

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. The documentation can be found at opencobra.github.io/COBRA.jl.

References

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