The perks of agent-based modelling with iDynoMiCS 2

Cockx, Bastiaan; Clegg, Robert J.; Lang, Stefan; Smets, Barth F.; Kreft, JanUlrich

Publication date:
2016

Document Version
Publisher's PDF, also known as Version of record

The perks of agent-based modelling with iDynoMiCS 2

Bastiaan J R Cockx*, Robert J Clegg, Stefan Lang, Barth F Smets, Jan-Ulrich Kreft
*Department of Environmental Engineering, Technical University of Denmark, Bygningstorvet 115, 2800 Kgs. Lyngby, Denmark, baco@env.dtu.dk

Introduction

In microbiology subtle differences can have a big impact. Both external effects such as local environmental gradients and internal effects such as stochasticity in gene expression levels may cause individual microbes of the same species to be in an entirely different physiological state. Also when comparing different species, small differences may tip the balance and favor one or the other microbial species, this effect may result in an entirely different community structure. In many cases a single outlier, such as one cell with a higher substrate affinity due to a mutation, can completely change the outcome of a modelled system. In such a scenario a model description based on averages (mean field) is not sufficient. Agent-based models (ABMs) can account for these effects. Any agent will act individually following a simple set of rules, responding to their local environment and all agents are represented as separate entities within the model. From the simple behavior of all individuals the structure and behavior of the community emerges.

Methods

The basic principles and methodology of microbial agent-based models are generally very similar:

- The computational domain typically has distinct size, shape and boundaries.
- The domain is discretized and so are all environmental gradients such as solute concentration, pH and temperature. This data is represented as a discretized grid within the domain.
- Solute concentrations and other environmental parameters may change over time in each grid cell due to diffusive or convective transport with neighboring grid cells as well as spontaneous reactions or reactions catalyzed by agents in the grid cell.
- Agents are represented as discrete entities, often with simple sphere or rod shaped morphologies. Agents can interact with their local environment by converting solutes, attracting or repelling neighboring agents or by attaching to surfaces.
- Time is discretized and the modelled processes are evaluated in a sequential fashion (Fig. 1)

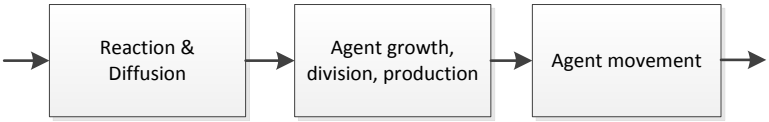

Figure 1: simplified representation of sequential processes as modelled in a single ABM time step.

The iDynoMiCS framework

Even though the structure and approaches used in ABMs are very similar, many research groups develop their own code. Developing this code separately takes a lot of resources from these groups and makes it difficult to compare models. In order to tackle these issues a collaborative project called iDynoMiCS was started (Lardon *et al*, 2011). The iDynoMiCS framework 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 iDynoMiCS: Learning how to use iDynoMiCS can be challenging and multiple 3th party tools are required to properly use the software, simulation protocols are sensitive to typos and difficult to validate, it is not possible to simulate more than 1 environment, it is difficult to combine agent types, only spherical agents can be modelled, agents can only interact with a single grid cell and it is not possible to evaluate processes at different timescales. To address these issues

we have developed the iDynoMiCS 2 framework. Because of its modular structure (Fig. 2) iDynoMiCS 2 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. A user interface has been developed to assist the user with the mode construction. This lowers the complexity for new iDynoMiCS users and reduces the changes of creating a protocol with errors.

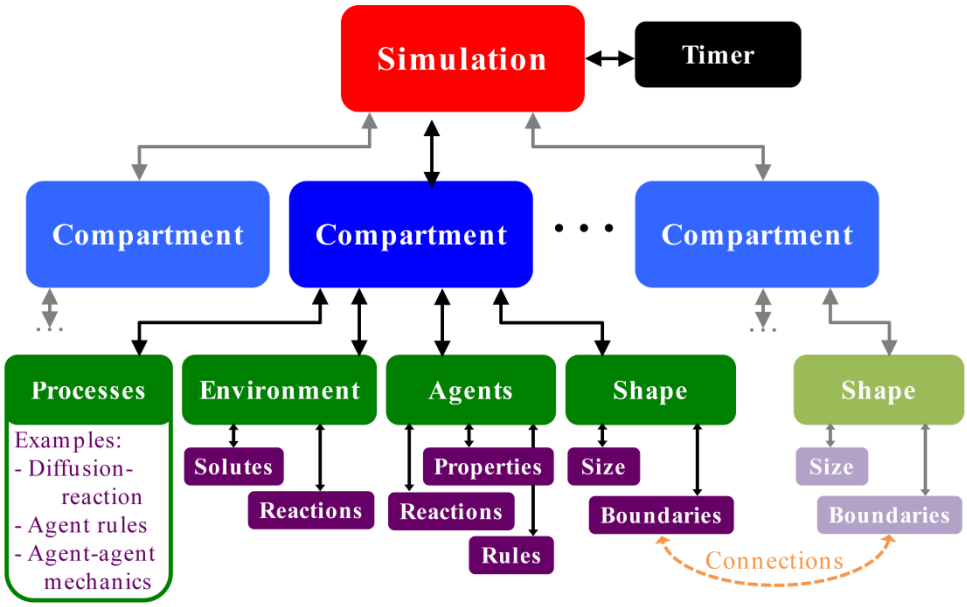

Figure 2: The general structure of iDynoMiCS 2. Each compartment has four main components: the shape of the computational domain (this includes size, dimensions, and any boundaries), an environment container (this holds any dissolved solutes modelled as continuous concentration fields), an agent container (this holds any agents modelled as discrete particles) and the processes that occur within the compartment, each process can be performed at a different timescale and the process sequence is determined by occurrence and priority.

Results and conclusions

With a case study (Fig. 3) we show how iDynoMiCS 2 can be used to study the effects of individual parameters on community development and can be used to answer relevant ecological questions in a fraction of the time that would be needed to answer these questions with an experimental approach.

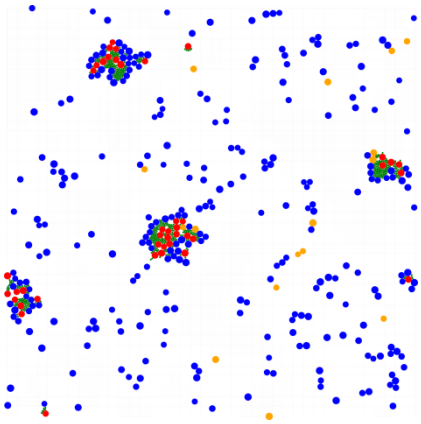

Figure 3: The benefit of aggregation. Blue agents consume solute A, red and orange agents are inhibited by solute A and consume solute B. Red agents also produce EPS particles (green) with strong attachment properties, at a metabolic cost. The blue agents can lower the local inhibitor concentration to sub-inhibitory levels and growth of the inhibited agent is enabled when blue agents are incorporated in the formed aggregates.

References:

Lardon *et al* (2011) *Environmental Microbiology* **13**: 2416-2434