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OptFlux is a new platform aimed at being the reference computational tool for Metabolic Engineering (ME) applications. It allows the use of stoichiometric models of microbial metabolism for simulation and optimization purposes. ME deals with designing organisms with enhanced capabilities regarding the productivities of desired compounds. Different approaches have been used to aid in ME efforts taking available models of metabolism and mathematical tools and/or experimental data to identify metabolic bottlenecks or targets for genetic engineering. However, the rational design of microbial strains has been limited to the developers of the computational/mathematical techniques, since a platform that provides a user friendly interface to perform such tasks was not yet available.

To change this scenario, we introduce the *OptFlux*, whose main features are:

- Open-source – users can use the tool freely and invites the contribution of other researchers;
- User-friendly – facilitates its use by users with no/little background in modelling/informatics;
- Modular – facilitates the addition of new features;

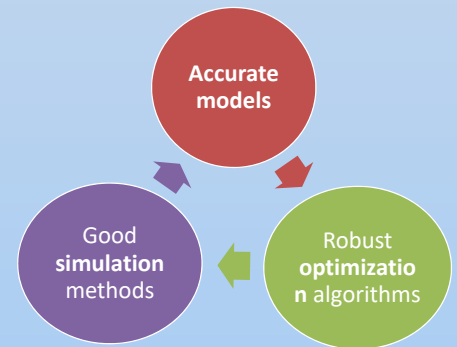
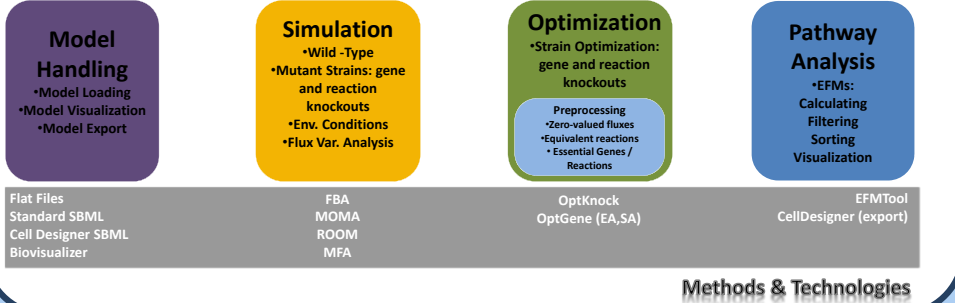
- Compatible with standards – compatibility with the Systems Biology Markup Language (SBML) and the layout information of CellDesigner.

Currently, the methods implemented for the simulation of wild-type or mutant strains are Flux Balance Analysis, Minimization of Metabolic Adjustment (MOMA), and Regulatory on/off Minimization of Metabolic flux changes (ROOM).

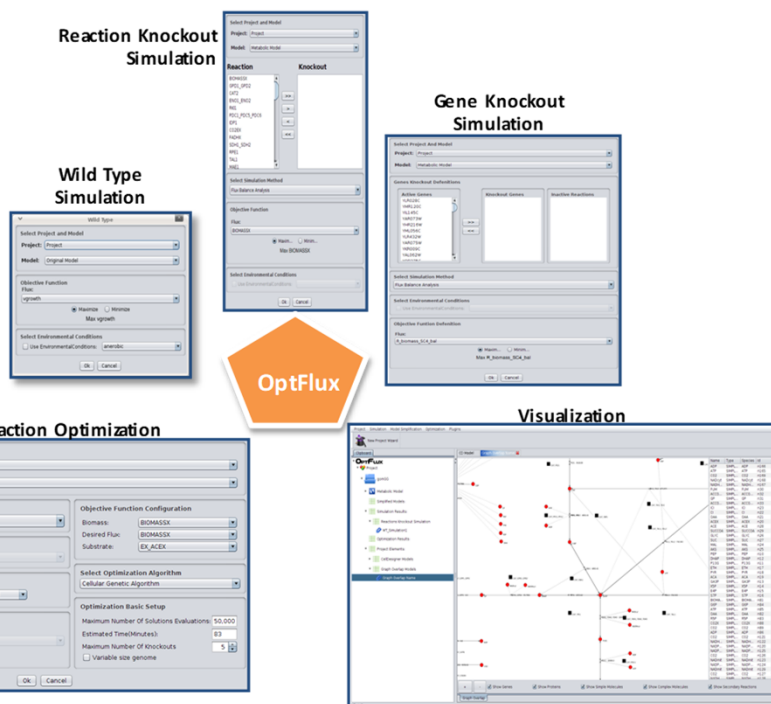
The optimization tasks, i.e., the identification of metabolic engineering targets can be performed with Evolutionary Algorithms or Simulated Annealing[1,2]. Furthermore, the software includes plug-ins to handle Elementary Flux Modes and Metabolic Flux Analysis.

The software is made available, together with other resources, in the home page: <http://www.optflux.org>.

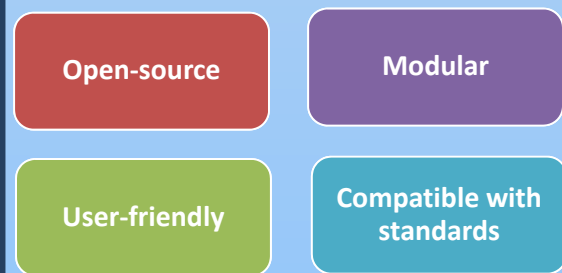
Functional Modules



Platform Overview



Main Features



Acknowledgments

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References

- [1] Patil, K.R. *et al.* (2005) Evolutionary programming as a platform for *in silico* metabolic engineering. *BMC Bioinformatics* 6
- [2] Rocha, M. *et al.* (2008) Natural computation meta-heuristics for the *in silico* optimization of microbial strains. *BMC Bioinformatics* 9, 499