Soliton automata and graph matchings

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A soliton automaton is the mathematical model of so called soliton valves in certain carbohydrate molecules, and has the potential to serve as a future molecular switching device. The underlying object of a soliton automaton is a soliton graph, which is an undirected graph G having a perfect internal matching, i.e., a matching that covers all the vertices of G with degree at least two. Such vertices are called internal, whereas vertices with degree one are called external in G. The states of the automaton are all the perfect internal matchings of G, and transitions are defined by making alternating walks connecting two external vertices in G.

In this paper we will characterize soliton automata through its underlying graph object. First we will show that a decomposition of any soliton graph can be given according to its global internal structure. The corresponding soliton automaton, too, can be decomposed into component automata determined by the above structural results. Then a full characterization is obtained for automata based on the internal components, therefore the main contribution of the above results is to reduce the general problem to a simpler one.

Context-free grammars are also frequently used for the description of certain graph properties. We will give the grammars defining exactly the soliton graphs. The above structural decomposition will play important role in this result.

The final topic of this paper is the characterization of deterministic soliton graphs. To this end a reduction procedure is given for soliton graphs, by which every graph has a minimal representation. It is then proved that a 1-extendable and minimal soliton graph with external vertices has an alternating cycle with respect to some of its states iff the graph contains an even-length cycle. This result leads to a characterization of deterministic soliton graphs, saying that every internal elementary component of such a graph is a single mandatory edge, and the minimal representation of each external component is a graph not containing even-length cycles. Using this characterization, the deterministic property becomes straightforward to check for any soliton automaton given by its underlying graph.