Individual-Based Modelling: an essential tool for Microbiology.

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THE ROLE OF IbM IN MICROBIOLOGY

Individual-based Modelling (IbM) and further simulation of the models have proven to be a very useful tool in the study of biological communities (Grimm, 1999. *Ecol. Model.* 115, 129-148). Increasing computer power and detailed experimental data coming from -omic studies allow the resurgence of modelling and simulation of microbial communities. Modelling of microbial systems can be a useful tool in microbiology.

REALITY

Microorganisms play a central role in every ecosystem and in the global biomass cycle. Hornerdevine MC. et al, 2004. *Proc. Roy. Soc. Lon. B. Bio.* 271, 113-122.

Microbial communities are complex systems hardly explained by reduction. Laboratory and field experiments with microorganisms are costly and often unfeasible. Nearly 99% of the known microbial species have not yet been successfully cultured *in vitro*. Sharma et al., 2005. *Curr. Sci. India* 89, 72-76.

Microbiology has proven its practical applicability in many fields: food industry, medicine, environmentalism and biotechnology, among others. Maloy and Schaechter, 2006. *Int. Microbiol.* 9,1-7

IbM SIMULATIONS

Bottom-up approaches to real systems. Rules apply to individuals and the outcoming behaviour of statistical systems is studied.

- Construe experimental data.
- Suggest new experiments.

- Isolate processes and reduce complexity at will.
- Suggest new questions.

CHECK THE SET RELATIONS REALITY-THEORY

THEORY

Theoretical approach to real systems consists on building coherent models with descriptive and predictive capacity. Microbiology tackles microorganisms through different approaches.

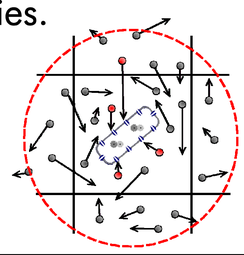
- Molecular level of description: chemical reaction kinetics, transport phenomena, etc. Seymour et al., 2004. *Phis. Rev. Let.* 93, 198103.

- Cellular level: metabolism and physiology, systems biology, cellular interactions, etc. O'Malley and Dupre, 2005. *Bioassays* 27, 1270-1276.

- Macroscopic level: whole system behaviour, population dynamics, microbial ecology. Bernaerts et al., 2004. *J. Food Protect.* 67, 2041-2052.

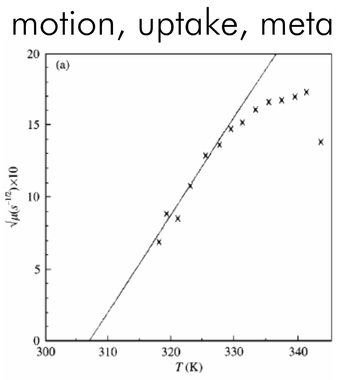
SOME EXAMPLES OF IbM APPLIED TO MICROBIAL SYSTEMS

INDISIM is a modelling tool designed from Molecular Dynamics' methodology and used to study microbial communities. Bermúdez et al., 1989. *Cabios 305-312*



PROKARYOTIC CELLS Ginovart et al., 2002. *J. Theor. Biol.* 214, 305-319.

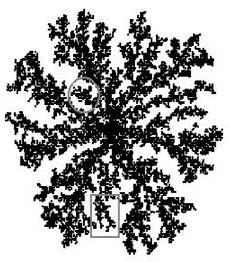
An Individual-based Model for simulating the growth and behaviour of bacterial communities was first developed. It rules individual motion, uptake, metabolism and reproduction. It studies the relation between the colony and its macroscopic constraints.



☜ Observed behaviour of the bacterial growth rate with temperature. Ratkowsky et al., 1983. *J. Bacteriol.* 154, 1222-1226.

Emergent Behaviours

A mechanistic and local definition of temperature at an individual level results on a global behaviour that reproduces the Ratkowsky observations.



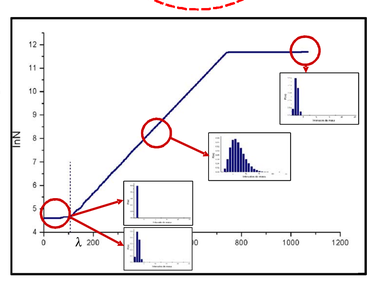
☜ Pattern formation obtained by computer simulations of a bacterial colony. Ginovart et al., 2002. *Physica A* 305, 604-618.

Spatial Complexity

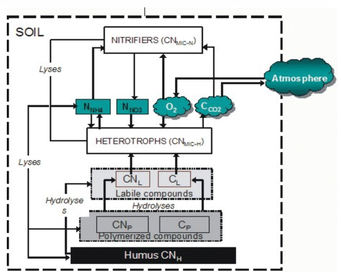
Different colony patterns are reproduced by changing the inoculation conditions and the nutrient distribution.

Temporal Complexity

The evolution of the biomass distribution provides useful information for tackling the microscopic causes of the bacterial lag phase.



Biomass distributions at different moments of the culture growth: lag, exponential and stationary. ☜ Prats et al., 2006. *J. Theor. Biol.* 241, 939-953.



Structural Complexity

An increase in the complexity of either the biological or the spatial model provides a tool to study more complexity covers improving the model for individuals and modelling ecosystems and communities with many species.

☜ Sketch of a model with many different microbial species and several sources of nutrient. Ginovart et al., 2005. *Nonlinear Anal. Real World Appl.* 6, 773-795.

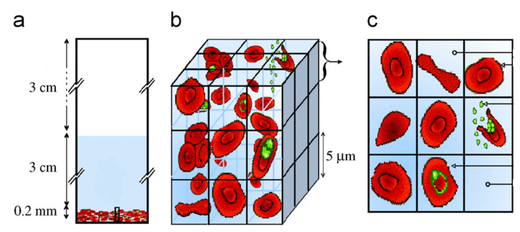
EUKARYOTIC CELLS

Models for eukaryotic cells deal with individuals with higher complexity. A couple of examples of published models are presented below:

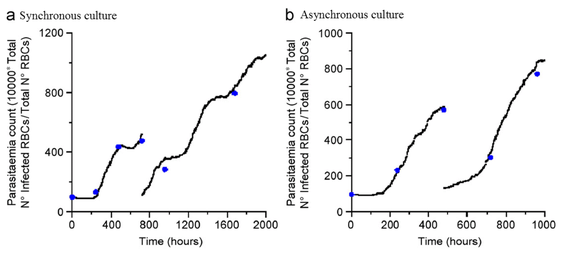
P. falciparum infected Red Blood Cells *in vitro* cultures

Ferrer et al., 2007. J. *Theor. Biol., in press.*

The model reproduces the propagation of the parasite through the henatocrit layer in a static culture of red blood cells. It tackles the effect of transport phenomena and macroscopic constraints on the evolution of the infection.



☜ Depiction of the model.

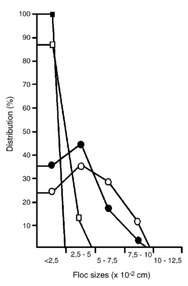


Results: • Experimental data · Simulation outcomes

Flocculation in brewing yeasts

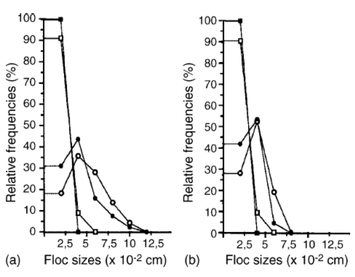
Ginovart et al., 2006. *BioSystems 83, 51-55.*

The model was used to compare two published theoretical mechanisms for flocculation of brewing yeasts at an individual level. The second one fits better to experimental data.



☜ Experimental data from: Brohan and McLoughlin, 1984 , *Appl. Microbiol. Biotechnol. 20, 16-22.*

Compared to simulation outcomes from: a) addition model, and b) cascade model for yeast flocculation. ☜



CONCLUSION: Individual-based Models are a useful tool in microbiology. They provide holistic understanding of the system under scope and fulfill requirements for specific practical applications.

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