FitMultiCell: Simulating and parameterizing computational models of multi-scale and multi-cellular processes

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Abstract

Motivation Biological tissues are dynamic and highly organized. Multi-scale models are helpful tools to analyze and understand the processes determining tissue dynamics. These models usually depend on parameters that need to be inferred from experimental data to achieve a quantitative understanding, to predict the response to perturbations, and to evaluate competing hypotheses. However, even advanced inference approaches such as Approximate Bayesian Computation (ABC) are difficult to apply due to the computational complexity of the simulation of multi-scale models. Thus, there is a need for a scalable pipeline for modeling, simulating, and parameterizing multi-scale models of multi-cellular processes. Results Here, we present FitMultiCell, a computationally efficient and user-friendly open-source pipeline that can handle the full workflow of modeling, simulating, and parameterizing for multi-scale models of multi-cellular processes. The pipeline is modular and integrates the modeling and simulation tool Morpheus and the statistical inference tool pyABC. The easy integration of high-performance infrastructure allows to scale to computationally expensive problems. The introduction of a novel standard for the formulation of parameter inference problems for multi-scale models additionally ensures reproducibility and reusability. By applying the pipeline to multiple biological problems, we demonstrate its broad applicability, which will benefit in particular image-based systems biology. Availability FitMultiCell is available open-source at https://gitlab.com/fitmulticell/fit Supplementary data are available at https://doi.org/10.5281/zenodo.7646287