

Software development of The Constraint-Based Reconstruction and Analysis Toolbox

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Project Goals: The aim of this project is to increase the robustness and enhance the stability of The Constraint-Based Reconstruction and Analysis Toolbox (The COBRA Toolbox). Since its release in 2011, The COBRA Toolbox v2.0 [1] is widely used for modeling, analysing and predicting a variety of metabolic phenotypes using genome-scale biochemical networks. Recently added new features include novel sampling algorithms, sparse optimisation code, new test functions and tools for integration of metabolomic data, to name a few. With an increasing number of contributions from developers around the world, the code base is evolving at a fast pace. In order to guarantee consistent, stable, and high quality code, the goal is to implement a continuous integration approach to development of The COBRA Toolbox.

The popularity of The COBRA Toolbox, its open-source nature, and the increasing number of collaborators bear the need for a continuous integration server. This automated environment ensure that every change in code, as minor as it may be, is fully tested before being released as part of a stable version. Each contribution is verified automatically, and for each code submission, a comprehensive test suite is run in order to detect bugs and integration errors before release. Consequently, the automated testing environment ensures higher quality code and the release of well tested computer code. The COBRA Toolbox provides researchers with a common high-level interface to a variety of optimization solvers, which allows users to easily select the most effective optimisation algorithm to solve genome-scale modeling problems. Within the continuous integration environment, the code is automatically run with multiple versions of MATLAB and several releases of the solvers, which guarantees its compatibility. The documentation is automatically deployed from the continuous integration server and generated based on the comments within the code. The code and the documentation are freely released as part of the openCOBRA project at github.com/opencobra/cobratoolbox.

References

- [1] Schellenberger J, Que R, Fleming RMT, Thiele I, Orth JD, et al. (2011) Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox v2.0. *Nature Protocols* 6: 1290–1307.

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