

# DistributedFBA.jl: High-level, high-performance flux balance analysis in Julia

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**Project Goals: Constraint-Based Reconstruction and Analysis (COBRA) [1] is a widely used approach for modeling genome-scale biochemical networks and integrative analysis of omics data in a network context. For kilo-scale models, flux variability analysis (FVA) can currently be performed efficiently using existing methods [2, 3, 4]. However, these implementations perform best when using only one computing node with a few cores, which becomes a temporal limiting factor when exploring the steady state solution space of larger models. Here, we exploit Julia [5], a high-level, high-performance dynamic programming language, to distribute sets of flux balance analysis problems and compare its performance to existing implementations.**

Flux balance analysis, and its variants, are widely used methods for predicting steady-state reaction rates in biochemical reaction networks. The exploration of high dimensional networks with such methods is currently hampered by software performance limitations. *DistributedFBA.jl* is a high-level, high-performance, open-source implementation of flux balance analysis in Julia. It is tailored to solve multiple flux balance analyses on a subset or all the reactions of large and huge-scale networks, on any number of threads or nodes. The code and benchmark data are freely available on [github.com/opencobra/COBRA.jl](https://github.com/opencobra/COBRA.jl). The documentation can be found at [opencobra.github.io/COBRA.jl](https://opencobra.github.io/COBRA.jl).

## References

- [1] Palsson BØ (2015) Systems Biology: Constraint-based Reconstruction and Analysis. Cambridge University Press, 1 edition.
- [2] Gudmundsson S, Thiele I (2010) Computationally efficient flux variability analysis. BMC Bioinformatics 11: 489.
- [3] Ebrahim A, Lerman JA, Palsson BO, Hyduke DR (2013) COBRApy: CONstraints-Based Reconstruction and Analysis for Python. BMC Systems Biology 7: 74.
- [4] 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.
- [5] Bezanson J, Edelman A, Karpinski S, Shah VB (2014) Julia: A Fresh Approach to Numerical Computing. arXiv:14111607 [cs] .

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