Soliton graphs and graph-expressions

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A graph having at least one vertex with degree one is called an open graph. A soliton graph is an open graph having a perfect internal matching, i.e., a matching that covers all the vertices of the graph with degree at least two. These vertices are called internal, whereas vertices with degree one are classified as external. Soliton graphs are the underlying objects of certain molecular switching devices called soliton automata.

The analysis of soliton automata is a very complex task, and only a few special cases have been successfully dealt with so far. Most of the difficult problems in the general case are still open.

This lecture addresses the issue of generating soliton graphs by context-free grammars over graph expressions. The relevance of describing soliton graphs in this specific way is that it highlights the structure of soliton walks defining the transitions of the corresponding soliton automata.

At first, a decomposition procedure is presented for soliton graphs in terms of their global internal structure. It is shown that the elementary components of soliton graphs can be grouped into pairwise disjoint families based on how they can be reached by alternating paths starting from external vertices. This decomposition is then carried over to soliton automata, using quasi-direct and α_0 products of their component automata.

As a second step, the families of elementary components is characterized. To this aim, the concept of factor-critical graphs is generalized for open graphs, and splitters are introduced as the "open" counterparts of barriers in graphs with perfect matchings. It is shown that all external families are factor-critical open graphs. On the other hand, internal families are characterized as graphs having a maximal splitter in which all vertices are inaccessible from external ones by an alternating path.

Finally, context-free grammars capable of generating graph expressions denoting external/internal families and soliton graphs in general are elaborated on the basis of the structural characterizations above.