

iDynoMiCS 2: Fully flexible computer modelling platform for microbial ecology

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Abstract

The source code is publicly available to download from <https://github.com/roughhawkbit/iDynoMiCS-2>.

Author Summary

Introduction

Individual-based modelling of microbial communities is becoming ever more widespread as software is developed and computational power increases [1]. Drive for more generic software: checked by more people, so more reliable [2]; easier to compare different model formulations, i.e. structural sensitivity [3]. Software based on [4–6].

The original iDynoMiCS framework [5] has seen a rise in popularity and is now used by many research groups all over the world. Half a decade later, we have initiated a rigorous overhaul of the framework. This is done to address several evident limitations of the original package: Learning how to use iDynoMiCS can be challenging and multiple 3rd party tools are required to properly use the software, simulation protocols are sensitive to typographical errors and difficult to validate, it is not possible to simulate more than a single environment, it is difficult to combine agent types, only spherical agents can be modeled, agents can only interact with a single solute grid cell and it is not possible to evaluate processes at different timescales.

To address these issues the iDynoMiCS 2 framework has been developed. This overhauled version of iDynoMiCS allows the user construct a new and unique model by combining simple building blocks that govern the processes and behavior of the agents and their environment. The user can use the default building blocks or develop own building blocks which are easily to implement because of the modular structure and

provided Java interfaces. A graphical user interface has been developed to assist the user with the model construction. This lowers the complexity for new iDynoMiCS users and reduces the changes of creating a protocol with errors.

Models

The model description follows the ODD (Overview, Design concepts, Details) protocol [7, 8]. Further details are available in Supporting Information for some parts of the model description.

Purpose

Entities, state variables, and scales

Process overview and scheduling

Each compartment is self-contained. No interaction between compartments within a global time-step, all transfers are stored and happen instantly between timesteps.

Process managers have own timestep; Compartment manages the order in which they are executed.

Design concepts

The iDynoMiCS 2 structure inherits many concepts from previous packages [4, 5], but also builds on these.

Basic principles

Emergence

Adaptation Agents may use species library for defaults, but overwrite these due to mutation, etc. Behaviours ("events") may depend on values of other local aspects.

Objectives

Learning

Prediction

Sensing

Interaction

Stochasticity

Collectives

Observation

Explanation

Other...? 50

Initialization 51

Native protocol file layout, but (hopefully!) able to read in other formats such as SBML [10] and CellML [11]. 52
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Input 54

Using input from external sources (data files or other models): there is potential to make a process manager that could handle this, but none are currently implemented. 55
56
Coupling with a fluid-flow package would be great. 57

Submodels 58

? 59

Results 60

Case study: agent force functions 61

Case study: filamentous organism and multi-grid-cell agents 62

Discussion 63

Ease of comparison Since iDynoMiCS 2 already adopts the hybrid approach to modelling (discrete) cells in (continuous) concentration fields, it is straightforward from a design perspective to instead treat cells as a continuum. This "retrofit" allows easy comparison of the hybrid IbM approach with more traditional population-based approaches [9] for the same system. Such calibration is already used often, but implementing this feature is, to our knowledge, the first time it has been offered *within a single software package*. 64
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66
67
68
69
70

Modularity Aids customisability 71

Supporting Information 72

Acknowledgements 73

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