Metabolic Engineering with OptFlux

Requirements and Synopsis

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- This is a fully hands-on workshop, programmed to last 2h. Contact me directly in case you run into any problems.
- Participants must have their own laptop with a valid internet connection;
- To minimize time wasting and avoid possible problems during the workshop, the participants are **strongly** advised to follow these requirements **prior** to the workshop date:

Installation

- Min HW Requirements: 64 bits operating system recommended and a minimum of 4GB RAM (8 GB preferred).
- Go to www.optflux.org and download the software - you will be redirected to OptFlux SourceForge page
- Download the **correct version for your computer architecture and operating system** (win32, win64, Mac, ...) - in windows, you can verify if your operating system is 32 or 64 bits by going to Control Panel -> System and Security -> System - if you install the wrong version, OptFlux will not work correctly (even if it's able to boot properly).
- Double-click the installation file and follow the installation steps.
- After the installation is done, start OptFlux. If updates are detected, make sure you perform them.
- Finally, restart OptFlux and everything should be ready.
- **[IMPORTANT - MAC USERS]**: for OSX El Capitan onwards (El Capitan, Sierra, High Sierra) with the introduction of the System Integrity Protection (SIP), OptFlux will not be able to work properly (even if it boots up). Please follow this tutorial for a workaround (**this is mandatory, OptFlux will be unusable otherwise**): https://sourceforge.net/p/optflux/support-requests/28/
- [OPTIONAL] – *If you have access to the CPLEX solver, this will greatly speed up OptFlux operations. Academic users have free access to CPLEX directly from IBM (if applicable, ask your supervisors for access).*
  A video tutorial on how to configure it in OptFlux is available here: https://vimeo.com/124835561

Test correct installation

1. Open OptFlux
2. Create a new Project (menu File -> New Project):
   - Set a project name (e.g.: "core") and select "OptFlux model repository"
   - Select the model: "Escherichia coli str. K12 substr. MG1655 / Ecoli core Model / 2010"
   - Select biomass equation: "R_Biomass_Ecoli_core_w_GAM"
3. Perform a simple wild-type simulation (menu simulation -> wild type -> ok)
4. If everything goes well and OptFlux does not throw any exception, everything should be okay for the workshop.

Synopsis

- Brief introduction to OptFlux
- Hands-on:
    - Model handling
        - Model formats;
        - Loading and exporting;
        - Model information/representation.
        - Loading, creating and exporting pathway layouts
    - Phenotype prediction / simulation
        - Wild-type prediction;
        - Mutant phenotype predictions and methods;
        - Flux Variability Analysis (FVA);
        - Solution robustness;
        - Maximum theoretical yields;
        - Defining and using environmental conditions;
    - Strain optimization
        - Configuration and execution;
        - Interpreting results