Biological functions and functional modules originated in the structure of chemical reaction network

Atsushi Mochizuki
Institute for Life and Medical Sciences, Kyoto University, Japan

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In living cells, chemical reactions are connected by sharing their products and substrates, and form a complex network system. Biological functions arise from the dynamics of chemical reaction networks, and are controlled by changes in the amount/activity of enzymes that catalyze reactions in the system. In this talk, I will introduce our recent theoretical approach to determine the behaviors of chemical reaction systems based solely on network topology. (1) We found that the qualitative response of chemical concentrations (and reaction fluxes) to changes in enzyme amount/activity can be determined from the network structure alone. (2) Non-zero responses are localized to finite ranges in a network, and each range is determined by a subnetwork called a "buffering structure". The buffering structure is defined by the following equation from local topology of a network $\chi := -(\#\text{ of chemicals}) + (\#\text{ of reactions}) - (\#\text{ of cycles}) + (\#\text{ of conserved quantities}) = 0$ where the index χ is analogous to the Euler characteristic. We proved that any perturbation of a reaction parameter inside a buffering structure only affects the concentrations and fluxes inside the buffering structure, and does not affect the concentrations nor fluxes outside. Finally, (3) buffering structures govern the bifurcation of the steady state of a reaction network. The bifurcation behaviors are localized to finite regions within a network, and these regions are again determined by buffering structures. These results imply that the buffering structures are the origin of the modularity of biological functions derived from reaction networks. We applied this method to the cell cycle system and demonstrated that the control of different checkpoints is achieved by buffering structures.