VISUALIZING AND ANALYZING LARGE SYSTEMS OF DIFFERENTIAL EQUATIONS

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ABSTRACT

At any given moment, there are 4.000–10.000 chemical reactions going on in each living cell (Jha and v.Schuppen 2001). Altogether, these reactions form a huge biochemical reaction network whose inherent structure and properties are still unknown for the most part. Current attempts use a number of differential equations to model this highly dynamic system with its subtle dependencies and interrelations between the said chemical reactions. Realistic models of this form contain 1.000–15.000 differential equations (v.Schuppen 2001). This large number of equations is virtually impossible to overlook in its written form. Yet, for instance visualization methods can be used to gain a better understanding of the vast amount of equations.

Now, there are many ways of visualizing differential equations (Schwalbe and Wagon 1997). But after one realizes that the uncertain parameters of these equations (like reaction rates, etc.) make it impossible to reach any conclusive, quantitative result, one has to come up with new ways of analyzing such models of reaction networks. Our approach to do so is, to describe only the dependencies between the different variables that occur in such a system of differential equations and to visualize these dependencies as a network itself. The use of graph visualization techniques allow for example to recognize causal dependencies between certain reactions (pathways), which is a valuable qualitative result. Also comparisons of different models can now be aided by the visualization and its interaction techniques. While a visualization can thus lead to first insights, it cannot provide a cast iron proof for these. Hence, we further propose to additionally combine the visualization with concrete analysis techniques from the field of graph and network theory. This provides a strong algorithmic foundation that supports the visual analysis and exploration process and permits to verify or falsify the perceived features.

Finally, to show the usefulness of this approach, we have built a software prototype for the analysis and visual exploration of large systems of differential equations. Among other first tests with models from the field of climate research, we also used this tool to analyze biochemical reaction data sets. So finally, some of the gained results are shown and commented on as well.

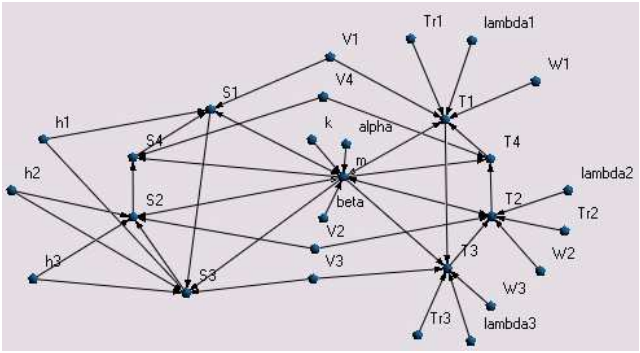

Figure 1: Visualization of a small part of a system of differential equations.

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