

# 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 3<sup>rd</sup> party tools are required use the software fully, simulation protocols are sensitive to typographical errors and difficult to validate, it is not possible to simulate more than a single environment at once, it is difficult to combine agent types, only spherical agents can be modelled, agents can only interact with a single solute grid voxel 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 behaviour of the agents and their environment. The user can use the default building blocks or develop their own; these are easily to implement thanks to the modular structure and provided Java

interfaces. A graphical user interface (GUI) has been developed to assist the user with model construction. This lowers the complexity for new iDynoMiCS users and reduces the chances 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

iDynoMiCS 2 is a software package with the capacity to model a wide range of systems in microbial ecology and, as such, this article does not set out to answer a specific question. Case studies are presented in the Results section which illustrate the power and flexibility of iDynoMiCS 2, but the purpose of iDynoMiCS 2 extends far beyond the questions they set out to answer.

## Entities, state variables, and scales

A simulation is composed of compartments, self-contained units of

## 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

<b>Interaction</b>	The exact nature of interactions between agents is the choice of the user, but we here highlight two common interactions.	51
	Cell-cell mechanics.	52
	Competition over resources.	53
	Other potential interactions include: communication via diffusible signals (quorum sensing), conjugation of plasmids, and phage predation.	54
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<b>Stochasticity</b>	Prevent synchronisation in division times.	57
<b>Collectives</b>	Biofilms, granules, etc, should be emergent rather than defined by the user.	58
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<b>Observation</b>	Can output simulation/compartment states as XML, as SVG, etc. GUI visualisation allows real-time observation.	60
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<b>Explanation</b>		62
<b>Other...?</b>		63
<b>Initialization</b>		64
	Native protocol file layout, but (hopefully!) able to read in other formats such as SBML [9] and CellML [10].	65
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<b>Input</b>		67
	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.	68
	Coupling with a fluid-flow package would be great.	69
		70
<b>Submodels</b>		71
	?	72
<b>Results</b>		73
<b>Case study: agent force functions</b>		74
<b>Case study: filamentous organism and multi-grid-cell agents</b>		75
<b>Discussion</b>		76
<b>Ease of comparison</b>	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 [11] 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 <i>within a single software package</i> .	77
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<b>Modularity</b>	Aids customisability	84
	Isolation of sub-models facilitates robustness analysis [12,13]	85

## Supporting Information

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## Acknowledgements

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