

Soliton automata: a computational model on the  
principle of graph matchings

Summary of the Ph.D. Thesis

*by*

Miklós Krész

Advisor:

Dr. Miklós Bartha

Associate Professor

University of Szeged

2004



## Introduction

Molecular computing is an emerging field in current theoretical and application-oriented research ([1],[27], [30]) as well. One of the most promising alternatives of the traditional semiconductor technology is the so-called bioelectronics or molecular electronics ([28]).

One interesting possibility of molecular electronic devices was proposed by F. L. Carter ([9]) and is about using single strands of the electrically conductive plastic polyacetylene. Electrons are thought to travel along polyacetylene in little packets called *solitons*. Hence, molecular scale electronic devices constructed from molecular switches and polyacetylene chains are called *soliton circuits*.

The practical research in soliton circuits (cf. [19], [20], [21], and [22]) has arisen the need to develop an applied mathematical arsenal in order to obtain a detailed understanding of the behavior of these circuits. Nevertheless, apart from the early work by M. P. Groves ([18]), no structural analysis has been given for the design and verification of soliton circuits.

This thesis deals with the mathematical model of soliton circuits called soliton automata. This model was introduced by J. Dassow and H. Jürgensen in 1990 ([10]) in order to capture the logical aspects of the "valve" effect by which soliton switches and soliton circuits might operate. Dassow's and Jürgensen's introductory work was followed by a series of papers (cf. [11], [12], and [13]) in which special cases of deterministic soliton automata were analyzed with respect to their transition monoids. Concerning another aspect of the computational power of deterministic soliton automata, in [17] a detailed analysis was given for homomorphically complete systems of these automata. However, no detailed theory has been developed for the description of the underlying topological structure of these automata, which explains the lack of more general results on soliton automata.

The precedings show that both from the side of automata theory and from the side of circuit design, there is a common need for a structural theory by which soliton circuits and soliton automata can be analyzed. This thesis is motivated by the above recognition and its goal is to provide a detailed structural description of soliton graphs and soliton automata. The impacts of our results on the practical design will also be outlined by giving the algorithmic consequences of the theory.

This work is strongly based on the papers [4], [5], [6], [7], [8], and [25].

## Soliton automata and matching theory

The structural analysis of soliton automata will be carried out on the basis of matching theory. By a *matching*  $M$  in graph  $G$  we mean a subset of  $E(G)$  such that no vertex of  $G$  occurs more than once as an endpoint of some edge in  $M$ . The connection between matching theory and soliton automata was recognized by M. Bartha and E. Gombás in [2] and [3].

The underlying object of a soliton automaton is the so-called soliton graph representing the topological structure of the corresponding molecule-network. In this model atoms (or groups of atoms) are represented by vertices and chemical bonds correspond to edges. The vertices with degree 1 are designated as *external vertices*, while a vertex with degree greater than one is called *internal*. External vertices correspond to the marginal parts of the system, which parts serve as electron donors or acceptors for the remaining part of the molecule-network. The internal vertices correspond to an atom (or group of atoms) with the property that among its neighbors there exists a unique one to which it is connected by a double bond. The above property is described by *perfect internal matchings*, matchings which cover all the internal vertices. Therefore a *soliton graph* is defined as an open graph (graphs having external vertices) possessing a perfect internal matching.

Considering the above facts it is justified to use the name *state* as a synonym for perfect internal matching. The set of states (set of perfect internal matchings) of a graph  $G$  will be denoted by  $S(G)$ .

For the study of the logical aspects of soliton switching we need to give a graph theoretic formalization of the state transitions induced by soliton waves. Ignoring the physico-chemical details, the effect of a soliton wave propagating along a polycetylene chain is to exchange all single and double bonds. This logical aspect is captured by the concept of soliton walk. In order to place this concept into a matching-theoretic framework, we need the following notation: For a walk  $\alpha = v_0, e_1, \dots, e_n, v_n$ , let  $n_\alpha(j)$  ( $j \in [n]$ ) denote the number of occurrences of the edge  $e_j$  in the prefix  $\alpha[v_0, v_j]$ .

**Definition.** A *partial soliton walk* with respect to state  $M$  in soliton graph  $G$  is a backtrack-free walk  $\alpha = v_0, e_1, \dots, e_n, v_n$  ( $n \geq 1$ ) subject to the following conditions:

- (a)  $v_0$  is an external vertex;
- (b) for every  $j \in [n-1]$ ,  $n_\alpha(j)$  and  $n_\alpha(j+1)$  have the same parity if and only if  $e_j$  and  $e_{j+1}$  are  $M$ -alternating, i.e.,  $e_j \in M$  iff  $e_{j+1} \notin M$ .

Furthermore, a partial soliton walk is called a *soliton walk* if  $v_n$  above is an external vertex.

*Making the walk*  $\alpha$  in state  $M$  means creating the edge set  $S(M, \alpha)$  by setting for every  $e \in E(G)$ :

$e \in S(M, \alpha)$  iff  $e \in M$  and  $e$  occurs an even number of times in  $\alpha$ , or  $e \notin M$  and  $e$  occurs an odd number of times in  $\alpha$ .

It can be proved that for any soliton walk  $\alpha$ ,  $S(M, \alpha)$  is also a state. Furthermore, it is also clear that *impervious edges*, i.e. edges not traversed by any partial soliton walk, have no effect on the operations of the system. Therefore, considering any soliton graph  $G$ , only the *viable* edges (edges which are not impervious) of  $G$  have role in the concept of soliton automata. The above observation motivates to define the *viable subgraph*  $G^+$  of any soliton graph  $G$ , by which we mean the subgraph of  $G$  determined by its viable edges only. It is also easy to prove that  $G^+$  is also a soliton graph.

For the definition of soliton automata, we need a further notation:

For any state  $M$  of a soliton graph  $G$  and any external vertices  $v_1, v_2 \in V(G)$ , let

$$\mathcal{S}_G(M, v_1, v_2) = \{S(M, \alpha) \mid \alpha \text{ is a soliton walk with respect to } M, \text{ which starts at } v_1 \text{ and ends at } v_2\}$$

**Definition.** A *soliton automaton* associated with underlying graph  $G$  is a non-deterministic finite automaton

$$\mathcal{A}(G) = ((S(G^+), (X \times X), \delta)$$

subject to the following conditions:

- (a)  $G$  is a soliton graph
- (b)  $S(G^+)$ , the set of states of  $\mathcal{A}(G)$ , is the set of states of  $G^+$
- (c)  $(X \times X)$  is the input alphabet, where  $X$  denotes the set of external vertices of  $G$
- (d)  $\delta : S(G^+) \times (X \times X) \rightarrow 2^{S(G^+)}$  is the transition function, such that

$$\delta(M, (v_1, v_2)) = \begin{cases} \mathcal{S}_{G^+}(M, v_1, v_2), & \text{if } \mathcal{S}_{G^+}(M, v_1, v_2) \neq \emptyset \\ \{M\}, & \text{otherwise} \end{cases}$$

for any  $M \in S(G^+)$  and  $v_1, v_2 \in X$ .

## Tutte type characterizations of soliton graphs

In [2], the exact counterpart of Tutte's theorem ([29]) on graphs with perfect matchings has been elaborated for graphs having a perfect internal matching. Here we strengthen the above result by proving two Tutte type theorems for splitters, which are introduced to take over the role of barriers ([26]) in graphs with perfect internal matchings. In order to state these theorems, we need the following concepts.

Given a soliton graph  $G$ , we say that an edge  $e \in E(G)$  is *allowed* (*mandatory*) if  $e$  is contained in some (respectively, all) perfect internal matching(s) of  $G$ . *Forbidden edges* are those that are not allowed. A nonempty set of internal vertices of  $G$  is a *splitter* if connecting any two of its elements by an edge  $e$ , the edge  $e$  will become forbidden in the resulted graph  $G + e$ .

Let  $M$  be a perfect internal matching in  $G$ . An edge  $e \in E(G)$  is said to be  *$M$ -positive* ( *$M$ -negative*) if  $e \in M$  (respectively,  $e \notin M$ ). An *alternating trail* with respect to  $M$  (or  *$M$ -alternating trail*, for short) in  $G$  is a trail stepping on  $M$ -positive and  $M$ -negative edges in an alternating fashion. We say that an internal vertex  $v$  is *accessible* from external vertex  $w$  in state  $M$ , if there exists an alternating path starting from  $w$  and terminating in a positive edge at  $v$ . *Accessible vertices* are those that are accessible from some external vertex in a state of  $G$ .

The concept of factor-critical graphs (cf. [26]) can be also generalized in a natural way: A connected graph  $G$  is *factor-critical* if for every internal vertex  $v$ ,  $G$  has a matching covering every internal vertex but  $v$ .

Finally, if  $X$  is a set of internal vertices in  $G$ , then a connected component of  $G - X$  which consists of a single external vertex is called *degenerate*.

**Theorem 1.**([8]) *Let  $X$  be a non-empty set  $X$  of internal vertices of a soliton graph  $G$ , and let  $c_{\text{in}}(G, X)$  denote the number of connected components of  $G - X$  containing internal vertices only. Then the following two statements are equivalent.*

- (i) *The set  $X$  is a maximal splitter.*
- (ii) *Each non-degenerate connected component of  $G - X$  is factor-critical such that*
  - (iia)  $|X| = c_{\text{in}}(G, X) + 1$ , or
  - (iib)  $|X| = c_{\text{in}}(G, X)$  with every external component of  $G - X$  being degenerate.

Furthermore, condition (iib) holds in (ii) above if and only if  $X$  is inaccessible, i.e. it does not contain accessible vertices.

**Theorem 2.**([8]) *An open graph  $G$  is a soliton graph if and only if  $c_{\text{in}}^{\circ}(G, X) \leq |X|$  for any set  $X$  of internal vertices, where  $c_{\text{in}}^{\circ}(G, X)$  denotes the number of odd connected components of  $G - X$  containing internal vertices only. Equality may hold for some non-empty  $X$  only if not all connected components of  $G$  are open factor-critical. In this case, the equation is guaranteed by any maximal inaccessible splitter  $X$ .*

Our concluding observation provides a characterization of factor-critical open graphs.

**Theorem 3.**([8]) *A connected open graph  $G$  is factor-critical if and only if  $c_{\text{in}}^{\circ}(G, X) \leq |X| - 1$  for any non-empty set  $X$  of internal vertices. In this case, equality holds for any maximal splitter  $X$ .*

## A structure theory for soliton graphs

Compositions and decompositions of finite automata have been intensively studied since the beginning of the sixties. The goal of this research is to characterize complex systems by products of smaller automata. In order to carry out this task for soliton automata, first we need to work out a decomposition of soliton graphs into smaller components such that the automata associated with these components should operate partly independently, i.e. the relationship among the components can be fully described. To meet the above goal, we develop a structure theory of soliton graphs on the basis of their elementary components.

An *elementary component* of a graph  $G$  having a perfect internal matching is a maximal connected subgraph of  $G$  spanned by allowed edges only. An elementary component is called *external* or *internal* depending on whether it contains an external vertex. A graph is *elementary* if it consists of a unique elementary component.

It is well-known (cf. [26]) that a canonical partition can be defined on the vertex set of any elementary graph with respect to perfect matchings (matchings covering all vertices). This result has been generalized for perfect internal matchings in [3]. As a first result, we show that this partition can be extended for any graph having a perfect internal matching.

**Definition.** Let  $G$  be a graph having a perfect internal matching. Then for any two internal vertices  $u, v \in V(G)$ ,  $u \sim v$  if there exists a splitter containing both  $u$  and  $v$ , and they belong to the same elementary component

of  $G$ .

**Theorem 4.**([6]) *The relation  $\sim$  is an equivalence on the set of internal vertices of  $G$ .*

The relation  $\sim$  is called *canonical equivalence*, and the blocks determined by  $\sim$  are called the *canonical classes* of  $G$ .

Based on this partition the elementary components containing viable edges are given a structure reflecting the order in which they can be reached by alternating paths starting from an external vertex (*external alternating paths*). The observations of this structure theory are summarized below.

**Theorem 5.**([6]) *The viable elementary components of a soliton graph  $G$  can be grouped into disjoint families such that the following conditions hold.*

- (i) *Any family contains at most one external elementary component.*
- (ii) *For any family  $\mathcal{F}$  consisting of internal elementary components only (internal families), there exists a unique canonical class  $P$  in some elementary component of  $\mathcal{F}$ , called the principal canonical class of  $\mathcal{F}$ , such that any external alternating path leading to a member of  $\mathcal{F}$  must reach  $P$  first.*
- (iii) *There exists a partial order  $\mapsto^*$  among the families reflecting the order by which any external alternating path reaches the families. The maximal elements are the families containing an external elementary component (external families).*
- (iv) *An internal vertex  $v$  belonging to a viable elementary component is inaccessible iff  $v$  is contained in a principal canonical class.*

The above structure plays a central role in the decomposition of soliton automata. Therefore it is important to isolate the families of any soliton graph by an efficient method. We have proved that a modification of the Edmonds algorithm ([14]) leads to a procedure running in linear time.

**Theorem 6.**([5]) *For any soliton graph  $G$ , the viable subgraph  $G^+$  and the families of the viable elementary components together with the partial order  $\mapsto^*$  can be determined in  $\mathcal{O}(|E(G)|)$  time.*

## Decomposition of soliton automata

Concerning soliton circuits and soliton automata two questions seem to be the most fundamental to address.



- (a) Given the underlying topology of interconnected molecules and molecule chains, verify the soliton circuit based on this system by describing its operations. (see e.g. [18])
- (b) Characterize the class of soliton automata.

Making use of our structure theory we reduce both of the above problems to the analysis of elementary soliton automata (soliton automata associated with an elementary graph).

Actually question (a) can be also easily translated into the language of soliton automata: a method which describes the automaton associated with a given soliton graph (Automaton Description Problem - ADP) is needed. First we investigate the following basic approach for solving the above problem.

**Automaton Construction Problem (ACP):** *Given a soliton graph  $G$ . Construct the automaton  $\mathcal{A}(G)$  associated with  $G$ .*

In order to solve ACP we need to determine the set of states and the transition function of  $\mathcal{A}(G)$ . The set of states can be constructed by an extension of the method suggested in [24] for bipartite graphs with respect to perfect matchings. In order to determine the transition function, we have given a matching-theoretic characterization of soliton transitions ([4]). This characterization leads then an  $\mathcal{O}(|V(G^+)| \cdot |E(G^+)|)$  time algorithm which decides for an arbitrary pair of states if there exists a transition between them. Therefore we obtain the following result.

**Theorem 7.** *Let  $G$  be a soliton graph,  $n = |V(G^+)|$ ,  $m = |E(G^+)|$  and  $k = |S(G^+)|$ . Then ACP can be solved in  $\mathcal{O}(k^2 \cdot n \cdot m)$  time.*

In [12], an important special case of deterministic soliton automata has been characterized: soliton automata with a single external vertex. Here we generalize this result for non-deterministic soliton automata.

**Definition.** Let  $M$  be a state of soliton graph  $G$  and  $v$  be an external vertex of  $G$ . An  $M$ -alternating  $v$ -racket  $\beta$  is an  $M$ -alternating trail starting from  $v$  which can be decomposed into an external alternating path  $\beta_h$  and an even-length alternating cycle  $\beta_c$ . An  $M$ -alternating double  $v$ -racket  $\alpha$  is a pair of  $M$ -alternating  $v$ -rackets  $(\alpha^1, \alpha^2)$  such that  $E(\alpha_h^1) \cap E(\alpha_c^2) = \emptyset$ ,  $E(\alpha_h^2) \cap E(\alpha_c^1) = \emptyset$ , and either  $\alpha_c^1 = \alpha_c^2$  or  $V(\alpha_c^1) \cap V(\alpha_c^2) = \emptyset$ .

**Definition.** Let  $\mathcal{A} = (S, X, \delta)$  be an automaton such that its alphabet is a singleton, i.e.  $X = \{x\}$ . We say that  $\mathcal{A}$  is a *full (semi-full)* automaton if for each  $s \in S$ ,  $\delta(s, x) = S$  (respectively,  $\delta(s, x) = S \setminus \{s\}$  with  $|S| > 1$ ).

**Theorem 8.** *Let  $G$  be a soliton graph with a single external vertex  $v$ . Then*

$\mathcal{A}(G)$  is either a full or a semi-full automaton. Moreover,  $\mathcal{A}(G)$  is semi-full iff  $G^+$  is a bipartite graph without double  $v$ -rackets.

The above result plays an important role in the elementary decomposition of soliton automata, which is carried out with a special type of  $\alpha_0^{\otimes}$ -product (cf. [15], [16], [23]), called canonical product. The formal definition of this product needs a few additional concepts.

**Definition.** Let  $\mathcal{A}(G) = (S(G^+), X \times X, \delta)$  be a soliton automaton. The *extension* of  $\mathcal{A}(G)$  is the automaton  $\mathcal{A}_e(G) = (S(G^+), X \times X, \delta_e)$ , where for any state  $M$  of  $G$  and any pair of external vertices  $(v, w) \in X \times X$ ,

$$\delta_e(M, (v, w)) = \begin{cases} \delta(M, (v, w)), & \text{if } v \neq w \\ \delta(M, (v, w)) \cup \{M\}, & \text{otherwise} \end{cases}$$

**Definition.** For  $i = 1, 2$ , let  $X_i$  be alphabets and  $\mathcal{A}_i = (S_i, X_i \times X_i, \delta_i)$  be automata. We say that  $\mathcal{A}_1$  and  $\mathcal{A}_2$  are *strongly isomorphic* if there exists a pair  $\psi = (\psi_S, \psi_X)$  of bijections  $\psi_S : S_1 \rightarrow S_2$  and  $\psi_X : X_1 \rightarrow X_2$  which satisfies the equation

$$\{\psi_S(s') \mid s' \in \delta_1(s, (x, x'))\} = \delta_2(\psi_S(s), (\psi_X(x), \psi_X(x')))$$

for every  $s \in S_1$  and every  $x, x' \in X_1$ .

We say that a *soliton isomorphism* exists between  $\mathcal{A}_1$  and  $\mathcal{A}_2$ , if for  $i = 1, 2$  there is a soliton automaton  $\mathcal{A}(G_i)$  such that  $\mathcal{A}_i$  is strongly isomorphic with  $\mathcal{A}(G_i)$ , and  $\mathcal{A}_e(G_1)$  is strongly isomorphic with  $\mathcal{A}_e(G_2)$ . The existence of a soliton isomorphism between automata  $\mathcal{A}_1$  and  $\mathcal{A}_2$  is expressed by  $\mathcal{A}_1 \cong_s \mathcal{A}_2$ .

Now we are ready to define the appropriate automata product.

**Definition.** Let  $G_1, \dots, G_n (n \in N)$  be soliton graphs and for each  $i \in [n]$  let  $\mathcal{A}_i$  denote the soliton automaton associated with  $G_i$ , i.e.  $\mathcal{A}_i = \mathcal{A}(G_i)$  with transition function  $\delta^i$  and set of states  $S_i = S(G_i^+)$ . Furthermore, let  $\mathcal{L} = \{\mathcal{A}_{n+1}, \dots, \mathcal{A}_m\}$  ( $n \leq m$ ) be a system of (not necessarily soliton) automata with  $\mathcal{A}_j = (S_j, X_j, \delta^j)$  ( $n+1 \leq j \leq m$ ), and  $\tau$  be a mapping, called *canonical dependency*, from  $\mathcal{L}$  to the power set of the set of canonical classes contained in some  $G_i$  ( $i \in [n]$ ). Then a *canonical product* from  $\mathcal{Q} = \{\mathcal{A}_1, \dots, \mathcal{A}_n\}$  to  $\mathcal{L}$  with respect to  $\tau$  is a product  $\mathcal{A} = (S, X \times X, \delta)$  of  $\mathcal{A}_e(G_1), \dots, \mathcal{A}_e(G_n), \mathcal{A}_{n+1}, \dots, \mathcal{A}_m$  with alphabet  $X \times X$  and feedback function  $\phi = (\phi_1, \dots, \phi_m)$  such that the following conditions hold.

- (a)  $X = X_1 \sqcup \dots \sqcup X_n$ , where for each  $i \in [n]$ ,  $X_i$  is the set of external vertices of  $G_i$

(b)  $S = S_1 \times \dots \times S_m$

(c) For each  $i \in [m]$ ,  $\phi_i$  is a mapping subject to the following conditions:

(c1) If  $i \leq n$ , then  $\phi_i : X \times X \rightarrow (X_i \times X_i) \cup \{\varepsilon\}$  such that for every  $v, w \in X$ ,

$$\phi_i((v, w)) = \begin{cases} (v, w), & \text{if } v, w \in X_i \\ \varepsilon, & \text{otherwise} \end{cases}$$

(c2) If  $n + 1 \leq i \leq m$ , then  $\phi_i : S_1 \times \dots \times S_n \times (X \times X) \rightarrow (X_i \times X_i) \cup \{\varepsilon\}$  such that for every  $M_1 \in S_1, \dots, M_n \in S_n$ , and  $v, w \in X$  with  $v \in X_k$  and  $w \in X_l$  for some  $k, l \in [n]$ ,

$$\phi_i(M_1, \dots, M_n, (v, w)) = \varepsilon$$

iff one of the following conditions holds:

(c2/i)  $\tau(\mathcal{A}_i) \cap \mathcal{P}_{G_k}(M_k, v) = \emptyset$ , where  $\mathcal{P}_{G_k}(M_k, v)$  denotes the set of canonical classes of  $G_k$  containing a vertex accessible from  $v$  in  $M_k$ .

(c2/ii)  $k \neq l$ .

(c2/iii)  $k = l$ ,  $v \neq w$  and  $\delta^k(M_k, (v, w)) = \{M_k\}$ .

(d) For every  $x, x' \in X$ , and  $(s_1, \dots, s_m) \in S$ ,

$$\begin{aligned} \delta((s_1, \dots, s_m), (x, x')) &= \delta_e^1(s_1, \phi_1((x, x'))) \times \dots \times \delta_e^n(s_n, \phi_n((x, x'))) \times \\ &\quad \times \delta^{n+1}(s_{n+1}, \phi_{n+1}(s_1, \dots, s_n, (x, x'))) \times \dots \\ &\quad \times \delta^m(s_m, \phi_m(s_1, \dots, s_n, (x, x'))) \end{aligned}$$

Furthermore, if  $n = m$  (i.e.  $\mathcal{L} = \emptyset$ ), then we speak of the *disjoint product* of  $\mathcal{A}(G_1), \dots, \mathcal{A}(G_n)$ .

Intuitively, a canonical product is a special type of  $\alpha_0^\varepsilon$ -product such that the automata in  $\mathcal{L}$  are connected to the soliton automata in  $\mathcal{Q}$  through their canonical classes, according to the canonical dependency, from  $\mathcal{L}$  to the power set of the canonical classes of soliton automata in  $\mathcal{Q}$ . A state transition is induced in an automaton of  $\mathcal{L}$  according to its "accessibility" from the first component of the input pair through a canonical class determined by the canonical dependency.

**Theorem 9.**[4] *The class of soliton automata and the class  $\mathcal{S}$  of automata obtained by a canonical product from a system of soliton automata to a system of full automata coincide up to soliton isomorphism.*

It is important to note that the proof of the above theorem is constructive,

it provides a procedure by which the suitable canonical product is obtained for any soliton automaton.

Finally, we return to the problem posed as Question (a).

**Automaton Description Problem (ADP):** *Given an arbitrary soliton graph  $G$ . Give a formal description of the automaton  $\mathcal{A}(G)$  associated with  $G$ .*

It is clear that ACP is a solution for the above problem, but the soliton automata with a single external vertex show that both the computational and the descriptonal complexity can be significantly reduced by the knowledge of the underlying graph structure. Such a reduction can be applied for any soliton graph, as we showed it in [4]. As a further development of this result, in the thesis we worked out the so-called Elementary Structure Encoding. Such an encoding of a soliton graph  $G$  consists of the followings: the external elementary components extended by some forbidden edges following certain rules, the set of interlinking vertices (vertices of the external elementary components which are adjacent to some vertex of an internal elementary component), the canonical partition of these components, the identifiers of the full automata corresponding to the internal elementary components with respect to their number of states, and a relation between the canonical classes and the full automata. The above reduced structure is equivalent to the automaton associated with  $G$ , but it provides a lower complexity for ADP.

Because of space restrictions, we omit the formal definition of our structure encoding, but we state its consequences for ADP.

**Theorem 10.** *Let  $G$  be a soliton graph such that each of its external elementary component has a polynomial number of states and the state complexity of each internal elementary component of  $G^+$  can be determined in polynomial time. Then ADP can be solved in polynomial time for  $G$ .*

## Deterministic soliton automata

In the analysis of complex systems it is a central question to describe the characteristics which make a given system deterministic. The operation of the internal part of any soliton automaton is captured by Theorem 9., hence it is an obvious generalization of determinism to introduce *partially deterministic soliton automata* as automata associated with a graph such that each of its external elementary components is deterministic. In order to obtain a matching independent characterization of deterministic and partially deterministic automata, we introduce a reduction method for soliton graphs.

**Definition.** A *redex*  $r$  in graph  $G$  consists of two adjacent edges  $e = (u, z)$  and  $f = (z, v)$  such that  $u \neq v$  are both internal and the degree of  $z$  is 2. The vertex  $z$  is called the *center* of  $r$ , while  $u$  and  $v$  ( $e$  and  $f$ ) are the two *focal vertices* (respectively, *focal edges*) of  $r$ .

Let  $r$  be a redex in  $G$ . *Contracting*  $r$  in  $G$  means creating a new graph  $G_r$  from  $G$  by deleting the center of  $r$  and merging the two focal vertices of  $r$  into one vertex  $s$ . The vertex  $s$  is called the *sink* of  $r$  in  $G_r$ .

The above reduction procedure is extended by another natural simplifying operation on graphs; which is the removal of a loop from around a vertex  $v$  if the degree of  $v$  is greater than 3. Such loops will be called *inner*. Let  $G_v$  denote the graph obtained from  $G$  by removing an inner loop at vertex  $v$ . Clearly, if  $G$  is a soliton graph, then so is  $G_v$ , and the states of  $G_v$  are exactly the same as those of  $G$ .

**Definition.** Graph  $G$  is called *reduced* if it does not contain a redex or inner loop.

For an arbitrary graph  $G$ , contract all redexes and remove all inner loops in an iterative way to obtain a reduced graph  $r(G)$ . Then it can be proved that for any soliton graph  $G$ ,  $\mathcal{A}(G) \cong_s \mathcal{A}(r(G))$ , and if  $G$  is deterministic, then  $\mathcal{A}(G)$  and  $\mathcal{A}(r(G))$  are strongly isomorphic. Therefore, it is enough to consider the reduced deterministic graphs for further analysis. The key to the characterization of deterministic and partially deterministic soliton automata is the following result.

**Definition.** A connected loop-free graph  $G$  is a *generalized tree* if it does not contain even-length cycles.

**Theorem 11.** ([7],[25]) *A non-mandatory elementary soliton graph is deterministic iff it reduces to a generalized tree.*

By the above result we can give the required characterization as products of automata associated with baby chestnuts (chestnuts consisting of two parallel edges and a number of external edges having their internal endpoints in common) and generalized trees.

**Theorem 12.** *Let  $\mathcal{T}$  denote the class of soliton automata associated with either a reduced generalized tree or a mandatory elementary graph. Furthermore, let  $\mathcal{D}$  denote the class of soliton automata  $\mathcal{A}(G)$  such that either  $\mathcal{A}(G)$  belongs to  $\mathcal{T}$  or  $G$  is a baby chestnut. Then the followings hold.*

(i) *The class of partially deterministic soliton automata and the class of*

*automata obtained by a canonical product from a system of soliton automata in  $\mathcal{T}$  to a system of full automata coincide up to soliton isomorphism.*

- (ii) *The class of deterministic soliton automata and the class of automata obtained by a disjoint product of soliton automata in  $\mathcal{D}$  coincide up to strong isomorphism.*

The above characterization of the graph structure of reduced deterministic elementary graphs results in a  $\mathcal{O}(n^3)$  time algorithm deciding if a graph is deterministic, where  $n$  denotes the number of vertices. This algorithm consists of three methods: the construction of the elementary decomposition of the given soliton graph, the reduction procedure for the external elementary components, and a method testing the existence of a cycle of even length in the reduced external elementary components.

**Theorem 13.**[25] *For any soliton graph  $G$  with  $n$  vertices, it can be checked in  $\mathcal{O}(n^3)$  time if  $G$  is deterministic.*

## Conclusion

In this thesis we have given a detailed structural analysis of soliton graphs and soliton automata on the basis of graph matchings. We believe that the above results will have a real impact on the design and verification of soliton circuits, as outlined by some algorithms obtained as consequences of our structure theory. Nevertheless, the further improvement of these results towards practical applications needs consultation with the engineering profession.

# Bibliography

- [1] A. Adamatzky, *Computing in Nonlinear Media and Automata Collectives*, IOP Publishing, Bristol-Philadelphia, 2001.
- [2] M. Bartha, E. Gombás, A structure theorem for maximum internal matchings in graphs, *Information Processing Letters* **40** (1991), 289–294.
- [3] M. Bartha, E. Gombás, On graphs with perfect internal matchings, *Acta Cybernetica* **12** (1995), 111–124.
- [4] M. Bartha, M. Krész, Elementary decomposition of soliton automata, *Acta Cybernetica* **14** (2000), 631–652.
- [5] M. Bartha, M. Krész, Isolating the families of soliton graphs, *Pure Mathematics and Applications* **13** (2002), 49–62.
- [6] M. Bartha, M. Krész, Structuring the elementary components of graphs having a perfect internal matching, *Theoretical Computer Science* **299** (2003), 179–210.
- [7] M. Bartha, M. Krész, Deterministic soliton automata defined by elementary graphs, in *Proceedings of the Kalmár Workshop on Logic and Computer Science* (2003) pp. 69–79.
- [8] M. Bartha, M. Krész, Tutte type theorems in graphs having a perfect internal matching, *Information Processing Letters* **91** (2004), 277–284.
- [9] F. L. Carter, The molecular device computer: Point of departure for large scale cellular automata, *Physica D* **10** (1984), 175–194.
- [10] J. Dassow, H. Jürgensen, Soliton automata, *J. Comput. System Sci.* **40** (1990), 154–181.

- [11] J. Dassow, H. Jürgensen, Soliton automata with a single exterior node, *Theoretical Computer Science* **84** (1991), 281–292.
- [12] J. Dassow, H. Jürgensen, Soliton automata with at most one cycle, *Journal of Computer and System Sciences* **46** (1993), 155–197.
- [13] J. Dassow, H. Jürgensen, The transition monoids of soliton trees, Research Report # 331, Department of Computer Science, The University of Western Ontario, London, Canada, 1992.
- [14] J. Edmonds, Paths, trees and flowers, *Canad. J. Math.* **17** (1965), 449–467.
- [15] Z. Ésik, J. Virágh, On products of automata with identity, *Acta Cybernetica* **7** (1986), 299–311.
- [16] F. Gécseg, *Products of Automata*, Akademie-Verlag, Berlin, 1986.
- [17] F. Gécseg, H. Jürgensen, Automata represented by products of soliton automata, *Theoretical Computer Science* **74** (1990), 163–181.
- [18] M. P. Groves, Towards verification of soliton circuits, in *Molecular Electronic Devices* (F. L. Carter, R. E. Siatkowski, H. Wohltjen Ed.), North-Holland, Amsterdam, 1988, pp. 287–302.
- [19] M. P. Groves, C. F. Carvalho, C. D. Marlin, and R. H. Prager, Using Soliton Circuits to Build Molecular Memories, *Australian Computer Science Communications* **15** (1993) pp. 37–45.
- [20] M. P. Groves, C. D. Marlin, Using Soliton Circuits to Build Molecular Computers, *Australian Computer Science Communications* **17** (1995) pp. 188–193.
- [21] M. P. Groves, C. F. Carvalho, and R. H. Prager, Switching the polyacetylene soliton, *Materials Science and Engineering* **C3** (1995) pp. 181–185.
- [22] M. P. Groves, Soliton Circuit Design Using Molecular Gate Arrays, in *Proceedings of the 20th Australasian Computer Science Conference* (1997) pp. 245–252.
- [23] B. Imreh, M. Ito, On  $\alpha_i$ -product of nondeterministic automata, *Algebra Colloquium* **4** (1997), 195–202.



- [24] A. Itai, M. Rodeh, S. Tanimoto, Some matching problems for bipartite graphs, *Journal of the ACM* **25** (1978), 517–525.
- [25] M. Krész, Alternating cycles in soliton graphs, *WSEAS Transactions on Mathematics* **1** (2002), 165–170.
- [26] L. Lovász, M. D. Plummer, *Matching Theory*, North Holland, Amsterdam, 1986.
- [27] T. Sienko, A. Adamatzky, N. Rambidi, and M. Conrad (Ed.), *Molecular Computing*, The MIT Press, London, 2003.
- [28] D. M. Taylor, Molecular nanostructures and their electrical probing, *Thin Solid Films* **331** (1998), 1–7.
- [29] W. T. Tutte, The factorization of linear graphs, *J. London Math. Soc.* **22** (1947), 107–111.
- [30] Y. M. Yin, X. Q. Lin, Progress on molecular computer, *Progress in Chemistry* **13** (2001), 337–342.