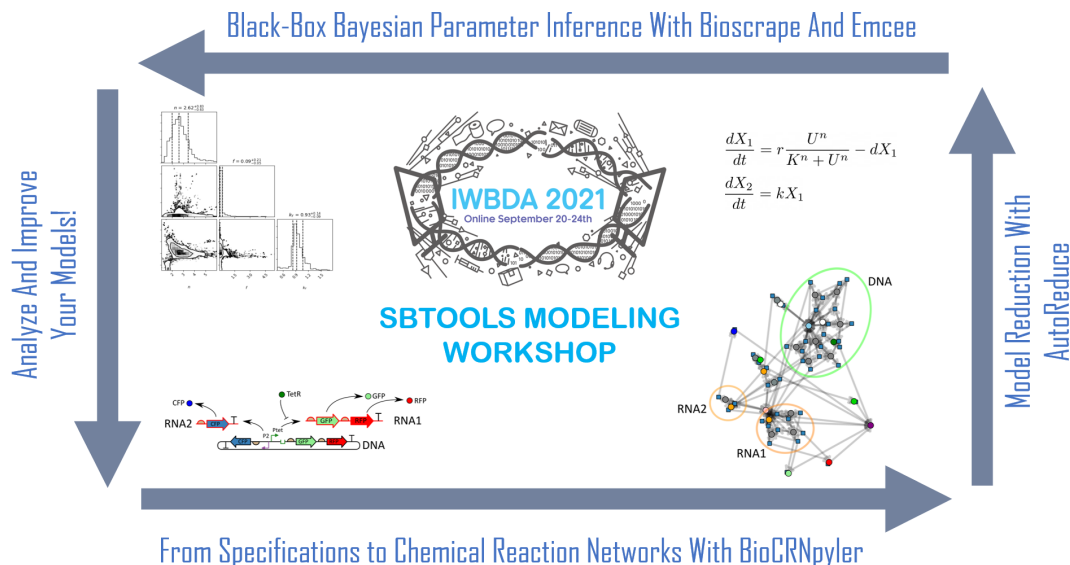


From Chemical Reaction Network Compilation to Bayesian Parameter Inference

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As the complexity of synthetic biological systems increases, software tools and pipelines will be necessary in order to efficiently deploy models and parameterize them based upon biological data. In this two part workshop we will showcase a modular pipeline which begins at a simple specification of a biochemical system, automatically compiles detailed chemical reaction network models, and finally parameterizes the model from experimental data. This workshop will be divided into two self-contained units which can be attended individually or jointly.

Part 1: Compiling Chemical Reaction Networks from Simple Specifications with BioCRNpyler. We will describe the [BioCRNpyler](#) software package [1] and provide a hands-on-tutorial demonstrating how this package can be used to compile diverse chemical reaction network models of biochemical systems. Attendees will also explore BioCRNpyler with a case study involving integrase circuits. We note that this package produces SBML files and can be integrated with existing pipelines. ~ 2 Hours

Part 2: Connecting Chemical Reaction Network Models with Data using Autoreduce, Bioscrape, and Black-box Parameter Inference (Emcee). We will begin by automatically reducing the dimensionality of a chemical reaction network model represented as SBML with [AutoReduce](#) [2] to simplify it for data-driven parameterization. Finally, attendees will use [Bioscrape](#)'s [3] black-box Bayesian parameter inference API (based on the [Emcee](#) package [4]) to parameterize the model from real experimental data. ~ 2 Hours

[1] Poole, W. A. Pandey, A. Shur, Z. Tuza, & R.M. Murray. [Bioarxiv](#), 2020.

[2] Pandey, A. & R.M. Murray. [Bioarxiv](#), 2020.

[3] Swaminathan, A. W. Poole, V. Hsiao, & R.M. Murray. [Bioarxiv](#), 2019

[4] Foreman-Mackey D, Hogg DW, Lang D, Goodman J. Publications of the Astronomical Society of the Pacific, 2013.