Challenges and Perspectives in Modeling Plant–Microbe Interactions

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Editorial Note

With the vast quantity of data being generated by high-throughput experimental techniques, new opportunities are arising to integrate theoretical and computational approaches with experiments. Potential synergies include designing hypothesis-driven experiments based on the results of modeled scenarios, or using modeling as a tool to mechanistically interpret the results of high-throughput experiments. In the bacterial field, there is currently a major initiative to integrate genomic sequencing data with computational modeling, in order to predict the function of individual bacterial strains and whole bacterial communities. Already, microbial engineering is a mature technology that exploits the power of computational modeling to optimize strains and communities for industrial processes like bioremediation and fermentation. Regarding the study of the rhizosphere microbiome, over the past 15 years this field has accumulated a huge volume of sequencing data, but these data are generally descriptive, and to date they have not been used to significantly further our mechanistic understanding of nutrient exchange processes in the rhizosphere. We see mathematical modeling as the most promising approach to bridge this gap, and in the following section we want to elucidate through examples the impact mathematical modeling can have for future improvement of rhizosphere interactions to boost plant growth.

One of the principal aims of mathematical models is the reduction of complexity in order to capture the fundamental principles behind the phenomena of interest. There is nowadays a positive trend in biology to develop predictive models of the system under study, with some disciplines at a more advanced stage than others in the integration of theory and experiments. The study of microbial communities is a clear illustrative example of a field where computational approaches are essential. While bioinformatics is instrumental to analyze high throughput data from meta-omics experiments, theoretical models are developed to gain mechanistic understanding of complex biological systems. Mathematical descriptions of population dynamics were pioneered in the 19th century by Verhulst's law of logistic growth and are now a fundamental part of ecology. In the same way, over the last five decades models of metabolism have started converging into sound mathematical methods to investigate cellular functions. It is also relevant to point out that another characteristic of mathematical models is that, as long as the described mechanism holds true, they can be easily generalized to different organisms. Therefore, as an example, a model originally built to describe bacteria might be also applied to other microbes.

Methods of Theoretical biology

Theoretical biology is a rapidly expanding field and it is nearly impossible to condense and classify it in few words, but we can roughly point out three main classes of methods: kinetic models, stochastic models, and network-based models. It is important to point out that depending on the system and phenomena under study, certain modeling techniques will be more suited than others. Kinetic models are dynamic and deterministic, typically constructed as systems of differential equations, solved nowadays with computational integration algorithms. These models can offer precise predictions but require either a priori knowledge or inference (e.g., through a fit to data) of the equation parameters. Typically, these models are well suited to describe small-scale metabolic pathways where most enzyme kinetic constants are measured and few parameters are reasonably constrained and then fit. Stochastic models encompass any representation that implements some random components with a Monte Carlo procedure and they are needed to capture effects like noise or individual variability.

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