WORKSHOP BIOCONNECT

Introduction to mathematical modeling tools for microbial interactions A digital toolbox



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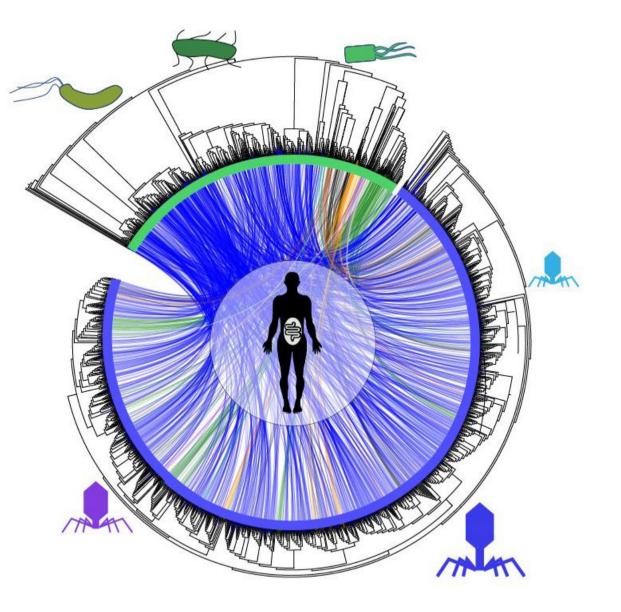
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1. Definition and Goals

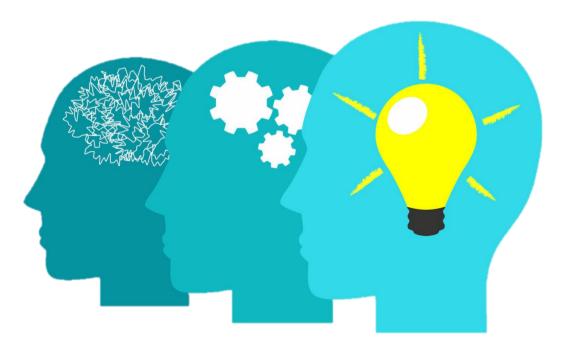
2. Methodology

- 3. Theoretical approach
- 4. Stochastic approach
- 5. Conclusions



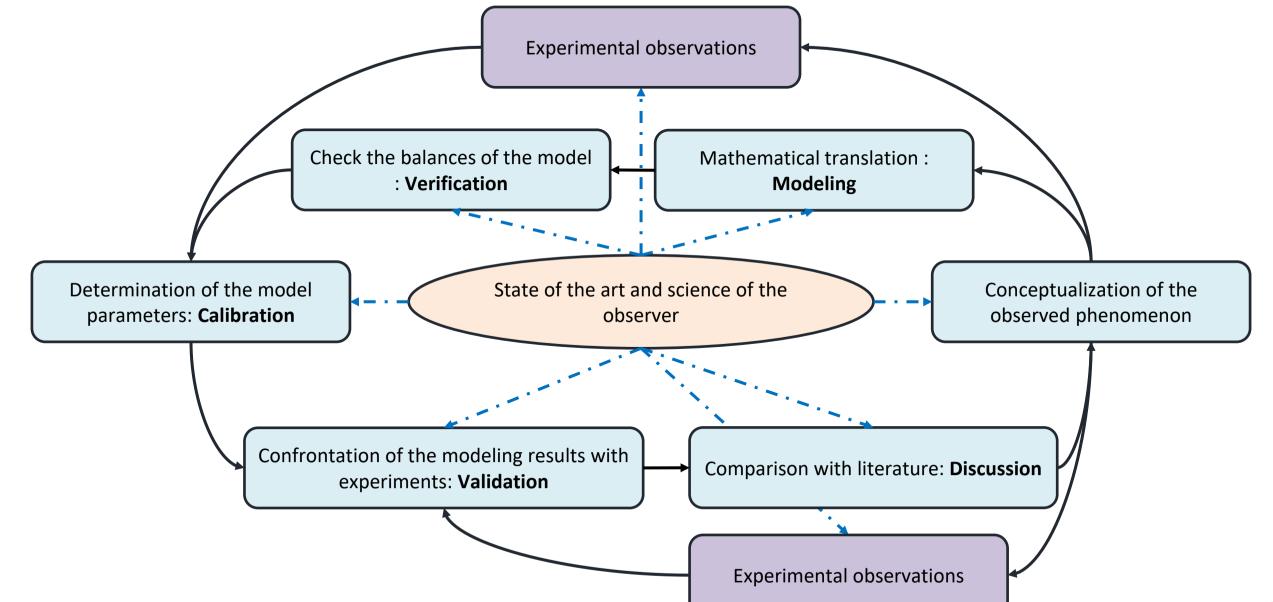
What is modeling ?

- Represents the biological kinetics and physical behavior
- Main goals :
- > Quantifying and simulate a system
- > Understanding of the phenomenon
- > Prediction and Control tools





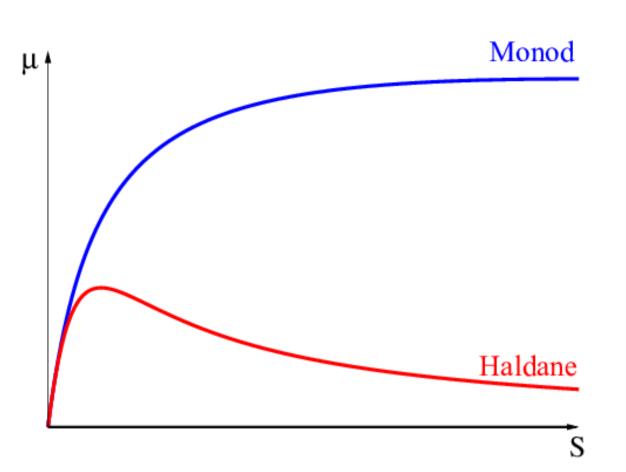
Modeling methodology



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Biological kinetics modeling

- First order kinetics
- Very easy to implement
- No consideration of inhibition phenomena
- Monod kinetics
- growth limiting factor
- Haldane kinetics
- Inhibition parameter
- Units : mol.g_{DW}⁻¹ / COD.g_{DW}⁻¹





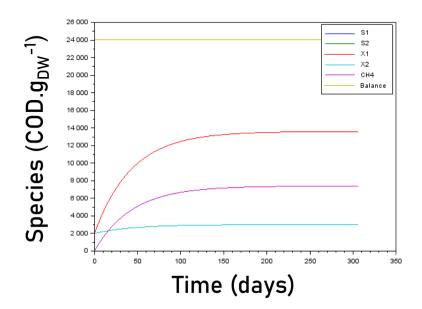
Example: biomass population modeling

- Anaerobic digestion modeling in a cow stomach
- Acidogenesis

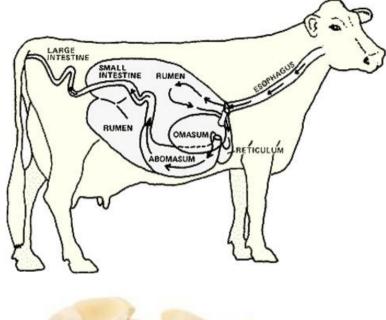
$$S_1 \xrightarrow{r_1} Y_{X1} X_1 + (1 - Y_{X1}) S_2$$

Methanogenesis

$$S_2 \xrightarrow{r_2} Y_{X2} X_2 + (1 - Y_{X2}) CH_4$$



$$\frac{dX_1}{dt} = Y_{X1}r_1(t) \text{ Monod kinetics}$$
$$\frac{dX_2}{dt} = Y_{X2}r_2(t) \text{ Haldane kinetics}$$



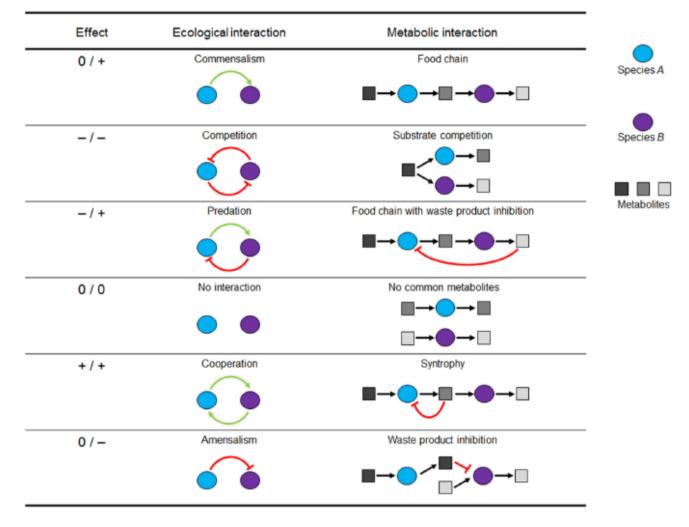
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Interactions and physical behavior

- Physico-chemical balances
- Ecological interactions
- Metabolic interactions
- Hydrodynamics
- Biomass mortality

• Etc.



Theoretical approaches in a brief



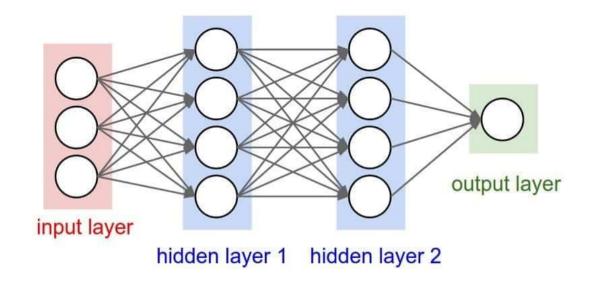
- Efficient in understanding the phenomenon
- Good tool to simulate and monitoring the phenomenon studied

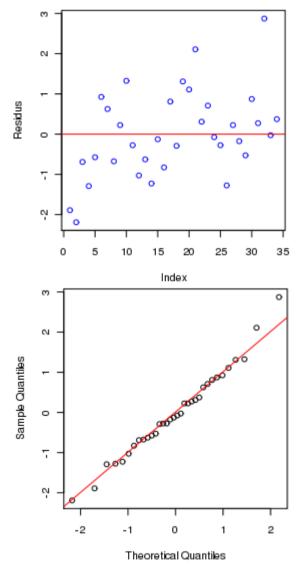


- Modeling could be very complex
- Sometimes kinetics parameters are not identifiables

Stochastic approaches

- Describe the random variations of the studied phenomena
- Numerous modeling are used in the literature
 - Linear modeling (linear regression, analysis of variance)
 - Non-linear modeling (GAM, neural networks)

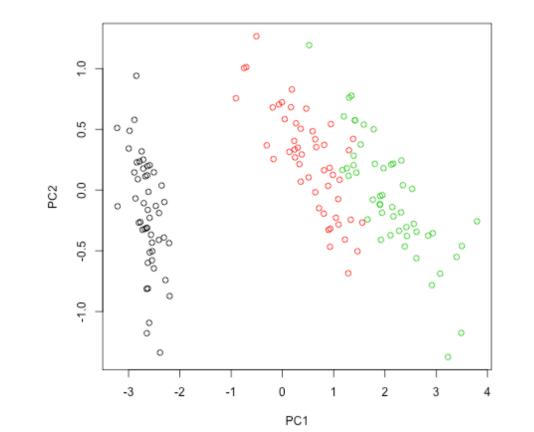






- Ensure there is no unnecessary or redundant variables
- Identify links and correlations between variables
- Different methods :
 - Principal component analysis (PCA)
 - Multiple correspondances analysis (MCA)
 - Etc.

Data analysis





Stochastic approaches in a brief



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- Provides robust and repeatable results
- It is not necessary to have a deep understanding of the phenomenon
- Data analysis provides supplementary contents for scientific studies



- It could be difficult to link results and understanding
- Data cleansing and analysis are unavoidable preliminary steps
- The data set must be large enough to have significant results

Conclusions

- A vector of potential for research and industry
- Actually modeling is a choice between understanding and robustness
- One of the main challenges of tomorrow is the marriage between theoretical and stochastic methods to describe complex phenomena with great results and understanding of the phenomenon

Thank you for your attention

