in silico simulation and analysis of microbial metabolism.\textsuperscript{1} SHENG HUI\textsuperscript{2}, SHENGHUA LIANG, LEI-HAN TANG, Department of Physics, Hong Kong Baptist University — Through evolution living organisms have developed an elaborate network of enzyme-facilitated reactions and transport to process and cycle biochemical compounds for cell growth. A majority of these reactions are unidirectional, yet the network allows an organism to live on a variety of carbon sources and synthesize a diverse set of compounds in varying amounts. We found that biosynthesis of the end products can proceed independently. In the three genome-wide in silico models examined, the optimal yield for simultaneous synthesis of two compounds is only about 3\% higher than what is achievable under separate production of individual compounds. In most cases, the residual correlation can be attributed to the requirement of energy, redox potential, or charge balance. These observations quantify, in the context of cellular metabolism, the bow-tie analogy which has been argued to provide a ubiquitous architecture for multi-input/multi-output networks.

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\textsuperscript{2}Present address: BioMaPS Institute, Rutgers University