Computational Biophysics

1: Introduction to Python (1 week):

– Introduction to the Python language; Ipython
– Python for scientific computing
– Basic data analysis with Python

2: Modeling processes in networks. Ecology and epidemiology. (3 weeks)

– Introduction to networks. Motivation and mathematical definitions
– Analyzing networks with python modules. Watts-Strogatz and Barabasi-Albert models.
– Models in ecology. Population dynamics. Chaos and controlling chaos.
– Individual-based modeling. The Gillespie algorithm.
– Models in epidemiology. SIS and SIR models.

3: Non-extended dynamical systems. Genetic networks (4 weeks)

–System biology. Introduction to ODE's. Fixed points and nullclines.
–Slaving and freezing conditions. Applications to cell reactions.
–Stability and bifurcations. Decisions in cell genetic networks.
–Limit cycles. Delays and nonlinearities. Application to cell metabolism.
–Stochastic modeling: Random number generator. Application to cell signaling.

4: Spatially extended systems. Pattern formation in biology (4 weeks)

–Introduction to Pattern formation: Linear Stability and Amplitude Equations.
–Reaction-diffusion systems. Morphogenesis and the Turing Mechanism.
–Reaction-diffusion-advection systems. Bioconvection
–Pseudo-Spectral methods. The Swift-Hohenberg Equation.
–Patterns in the Brain: Neural fields.

5: Seminar series on complex modeling (1 week)

–Modeling self-organization in biology (Dr. Sergio Alonso).
–Modeling infectious diseases (Dra. Clara Prats).

Methodology:

The course will be centered in code-implementation classes and its theoretical and biological interpretation. Six different hands-in will be ordered related with the codes done in class. Besides the normal classes, a few seminars showing examples of different types of modeling in biology will be given. A personal laptop every two students will be very handy.

Project:

All students should pair to reproduce, understand, explain and work on a biophysical model. A set of different projects with the explanation of the biophysical model to be developed will be listed in Atenea. One of these projects will be assigned to each group according to interests. At the end of the semester, every pair of students will hand a working code and an explanation related with the project. A formal examination of the simulations performed by the group will be held. The possibility to do an extended project with a very strong biological context will be available upon demand.

Project tutors:

Clara Prats, and Sergio Alonso

Instructors:

Enric Alvarez-Lacalle (coordinator) , Romualdo Pastor, and Antonio J. Pons

Exams and grading policy:

The students' evaluation will consist on grading the work done in class and at home through handed-in homework (HE), and the formal evaluation of the project (PE). There will not be a mid-term exam nor a final exam. The final mark will be given by:

$$0.6*HE+0.4*PE$$

Bibliography:

Basic:

–Brian P. Ingalls *Mathematical Modeling in Systems Biology*

–Paul Gries, Jennifer Campbell, Jason Montojo *Practical Programming (Python), 2nd Edition, T*he Pragmatic Bookshelf, 2013

–A. Barrat, M Barthélemy, A. Vespignani. *Dynamical Processes on Complex Networks*

–M. Cross, H. Greenside. *Pattern Formation and Dynamics in Nonequilibrium Systems,* 1st Edition, Cambridge University Press, 2009

Complementary:

–Y. Vodovotz, and G. An *Systems biology: mathematical modeling and model analysis*

–M. Walhout, M Vidal, and J. Dekker. *Handbook of system biology. Concepts and insight*

–F. Brauer and C. Castillo-Chavez. *Mathematical models in population biology and epidemiology*

–J.D. Murray. *Mathematical Biology I: An Introduction,* 3rd Edition, Springer-Verlag, 2013

– J.D. Murray. *Mathematical Biology II: Spatial Models and Biomedical Applications,* 3rd Edition, Springer-Verlag, 2013