Numerical Properties Of Stoichiometric Matrices

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Project URL: https://stanford.edu/group/SOL/multiscale/

Project Goals: This project aims at determining the numerical characteristics of stoichiometric matrices, identifying ill-scaled models requiring high precision computations, and drawing biologically inspired conclusions and determine possible avenues to accelerate Constraint-Based Reconstruction and Analysis computations for multiscale microbial communities.

Over the last 20 years, Constraint-Based Reconstruction and Analysis (COBRA) reconstructions gained considerably in complexity. A challenge, especially for huge scale networks and communities of organisms, is to accelerate related COBRA analyses using the COBRA Toolbox [1] or distributedFBA, part of COBRA.jl [2]. Knowledge of the numerical properties of the underlying metabolic network represented as the stoichiometric matrix is key to tackle this challenge. We present the numerical characteristics of the 773 microbial reconstructions [3], and link the properties to practical considerations in biology and scientific computing. It is shown that key numerical characteristics are correlated to inherent biological traits. Hints are provided to accelerate the analysis of large and huge-scale biochemical networks, especially for microbial community models.

References

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This work was supported by the U.S. Department of Energy, Offices of Advanced Scientific Computing Research and the Biological and Environmental Research as part of the Scientific Discovery Through Advanced Computing program, grant #DE-SC0010429, the National Centre of Excellence in Research, the Luxembourg National Research Fund (FNR) ATTRACT program grant (FNR/A12/01), and the Luxembourg National Research Fund (FNR) CORE program grant (C16/BM/11332722).