

Complex Systems modelling in Ecology: emergent diseases and climate change

1 Introduction

The most unique feature of Earth is the existence of life, and the most extraordinary feature of life is its diversity, with approximately 9 million types of live beings [1]. This huge biodiversity sustains the overall proper functioning of ecosystems [2], which ultimately provides humankind with air to breathe and food to eat. Unfortunately, the diversity of life on Earth is dramatically diminishing [3–5]. Nowadays, wildlife extinction rates are estimated to be much higher than before, and up to 50% of higher taxonomic groups are already critically endangered [6]. The main drivers of such global biodiversity loss were defined in the Millennium Ecosystem Assessment [7], including several biological and climatic factors such as emergent diseases and climate change. Wildlife emergent diseases threaten global biodiversity by potentially producing catastrophic declines in new and not adapted host populations. Furthermore, if the diseases become endemic, initial depopulation may be followed by chronic population depression, which could even lead to local extinction [8]. On the other hand, climate change may be a major threat to global biodiversity in the next 100 years [9–14], with predictions for species loss ranging from as low as 0% to as high as 54% [13]. Overall, many species and ecosystems are already threatened by emerging diseases and climate change, so that urgent intervention is needed for their conservation.

Mathematical and computational modelling in ecology have been recently recognised as some of the most powerful approaches to guide empirical work and provide a framework for synthesis, analysis, development of conservation plans and policy making [15–17]. The most important feature of these approaches is possibility of performing quantitative estimations that can be relatively easily contrasted. This allows to address fundamental questions to enrich the understanding of ecosystem functioning [18]. Moreover, the quantitative nature of these models allows to perform precise estimations of the future development of the system. For instance, if the effect of temperature in the system under study is included in the model, predictions of its evolution over different climate change scenarios can be carried out. Altogether, mathematical and computational models allow to simulate realistic situations and test different conservation plans previous to its implementation in natural systems.

In this project we aim to study some threatened species and ecosystems by emergent diseases and climate change from the perspective of mathematical and computational ecology. In particular, the following following topics will be covered:

- **The Mass Mortality Event of *Pinna nobilis***

The parasite *H. pinnae* is responsible for the Mass Mortality Event of the pen-shell *Pinna nobilis* [19, 20], an endemic filter-feeder bivalve of the Mediterranean sea. The first mortality events occurred in September 2016 in southeastern Spain [21], and has since spread to all Spanish Mediterranean coasts, reaching France, Italy, Greece, Cyprus and other Mediterranean countries in less than two years [22]. To date, data indicate that the protozoan species is specific to *P. nobilis*, without affecting other invertebrates, including the congener species *P. rudis* [19]. The prevalence and consequent subsequent mortality reaches almost 100% in infected populations, an unprecedented figure given the precedents of similar epidemics in commercial bivalve species [23, 24]. Follow-up of the event has helped to better understand the spread of the disease, with surface currents being the main factor influencing local dispersal, while disease expression appears to be closely related to temperatures above 13.5 C and salinity between 36.5 and 39.7 psu [20]. This phenomenon has mainly affected the coastal ecosystems of the eastern Mediterranean Sea [21], introducing a serious risk of extinction of the species [22].

- **Diseases produced by *Xylella fastidiosa***

The bacterium *Xylella fastidiosa* (Xf) [25], is native to the Americas, where it causes vector-borne diseases such as those produced in many economically important crops, such as vineyards, citrus, almond, coffee and olive trees [26, 27]. Xf is phylogenetically subdivided into three formally recognized subspecies: *fastidiosa*, *multiplex* and *pauca*, originally from Central America, North America and South America, respectively [28, 29]. Since 2013, several standard sequences of the three subspecies associated mainly with crop and ornamental plants have been detected in Europe [30–32]; among these, the clonal lineage (ST1 / ST2) of the subsp. *fastidiosa* responsible for the well-known diseases “Pierce Disease” (PD) [33] and “Almond Leaf Scorch Disease” (ALSD) [34]. The epidemic situation is especially delicate in Mallorca, where the disease is widespread in almond and vineyard plantations, affecting 81% of almonds [35] and more than 23 grape varieties [36]. To date, xylem-sap feeder insects, such as sharpshooters leafhoppers and spittlebugs appear to be the main epidemiological relevant vectors ¹ for Xf-related diseases [36–38], being *Philaenus spumarius* and *Neophilaenus campestris* the main relevant vectors in Europe.

- ***Posidonia oceanica* meadows**

Posidonia oceanica is an endemic seagrass of the Mediterranean sea that forms the dominant ecosystem on its coastline. Posidonia meadows have an enormous ecological, economic and social importance, protecting the beaches from erosion, improving water quality, giving life support to numerous species, absorbing CO₂, etc [39]. Nowadays, given its high sensitivity to temperature changes, this species is in decline in many areas of the Mediterranean [40, 41]. In addition, *P. oceanica* coexists in the bed with *Cymodocea nodosa*, another marine plant with greater tolerance to high temperatures. In a climate change context, the competition between both species will play a key role in how coastal marine ecosystems will change in the near future.

- **Coral reefs**

Coral reefs are one of the most biodiverse ecosystems in Earth, holding more than 25% of marine life with only 1% of ocean floor coverage [42]. Corals are colonies of live organisms called polyps, held together by a self-produced exoskeleton made of calcium carbonate. Polyps host photosynthetic microalgae in a mutualistic interaction: polyps obtain nutrients from microalgae while microalgae are compensated with protection and some nutrients too [43]. Consequences of global change, such as temperature increases and ocean acidification, represent a substantial threat to coral reef ecosystems [44]. High ocean temperatures promote the “bleaching” phenomenon, in which individual polyps expel the microalgae symbionts, losing their characteristic color and getting rid of their primary source of nutrients [45]. On the other hand, ocean acidification promotes the dissolution of the calcium carbonate exoskeleton of corals [46].

2 Objectives

The general objective of the thesis is to study different threatened species and ecosystems through the lens of mathematical and computational ecology. Specifically, we can identify four main specific objectives each corresponding to the study of one particular species or ecosystem:

1. Develop mathematical and computational models to describe the Mass Mortality Event of *Pinna nobilis* at different spatial scales, explicitly modelling the parasite population and addressing the effect of its mobility.
2. Develop mathematical and computational models to describe the different diseases produced by *Xylella fastidiosa*, explicitly modelling the vector population and addressing the effect of its mobility.
3. Develop AI-based models to monitor the extent and health of *Posidonia oceanica* meadows. Develop computational tools to perform large scale measures of different meadow properties.

¹In epidemiology, a vector is the organism responsible for disease transmission.

4. Develop computational tools to obtain worldwide measures of coral reefs features, such as the atoll size distribution, the typical inter-atoll distance, etc. Develop basic models of reef formation explaining the observed measures.
5. Study the effect of temperature in the systems under study. Perform predictions of their evolution under climate change scenarios.

3 Methodology

3.1 General methodology

Throughout the project, several training, dissemination and collaboration activities will be performed continuously. To do so, we will apply the following methodology:

- Constant revision of literature relevant to the different research topics of the project.
- Publication of articles in indexed journals.
- Attendance to IFSC seminars and talks.
- Research group meetings.
- Meetings with collaborators.
- Contribution as speaker in IFSC seminars and talks.
- Attendance and contribution (both oral talks and posters) in national and international congresses, workshops, summer schools and symposia.

3.2 Specific methodology

In order to achieve the proposed objectives we will apply the following specific methodology

1. Develop mathematical and computational models to describe the Mass Mortality Event of *Pinna nobilis* at different spatial scales, explicitly modelling the parasite population and addressing the effect of its spatial diffusion.

In order to develop our epidemic model we will apply the following considerations. First, invertebrate organisms such as pen-shells do not have an immune system with memory, so they can become infected again if they overcome a first infection [47]. Second, infected pen-shells excrete parasites through the respiratory and excretory systems. In general, this excretion process depends on many factors: the proliferation/reproduction rate of parasites, the mortality rate of the parasite within the pen-shell (which could be different from the mortality rate in the external environment), some type of excretion efficiency, etc. In addition, the population of parasites excreted would also depend on the current population of parasites within the infected pen-shell, which may change over time. However, we will consider that the evolution of the parasite within infected individuals occurs on a much faster time scale than the excretion process itself, so the population of parasites within infected pen-shell is constant. Thus, we consider that all the subprocesses within the infected pen-shell are in a steady state and finally the excretion process is given by an effective rate. Third, we consider that parasites only reproduce within infected pen-shells, and not alone in the aquatic environment. Finally, although the parasite develops different phases (unicellular, bicellular, plasmodium and spore) [19] these will not be considered in a first model. Following these considerations we will construct a compartmental model with 4 variables: S, pen-shell susceptible to infection; I, infected pen-shell; R, dead pen-shell and P, referring to the parasite population in water. The first version of the mathematical model will be a system of differential equations, deterministic, being an adaptation of the models presented by Anderson and May [48]. The model will be analysed analytically in depth (fixed points, conserved quantities, approximations, etc.) and will be accompanied by a numerical characterisation.

The second version of our epidemic model will be stochastic, built from master equations [49], and both analytical and computational treatment will be performed. Numerical simulations will be performed according to the well-known Gillespie method [50], which allows Monte Carlo simulations of master equations. As for the analytical analysis of the model, the effect of parasite mobility on disease incidence and outbreak probability will be quantified. The model will allow to study the influence of the distribution of the hosts in the development of the disease, so that it will be possible to design optimal strategies for the conservation of the species.

Studies on mass mortality in pen-hell populations throughout the Mediterranean Sea have recently been published, showing the serious situation of this species [20, 22]. With the collaboration of some of these authors, such as Dra. Iris Hendriks (IMEDEA) or Dr. J.R. García-March (IMEDMAR), with whom we are already in contact, will use the data from these and possibly future articles to adjust our epidemic model. Data will be grouped according to salinity and temperature conditions to include the effect of these variables in the study. The fit of the deterministic model of differential equations will be given by a minimisation of the sum of the mean square error (*least squares method*) [51].

2. Develop mathematical and computational models to describe the different diseases produced by *Xylella fastidiosa*, explicitly modelling the vector population and addressing the effect of its mobility.

In order to develop the models for Xf diseases the following assumptions will be taken into account. First, the disease is transmitted by xylem-sap feeder vectors, e.g. the insects *Philaenus spumarius* and *Neophilaenus campestris* in Europe [36, 52]. Second, infected hosts show a latent (asymptomatic) period and cannot recover naturally from infection, [26, 34, 36, 53–57]. Third, latent periods do not need to be considered for vectors [58]². Fourth, European vectors have an annual life cycle [59] in which they cannot recover from the infection [59, 60]. Following these considerations, four compartments will be considered by the hosts: susceptible (S), exposed (E), infected (I), dead (R) while only two for vectors, susceptible (S_v) and infected (I_v). Analogous to the previous point, an individual-based stochastic model will be developed in order to study the effect of the spatial distribution of the hosts and the mobility of the vectors on the development of the disease. The models will be analysed analytically in depth (fixed points, conserved quantities, approximations, etc.) and numerically characterised. Then, it will be validated with experimental data of incidence in the Balearic Islands [34] following a Bayesian approach.

Furthermore, we will explore the effect of temperature to the development of one specific disease caused by Xf in vines, Pierce’s Disease (PD). Experimental data from Xf inoculations in vine plants will be used to correlate the accumulated temperature with the probability that the inoculations will infect the plant prevalently. The so-called *winter curing* [61] will be modelled by correlating the accumulation of temperatures below a threshold (cold temperatures) with the probability that an infection is not prevalent. The transmission of disease from infected plants to healthy ones will be modelled following a SIR scheme [62]. The model will be validated / calibrated using PD prevalence data in the United States and, once validated/calibrated, will be predicted globally, with special reference to the most important wine areas. For temperature-related calculations, the ERA5-Land reanalysis [63] database will be used, with a resolution of 0.1° , and data from some weather stations in Mallorca. The ROC [64] curve method will be used to validate the model.

This goal will be carried out with the collaboration of Mr. Eduardo Moralejo (TRAGSA, Palma de Mallorca), Dr. Alberto Fereres and Dr. José Ramasco (IFISC-CSIC, UIB campus), with whom we are already in contact.

²Vectors acquire the bacterium while feeding on infected trees. The bacterium then multiplies in the anterior cavity of the vector, which is external to its body and, for this reason, can be re-transmitted immediately without latency during subsequent feeds.

- 3. Develop AI-based models to monitor the extent and health of *Posidonia oceanica* meadows. Develop computational tools to perform large scale measures of different meadow properties such as its spatial extension, cluster distribution, death rate, etc.**

The availability of multi-spectral satellite images opens the possibility to perform a large-scale mapping of different seagrasses species, such as *Posidonia oceanica* or *Cymodocea nodosa*, in an efficient manner and at a low cost. We will train AI models like Artificial Neural Networks (ANN) to classify different species of seagrass based on their particular spectral signature, this is, the particular way each seagrass reflects light, which is captured by satellites. The ground truth data (needed to train this kind of unsupervised machine learning models) will come from the ATLAS POSIDONIA project from the Balearic Islands [65]. We will explore different hyper-spectral satellite image sources such as WorldView (1.6 m resolution but expensive) or Planet (~ 3 m resolution with some availability for academic institutions), comparing the accuracy of the model when using each image.

Once the AI model is completed, we will develop computational tools to obtain large-scale measures of these meadows, such as its total spatial coverage and density, cluster distribution, etc. Furthermore, applying the model to a set of images from different years, we will track the evolution of the classified seagrass meadows through time. In addition, we will correlate the obtained results with the evolution of sea surface temperature in the study sites, which will allow to study the effect of temperature into these seagrasses and perform predictions of their evolution under different climate change scenarios.

This goal will be carried out with the collaboration of different scientists such as Dr. Tomàs Sintès, Dr. Damià Gomila and Dr. Nuria Marbà

- 4. Develop computational tools to obtain worldwide measures of coral reefs features, such as the atoll size distribution, the typical inter-atoll distance, etc. Develop basic models that reproduce the measured features to understand the fundamental processes of reef formation.**

We will develop computational tools to obtain worldwide measures of coral reefs, such as the atoll size distribution or typical inter-atoll distance. Once the measures are done, we will develop basic models that reproduce these measures. This will allow to understand the most fundamental processes driving reef formation.

This goal will be carried out with the collaboration of other scientists such as Dr. Carlos M. Duarte.

- 5. Study the effect of temperature in the systems under study. Perform predictions of their evolution under climate change scenarios.**

As already commented in some of the points above, a general objective of the project is to include the effect of temperature in the systems under study. This will allow to perform qualitative and quantitative estimations of the future development of these systems under different climate change scenarios.

This goal will be done in collaboration with other scientists such as Dr. José M. Gutiérrez (IFCA).

We are already in contact with the scientists mentioned in the different objectives of this section and, indeed, some results are already published [66–68].

4 Timeline

Objective	1st year				2nd year				3rd year				4th year			
1.	X	X	X	X	X	X										
2.				X	X	X	X	X	X	X						
3.							X	X	X	X	X	X	X			
4.										X	X	X	X	X	X	X
5.					X	X	X	X	X	X	X	X	X	X	X	X

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