

Numerical Properties Of Stoichiometric Matrices

Laurent Heirendt¹, Sylvain Arreckx¹, Almut Heinken¹, Dmitry Ravcheev¹, Ines Thiele¹, and **Ronan M.T. Fleming**^{1*}(ronan.mt.fleming@gmail.com)

¹ Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Esch-sur-Alzette, Luxembourg

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

- [1] Laurent Heirendt, Sylvain Arreckx, Thomas Pfau, Sebastian N. Mendoza, Anne Richelle, Almut Heinken, Hulda S. Haraldsdottir, Sarah M. Keating, Vanja Vlasov, Jacek Wachowiak, Stefania Magnúsdóttir, Chiam Yu Ng, German Preciat, Alise Zagare, Siu H.J. Chan, Maike K. Aurich, Catherine M. Clancy, Jennifer Modamio, John T. Sauls, Alberto Noronha, Aarash Bordbar, Benjamin Cousins, Diana C. El Assal, Luis V. Valcarcel, Inigo Apaolaza, Susan Ghaderi, Masoud Ahookhosh, Marouen Ben Guebila, Andrejs Kostromins, Hoai M. Le, Ding Ma, Yuekai Sun, Lin Wang, James T. Yurkovich, Miguel A. P. Oliveira, Phan T. Vuong, Lemmer P. El Assal, Scott Hinton, William A. Bryant, Francisco J. Aragón Artacho, Francisco J. Planes, Egils Stalidzans, Alejandro Maass, Santosh Vempala, Michael Hucka, Michael A. Saunders, Costas D. Maranas, Nathan E. Lewis, Thomas Sauter, Bernhard O. Palsson, Ines Thiele, and Ronan M. T. Fleming. Creation and analysis of biochemical constraint-based models: the COBRA Toolbox v3.0. *Nature Protocols (accepted)*, 2018.
- [2] Laurent Heirendt, Ines Thiele, and Ronan M. T. Fleming. DistributedFBA.jl: high-level, high-performance flux balance analysis in Julia. *Bioinformatics*, 33(9):1421–1423, May 2017.
- [3] Stefania Magnúsdóttir, Almut Heinken, Laura Kutt, Dmitry A. Ravcheev, Eugen Bauer, Alberto Noronha, Kacy Greenhalgh, Christian Jäger, Joanna Baginska, Paul Wilmes, Ronan M. T. Fleming, and Ines Thiele. Generation of genome-scale metabolic reconstructions for 773 members of the human gut microbiota. *Nature Biotechnology*, 35(1):81–89, January 2017.

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).