OpenFLUX 2019 (DRAFTING IN PROGRESS)

A MATLAB-based application to perform steady-state and dynamic 13C-MFA based on the EMU framework. The application facilitates the inference of metabolic pathway activities from 13C enrichment data (mass isotopologues) using simple text inputs and scripting interfaces. Each object of the OpenFLUX class encapsulates data, model and allowable operations, and is designed to be self-contained/portable.

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Code repository: <https://github.com/lakeeeq/OpenFLUX>

Available input and models:

* OpenFLUX version 2009 steady-state toy model
* Steady-state toy model (similar to version 2009)
* Dynamic toy model
* Adipocyte insulin response model

Workflow:

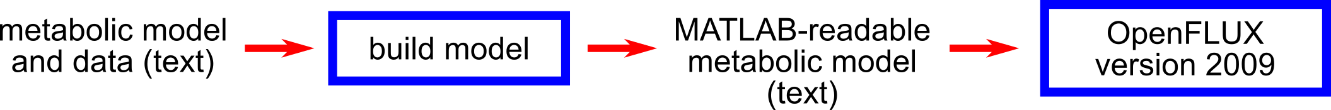
1. Edit OFspec\_\*.m to specify parameters of the OpenFLUX object.
2. Run the required task in OFstartHere.m by toggling on/off the specification file and task.

A clock sitting in the dark

Description automatically generated

You can still implement steady-state analysis using scripts from OpenFLUX version 2009, but the JAVA component may not be functional any more due to the lack support/update. Hence OpenFLUX 2019 can be used instead to generate the MATLAB-readable model files previously generated by the JAVA script.

1. Add “mFiles” folder (version 2009) to MATLAB path.
2. Specify model file location in OFstartHere\_2009.m (on line 8).
3. Run OFstartHere\_2009.m to generate MATLAB-readable model files (contained in the same folder as the model file).
4. Run start13OF.m (resume OpenFLUX 2009 workflow).



Task-based tutorial, step-by-step (DRAFTING IN PROGRESS)

* isotopic steady state, constant fluxes
* isotopic non-steady state, constant fluxes
* isotopic non-steady state, dynamic fluxes