

Chapter IX

Modelling and Simulation of Biological Systems

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ABSTRACT

It is unanimously accepted that a theoretical approach of a system or phenomenon reveals new features and offers a deeper insight into the intimate mechanisms. In life science, this approach is mainly based on mathematical modeling, followed naturally by computer simulation. The chapter presented here tries to give the reader a comprehensive view over the main issues arising when attempting to build models of biological systems. A series of applications is shortly presented. The second half of the chapter is dedicated to one of the most interesting models: protein synthesis regulation. The example follows the classical steps: the scheme of the processes to be described, the set of differential equations and the results, including their possible interpretation.

INTRODUCTION

Mathematical modelling proved to be a useful research tool, offering an elegant and simple description of a system (Ingram & Bloch, 1984). The computer's advent stimulated its use also in complex systems, like biomedical systems (Garfinkel, 1965). There are several ways to approach a formal description of biological systems, yielding several types of models (Brown & Rothery, 1993, Fishwick & Luker, 1991). We can classify the models from various

viewpoints (Mihalas, Lungeanu, Kigyosi, & Vemic, 1995):

- a. A system's structure
 - Continuous models
 - Discrete models
- b. An input-output relationship
 - Deterministic models (subdivided into analytical models and models based on differential equations)
 - Stochastic models

- c. A modeled feature
 - Models for structure
 - Models for function

BUILDING MATHEMATICAL MODELS OF BIOLOGICAL SYSTEMS

There are several typical steps followed for building mathematical models (Keen & Spain, 1992).

- Defining and delimiting the system and the process to be modelled
- Selecting the variables, both independent and dependent variables
- Establishing the relations between the variables
- Defining the input and output
- Setting initial conditions and the values of parameters and constants
- Choosing the results representation
- Establishing the validation mode

APPLICATIONS IN BIOMEDICAL RESEARCH

The results of a simulation are usually presented as a graphical plot representing the system evolution over time; the experimental conditions are represented by a set of input parameters.

There are several possible applications of mathematical models and their corresponding simulation programs in biomedical research (Mihalas, 1998).

- **Experimental Design:** The system behaviour for various values of input parameters is analyzed, letting us choose the best set of parameters corresponding to

the experimental conditions that yield measurable results.

- **Testing Hypotheses:** Sometimes there are no direct experimental procedures to test two different hypotheses concerning a certain phenomenon or process; in this case, we can simulate a system's behaviour under the two conditions and compare the simulation output with the real behaviour.
- **Determining Parameters:** For the parameters that are not (easily) accessible by direct measurements, we can simulate the process for a wide range of values of the studied parameter. By comparing the results with the real experimental behaviour, we can estimate the parameter.
- **Prognosis:** It is one of the largest applications and lets us analyze possible system evolution.
- **Feeling the Phenomenon:** A better understanding of the process is achieved when a system's behaviour is analyzed over several conditions.
- **Didactic Applications:** These are used for educational purposes.

AN EXAMPLE: COMPUTER SIMULATION OF PROTEIN-SYNTHESIS REGULATION

Delimiting the System and the Process

The system is represented by a reduced (simplified) cell (Mihalas, Niculescu-Duvaz, & Simon, 1985). We take into account only three components (Figure 1).

- A DNA sequence on which we can distinguish two genes: the synthesis gene (SG) and the control gene (C)

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