

Abstract Submitted
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Regulatory schemes to achieve optimal flux partitioning in bacterial metabolism¹ LEI-HAN TANG, Department of Physics, Hong Kong Baptist University and Beijing Computational Science Research Center, ZHU YANG, Department of Physics, Hong Kong Baptist University, SHENG HUI, Department of Physics, UCSD, PAN-JUN KIM, APCTP, Korea, XUE-FEI LI, Department of Physics, Hong Kong Baptist University, TERENCE HWA, Department of Physics, UCSD — The flux balance analysis (FBA) offers a way to compute the optimal performance of a given metabolic network when the maximum incoming flux of nutrient molecules and other essential ingredients for biosynthesis are specified. Here we report a theoretical and computational analysis of the network structure and regulatory interactions in an *E. coli* cell. An automated scheme is devised to simplify the network topology and to enumerate the independent flux degrees of freedom. The network organization revealed by the scheme enables a detailed interpretation of the three layers of metabolic regulation known in the literature: i) independent transcriptional regulation of biosynthesis and salvage pathways to render the network tree-like under a given nutrient condition; ii) allosteric end-product inhibition of enzyme activity at entry points of synthesis pathways for metabolic flux partitioning according to consumption; iii) homeostasis of currency and carrier compounds to maintain sufficient supply of global commodities. Using the amino-acid synthesis pathways as an example, we show that the FBA result can be reproduced with suitable implementation of the three classes of regulatory interactions with literature evidence.

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