

Elementary Modes of Metabolism, and Software for their Determination and Analysis

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ABSTRACT

Historically, the most common approach to the modelling of metabolic systems has been via kinetic modelling. That is, the system is represented as a set of kinetic equations, one for each reaction in the system. Despite the great utility of this approach, problems exist: the kinetic equations, and their associated parameters, may not be well known and the kinetics of individual reactions may vary between organisms, or even cell types within the same organism. These considerations lead to considerable difficulty in making generalisations about a system on the basis of kinetic modelling alone. Furthermore, a realistic description of a system may contain several partially overlapping, but independent, pathways. The determination of such pathways is not possible using kinetic modelling.

A complementary approach to kinetic modelling is structural modelling, in which a model is defined solely in terms of reaction stoichiometries, and is therefore immune to problems caused by uncertain kinetic knowledge. One such approach, "Elementary Modes Analysis", is described here. The utility of Elementary Modes Analysis is illustrated by its application to a problem that arose in the course of the investigation of a kinetic model of photosynthesis. Software, currently under development by this group, for the investigation of Elementary Modes, and some of the design philosophy thereof, is also described.

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