**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>

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<http://www.sciencedirect.com/science/article/pii/S2589004220300389>

**Available input and models:**

* OpenFLUX version 2009 steady-state toy model ([10.1186/1475-2859-8-25](https://doi.org/10.1186/1475-2859-8-25))
* Steady-state toy model (same as version 2009, but to be implemented using this version)
* Dynamic toy model
* Adipocyte insulin response model (manuscript)

**Folder information:**

|  |  |
| --- | --- |
| Name | Details |
| inputs\_adipocytes | * Input model (adipocytes) and data (control, insulin) described in the manuscript. * Least-square (objective) functions for ODE and SBR implementations. * OFspec\_\*.m specification files; ODE and SBR configurations provided as separate files. * Additional data and constraints. |
| inputs\_DYNAMICtoy | * Input model (toy) and data described in Figure 2E of manuscript. * Least-square function (ODE and SBR). * OFspec\_\*.m specification files; ODE and SBR configurations provided as separate files. * No (empty files) additional data and constraints. |
| inputs\_SStoy | * Toy steady-state model and data (constant fluxes, isotopic steady-state) same as OpenFLUX version 2009. * Least-square function. * OFspec\_SStoy.m specification files. * No (empty files) additional data and constraints. |
| MCinstances | * Folder to store Monte-Carlo optimisation instances (runner\_5). |
| OF\_2009\_projectFolder | * Folder containing model/data for implementation using OpenFLUX version 2009. |
| OFfunctions | * Folder containing OpenFLUX scripts. |
| OPinstances | * Folder to store optimisation instances (runner\_3). |
| SIMinstances | * Folder to store simulation instances (runner\_2) |

**Workflow:**

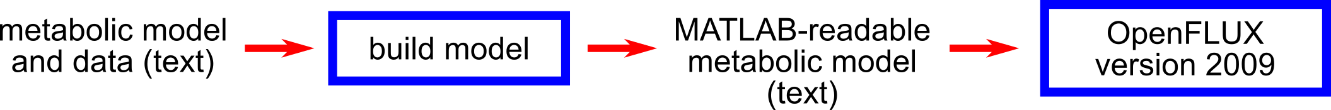
1. Edit OFspec\_\*.m (contained in inputs\_\* folders) to specify parameters of the OpenFLUX object.
2. Run the required task in OFstartHere.m by toggling on/off the specification file name and task to run.

A clock sitting in the dark

Description automatically generated

You can still implement MATLAB scripts from OpenFLUX version 2009, but the JAVA component may no longer be functional due to the lack support/update. Hence OpenFLUX 2019 can be used instead to generate the MATLAB-readable model files previously handled 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