

Goulet, D. 2017. Modeling, Simulating, and Parameter Fitting of Biochemical Kinetic Experiments. *SIAM REVIEW*. 58(2): 331–353.

See <https://arxiv.org/abs/1508.05359> . Accessed 30 March 2023.

**Abstract.** In many chemical and biological applications, systems of differential equations containing unknown parameters are used to explain empirical observations and experimental data. The differential equations are typically nonlinear and difficult to analyze, requiring numerical methods to approximate the solutions. Compounding this difficulty are the unknown parameters in the differential equation system, which must be given specific numerical values in order for simulations to be run.

Estrogen receptor protein dimerization is used as an example to demonstrate model construction, reduction, simulation, and parameter estimation. Mathematical, computational, and statistical methods are applied to empirical data to deduce kinetic parameter estimates and guide decisions regarding future experiments and modeling. The process demonstrated serves as a pedagogical example of quantitative methods being used to extract parameter values from biochemical data models.

**Keywords.** biology, biochemistry, chromatography, cluster analysis, conservation laws, differential equations, dimerization, estrogen receptor protein, mass action, parameter fitting, optimization, sensitivity analysis