Presenter:
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Title:
Calculating Detailed-Balanced Equilibrium by Fixed-Point Iterations and Cell Exclusion

Abstract:
We will report on our quest for an unconditionally convergent algorithm to compute the (detailed-balanced) equilibrium of complete networks of reversible binding reactions. Several networks used in pharmacology for simulation and parameter estimation are in this class, and methods used to compute equilibrium are often questionable or even inapplicable. We turned the algebraic equation for equilibrium into a fixed-point problem. We will present network-structural conditions that guarantee the convergence of fixed-point iterations, and a cell-exclusion algorithm that applies more generally.