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Modeling the Mass Action Dynamics of Metabolism with Fluctuation Theorems and Maximum Entropy. WILLIAM CANNON, DENNIS THOMAS, DOUGLAS BAXTER, JEREMY ZUCKER, GARRETT GOH, Pacific Northwest National Laboratory — The laws of thermodynamics dictate the behavior of biotic and abiotic systems. Simulation methods based on statistical thermodynamics can provide a fundamental understanding of how biological systems function and are coupled to their environment. While mass action kinetic simulations are based on solving ordinary differential equations using rate parameters, analogous thermodynamic simulations of mass action dynamics are based on modeling states using chemical potentials. The latter have the advantage that standard free energies of formation/reaction and metabolite levels are much easier to determine than rate parameters, allowing one to model across a large range of scales. Bridging theory and experiment, statistical thermodynamics simulations allow us to both predict activities of metabolites and enzymes and use experimental measurements of metabolites and proteins as input data. Even if metabolite levels are not available experimentally, it is shown that a maximum entropy assumption is quite reasonable and in many cases results in both the most energetically efficient process and the highest material flux.

William Cannon
Pacific Northwest National Laboratory

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