Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression - DTU Orbit (11/01/2019)

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Constraint-Based Reconstruction and Analysis (COBRA) is currently the only methodology that permits integrated modeling of Metabolism and macromolecular Expression (ME) at genome-scale. Linear optimization computes steady-state flux solutions to ME models, but flux values are spread over many orders of magnitude. Data values also have greatly varying magnitudes. Standard double-precision solvers may return inaccurate solutions or report that no solution exists. Exact simplex solvers based on rational arithmetic require a near-optimal warm start to be practical on large problems (current ME models have 70,000 constraints and variables and will grow larger). We have developed a quadrupledprecision version of our linear and nonlinear optimizer MINOS, and a solution procedure (DQQ) involving Double and Quad MINOS that achieves reliability and efficiency for ME models and other challenging problems tested here. DQQ will enable extensive use of large linear and nonlinear models in systems biology and other applications involving multiscale data.

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