Limit self-simplification in multiscale networks

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The concept of limiting step gives the limit simplification: the whole network behaves as a single step. This is the most popular approach for model simplification in chemical kinetics. However, in its simplest form this idea is applicable only to the simplest linear cycles in steady states. For such the simplest cycles the nonstationary behaviour is also limited by a single step, but not the same step that limits the stationary rate. In this paper, we develop a general theory of static and dynamic limitation for all linear multiscale networks. Our main mathematical tools are auxiliary discrete dynamical systems on finite sets and specially developed algorithms of "cycles surgery" for reaction graphs. New estimates of eigenvectors for diagonally dominant matrices are used.

Multiscale ensembles of reaction networks with well separated constants are introduced and typical properties of such systems are studied. For any given ordering of reaction rate constants the explicit approximation of steady state, relaxation spectrum and related eigenvectors ("modes") is presented. In particular, we proved that for systems with well separated constants eigenvalues are real (damped oscillations are improbable). For systems with modular structure, we propose to select such modules that it is possible to solve the kinetic equation for every module in the explicit form. All such "solvable" networks are described. The obtained multiscale approximations that we call "dominant systems" are computationally cheap and robust. These dominant systems can be used for direct computation of steady states and relaxation dynamics, especially when kinetic information is incomplete, for design of experiments and mining of experimental data, and could serve as a robust first approximation in perturbation theory or for preconditioning.