

Flux balance analysis of multi-scale biochemical reaction networks Yuekai Sun *, Ronan M.T. Fleming, Ines Thiele, Michael A. Saunders.

Biological processes, such as metabolism, signalling and macromolecular synthesis, can be modelled as large networks of biochemical reactions. Such network reconstructions of biological systems are inherently multi-scale because reaction rates can vary over many orders of magnitude. Larger, more comprehensive networks, like integrated networks that represent metabolism and macromolecular synthesis, require special methods for accurate analysis because naive use of off-the-shelf software packages can produce inaccurate or erroneously infeasible results. We describe techniques enabling off-the-shelf optimization software to compute accurate solutions to the poorly-scaled optimization problems arising from flux balance analysis of multi-scale biochemical reaction networks. We implement lifting techniques for flux balance analysis and demonstrate our techniques using the first integrated reconstruction of metabolism and macromolecular synthesis for *E. coli*. Our techniques enable accurate flux balance analysis of multi-scale networks using off-the-shelf optimization software. Although we describe lifting techniques in the context of flux balance analysis, our methods can be used to handle a variety of optimization problems arising from analysis of multi-scale network reconstructions.

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