

Modelling of eco-evolutionary dynamics in microbial communities with haploid evolutionary constructor

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Motivation and Aim: Being compact ecosystems of small organisms, microbial communities act as a brilliant trade-off between biological complexity and controllability. These communities exhibit significant range of essential life processes while providing broad opportunities to investigate different layers of their biological organization. Meanwhile, microorganisms are known for a rapid mutation rate and volatile genomes affected by such processes as horizontal gene transfer and loss of genetic material. Thus, microbial communities present a fascinating object for investigating eco-evolutionary dynamics.

Methods and Algorithms: “Haploid evolutionary constructor” (HEC), a software developed for the modelling of eco-evolutionary processes in microbial communities, considers the following levels of biological organization: genetic, metabolic, cellular, population, and ecological ones. It simulates both high-level (cellular chemotaxis and diffusion, substrates flow and diffusion) and low-level (mutations, horizontal gene transfer, gene regulation and metabolism) processes allowing combining various mathematical modeling approaches (agent-based modeling, differential equations, automata, etc.) in one model. HEC employs the concept of multi-layer modelling to integrate the models describing different biological levels into a unified modelling framework.

Results: Haploid evolutionary constructor modelling approach and simulation software package have been extended to describe eco-evolutionary dynamics in spatially structured environments more accurately. HEC has been used to address such problems as investigation of genetic variation in the models of populations inhabiting spatial environment of different structure, modelling of horizontal gene transfer between bacterial cells in changing environmental conditions [1], simulation of evolution of bacterial communities under phage infection [2], eco-evolutionary scenarios in self-organizing microbial communities [3], and competition of motile and sedentary bacterial populations in aquatic environments [4] among others.

Conclusion: Haploid evolutionary constructor modelling approach meets the challenge of the integration of cellular and population level models of microbial communities to get the knowledge of how population heterogeneity and complex behavior arises from the variation on individual level. Using multiscale data integration, including but not limited to multi-(meta-)omics data, as a foundation for such a research is essential for the further development in this field starting from the whole-cell models and up to a population level.

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