Using mathematical methods to study complex biological networks

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Complex biological processes such as metabolism often involve thousands of compounds coupled by chemical reactions. These process chains are described by researchers as chemical reaction networks. Researchers from the University of Luxembourg have developed new mathematical methods to study the energetic properties of these networks. The scientists published their findings in the scientific journal *Physical Review X*.

The paper prepared by the research group of Prof Massimiliano Esposito investigates how very small biological systems work at the molecular level. These systems are subject to large fluctuations in mass, which make their behavior difficult to predict. In order to describe them, the researchers use a probabilistic approach that calculates the dynamics of these systems based on the statistical likelihood that changes will occur. Using these probabilistic descriptions, the group studies how these systems exchange energy and matter with their environment and how much energy they dissipate during these processes – a discipline known as stochastic thermodynamics. However, in the realm of complex chemical reaction networks, probabilistic descriptions become unfeasible since thousands of molecules are involved. The authors showed how the mathematical methods developed for small systems can be used to investigate these networks.

"Currently, rigorous thermodynamic models for this kind of network are lacking. Our work paves the way for thermodynamic characterizations of real chemical networks, such as metabolism," explains Riccardo Rao, the

main author of the paper. "We think of these networks as machines transforming some compounds into others. Some compounds are consumed as they 'fuel' the processes. Our description answers questions such as: Is this process efficient? How much energy does it dissipate? If we slightly tweak the system, how will it react?"

At the moment, their research focuses on models of metabolic networks, for which some simplifying approximations are required. "We are now using this framework to investigate specific classes of chemical reaction networks, such as metabolic networks," Riccardo Rao said. Also, the research team will work with biologists and chemists to test and apply the results to concrete biological systems. Research in this direction with groups from the Luxembourg Center for Systems Biomedicine is already ongoing.

More information: Riccardo Rao et al. Nonequilibrium Thermodynamics of Chemical Reaction Networks: Wisdom from Stochastic Thermodynamics, *Physical Review X* (2016). DOI: 10.1103/PhysRevX.6.041064

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