic digraph obtained by construction in Theorem 3.1. The construction in Theorem 4.1 produces the unit with red arrows and vertices $\{(a, 0), (b, 0), (c, 0)\}$, sucn that $L(\Gamma, \{(b, 0)\}, \zeta, (a, 0))$ corresponds to the language of the DCM to the left. In both digraphs, in order to keep the figure easier to follow, the ζ-labelings are omitted. We note that the unit in this case is not necessarily connected.

Consider Fig. 10. The 1-periodic digraph to the right is isomorphic to the 1-periodic digraph to the right of Fig. 8 (map $(a, x) \mapsto (p, x)$, $(b, x) \mapsto (q, x-1)$ and $(c, x) \mapsto (r, x)$ for $x \in \mathbb{Z}$). In this case, the language $L((\Gamma, \{(g, 0)\}, \zeta, (p, 0))$ is recognized by the 1-counter machine in Fig. 10 to the left. We point out that the two different units of two isomorphic 1-periodic digraphs in Figs. 8 and 10 produce two non-isomorphic counter machines that recognize two distinct languages.

5 Concluding remarks

This paper proposes a formal language theory approach in understanding crystallographic structures. We consider this as a first step in the development of a larger algebraic model which would capture both rigid and flexible assemblies. We observed that labels of walks in periodic digraphs that start and terminate in the same unit are closely related to new classes of languages. They form a hierarchy of intersection languages, denoted here $\mathscr{DCL}$, that is included within the hierarchy of intersection of deterministic context free languages. The classes within this newly defined hierarchy are recognized with specific deterministic counter machines. We anticipate that all inclusions depicted in Fig. 1 are proper. These inclusions and further properties of $\mathscr{DCL}$ languages remain to be studied. We point out that several observations, such as Theorem 3.1, hold for arbitrary groups (groups that are not necessarily free abelian); while we do not know what types of languages could be associated with such general structures, such studies are of further interest.

Here we concentrate on periodic structures which are described by periodic digraphs and types of cyclic walks that appear in these structures. We hope that properties of these languages would improve our understanding of the structures they are associated with. In particular, we expect that in certain cases equality of languages associated with the structures (digraphs) may imply the digraphs are isomorphic. Also, the proof of Theorem 4.1 indicates that the transition diagram of the counter machine identifies a unit cell of the periodic graph. Hence, by examining different transition diagrams of counter machines may help in constructing new crystallographic structures.

Acknowledgments

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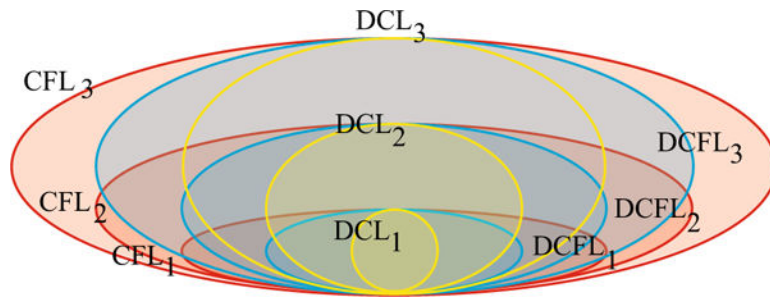
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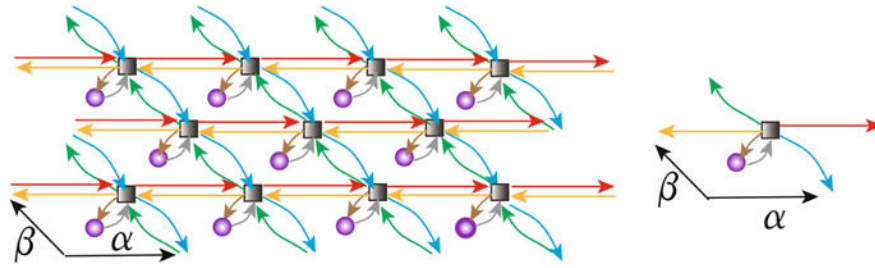
Fig. 1.
Nested hierarchies of intersections of context-free languages (CFL) in *red*, deterministic context free languages (DCFL) in *blue*, and deterministic counter languages (DCL) in *yellow*. (Color figure online)

Fig. 2.
At *left*, a digraph with two orbits of vertices and three orbits of arcs. At *right*, a fundamental transversal isolated
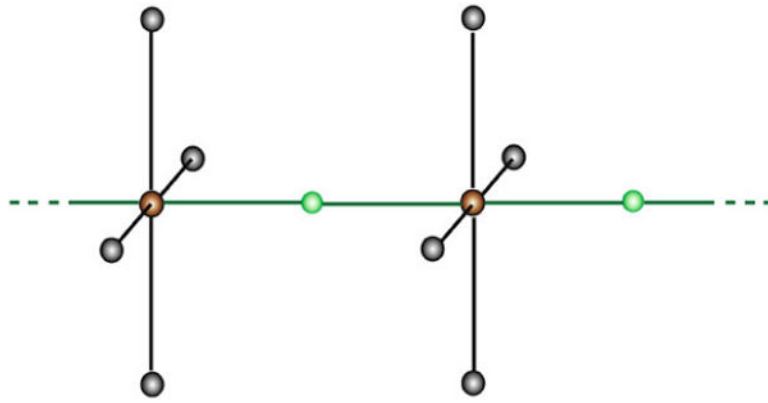
Fig. 3.
A 1-periodic net that cannot be isometrically embedded in any Euclidean space of dimension <3. This is an example of a "rod"
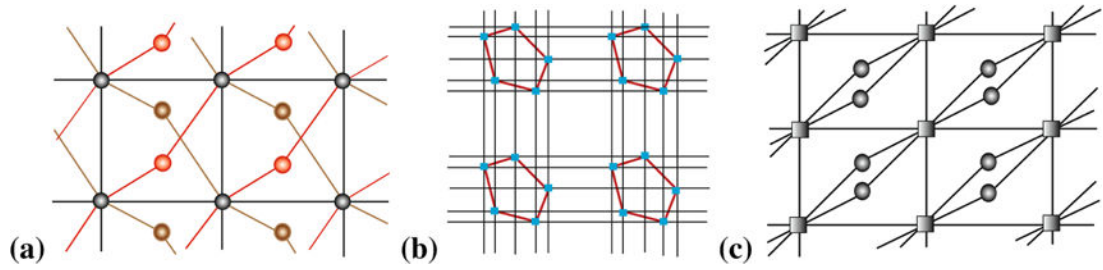
Fig. 4.
a An example of a 2-crystallographic non-barycentrizable graph; **b** an example of a 2-abstractly periodic graph that is not 2-crystallographic and **c** an example of a 2-abstractly periodic graph whose automorphism group is not a subgroup of any crystallographic group
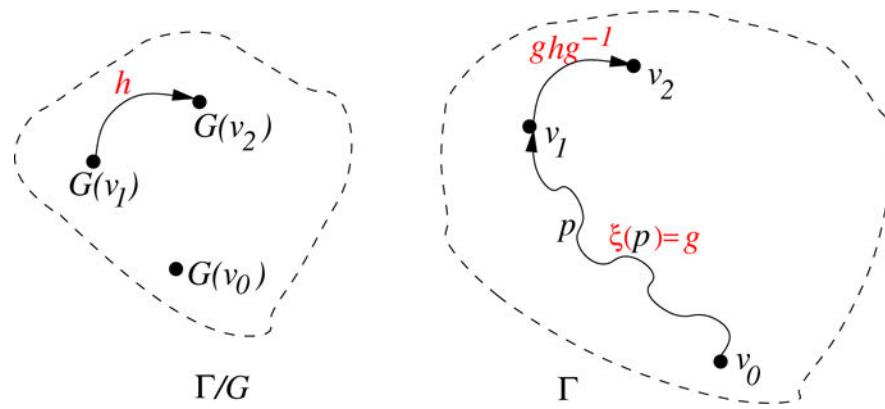
Fig. 5.
Map ξ honoring $\xi_{\Gamma/G}$. The group elements labeling arcs are indicated in *red*. (Color figure online)
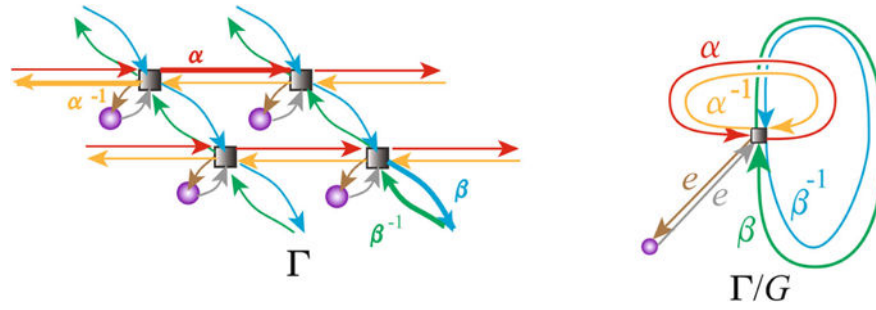
Fig. 6.
The graph Γ of Fig. 2 (*left*), where the group *G* is generated by the translations α and β and the quotient graph Γ/*G* (*right*)
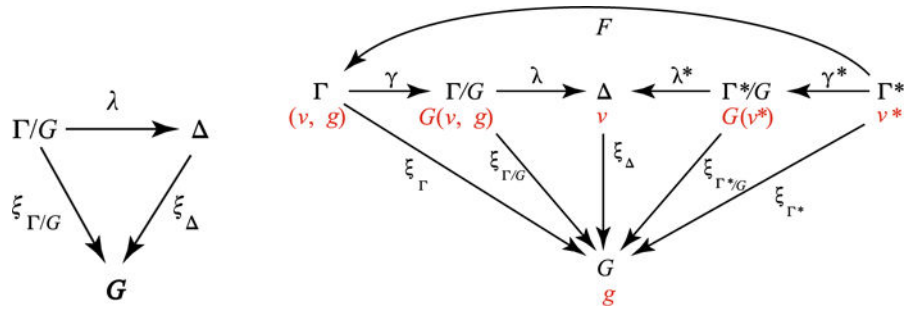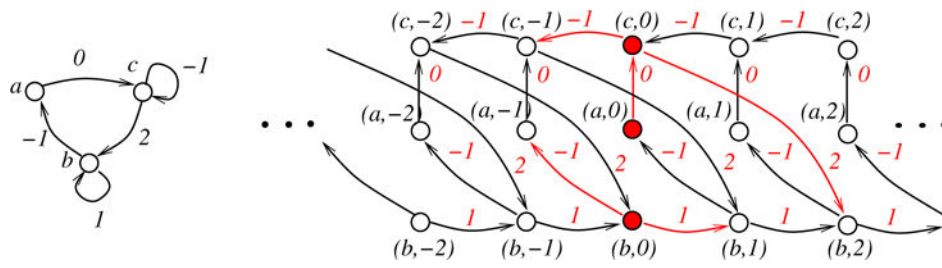
Fig. 7.
(*left*) The diagram for isomorphism $\lambda\colon \Gamma/G \to$ and (*right*) the diagram for the isomorphism between Γ^* and Γ
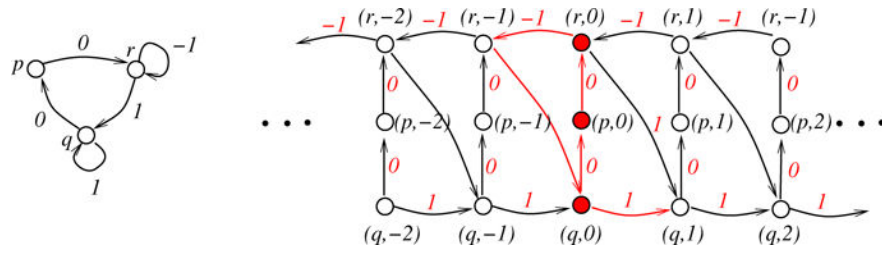
Fig. 8.
A weakly connected digraph with $\mathbb{Z}$-labeling to the *left* and the graph Γ obtained from the construction in Theorem 3.1. The unit $V_0 = V \times 0$ as generated in the proof of Theorem 4.1 is indicated in *red*. (Color figure online)
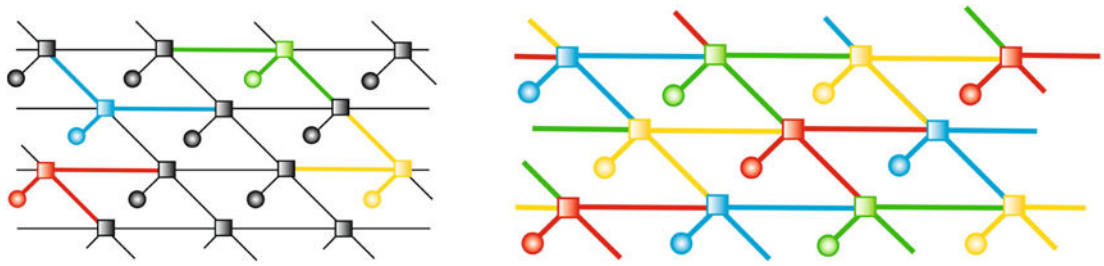
Fig. 9.
(*left*) Four types of units in a 2-periodic (Euclidean) graph shown in *red*, *blue*, *yellow*, and *green*. (*right*) Periodic graph being partitioned by units. (Color figure online)

Fig. 10.

A transition diagram of a 1-counter DCM to the *left* and the graph Γ obtained from the construction in Theorem 3.1 to the *right*. The unit $V_0 = V \times 0$ as generated in the proof of Theorem 4.1 is indicated in *red*. The ξ-labeling is omitted. (Color figure online)