

Computer implementation of simplification for stiff metabolic systems

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In many cases, metabolic network is composed of chains of fast reversible reaction for substrate to intermediate and relatively slow reaction for intermediate to product. This means co-existence of multiple time scale in these kinds of systems.

Therefore, metabolic problems for dynamic simulation are usually stiff systems. When a system is stiff, it's highly possible that model parameters are inaccurate in the view of measurability, and furthermore numerical algorithms are supposed to require much smaller time step compared to time horizon of the problem, which can result in loss of computational efficiency and numerical error accumulation.

Traditionally, quasi steady state approximation has been used in simplifying stiff dynamic problem. However, scale analyses in QSSA have been dependent on researchers' experience and intuition about corresponding systems. For practical computer implementation in metabolic problem, it is necessary to establish systematic and consistent approach toward proper model simplification. In this paper, computer implementation of those schemes was introduced with window interface and few systems were tested with automatic simplification process.