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## 1. Title: Deep process-based learning networks in Biodiversity research

**Duration of the sabbatical:** 6 months

**Research Institute:**

Institute for Cross-Disciplinary Physics and Complex Systems

[https : //ifisc.uib – csic.es/en/](https://ifisc.uib-csic.es/en/)

Mallorca, Spain.

## 2. Summary

We are in a enthralling scientific era. We have the computer power, the open-source tools, the know-how in many highly specialized fields and the team capabilities to integrate Earth science and Biodiversity research in open and decentralized automated research platforms. We are in a period where novel analytical methods and data are being fused at an incredible speed to decipher the complexity and feedbacks between the Earth system and the diversity of life. Yet, we are in a massive human-driven biodiversity extinction with large uncertain consequences for Earth climate, life conditions and the stability of Earth (Figure 1). This combination of an enthralling scientific era and rapid global change put us in an edge to team up to go beyond our disciplinary boundaries to contrast scenarios accounting for feedbacks between the Earth system and Biodiversity (Figure 2). For this to happen we need to connect fundamental and applied science (Figure 3.) One way to do it is throughout distributed and open research platforms to provide information for management forums in applied conservation and sustainability centers. During my sabbatical I will team up with researchers at different institutions to develop a distributed open-source and automated research platform to integrate multiple databases into contrasting Biodiversity scenarios and function decline taking into account the interdependencies among levels and scales in ecological and evolutionary networks (Box 1 and Figures 3 and 4).

## 3. Milestones

**M1** Submission proposal “Distributed open-source automated research platform (*ROBHOOT*)”  
FETOPEN-EU Challenging Current Thinking

Deadlines: September 2019 and March 2020)

Team:

Switzerland (SDSC, Christine Choirat, and EAWAG (Carlos Melian))

Spain, IFISC (Victor Eguiluz)

Estonia, U. Tartu (Raul Vicente)

**M2** Working prototype of a distributed open-source automated research platform based in Box 1 and Figure 4 of this proposal

Deadline: end of the sabbatical.

#### 4. Deep process-based learning networks in Biodiversity research

Specialization has produced an immense gain in detailed knowledge at each of the levels and scales studied in Biodiversity research. Yet, the information gained and the data obtained in specialized fields are not sufficiently integrated to understand the consequences of biodiversity decline in predicting the outcome of feedbacks between Bio-

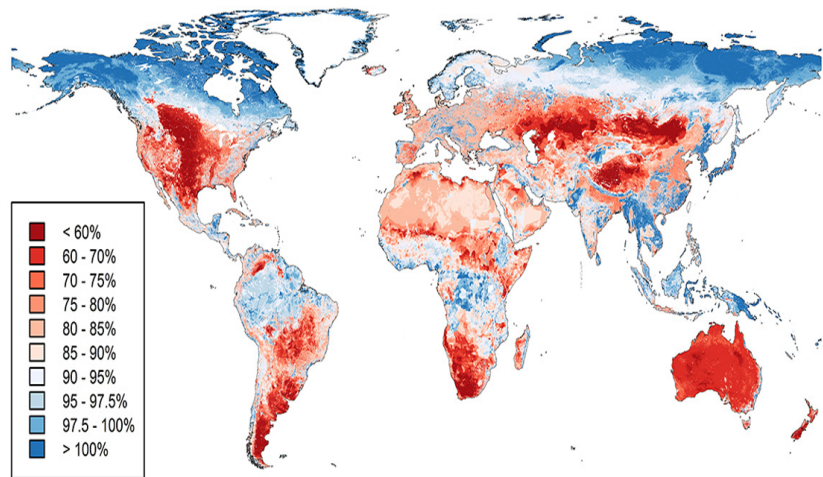


Figure 1: **Biodiversity is declining globally at unprecedented rates.** Map showing the remaining populations of native species across many taxa as a percentage of their original populations. Blue areas are within proposed safe limits, and red areas are beyond these limits. For further information please check the original work at <http://www.nhm.ac.uk/discover/news/2016/july/biodiversity-breaching-diversity-and-Earth-safe-limits-worldwide.html>.

system. Despite

the development of automated research platforms integrating different aspects of the scientific cycle is rapidly advancing<sup>1</sup> distributed open-source automated research platforms in Biodiversity research are still at a very incipient stage.

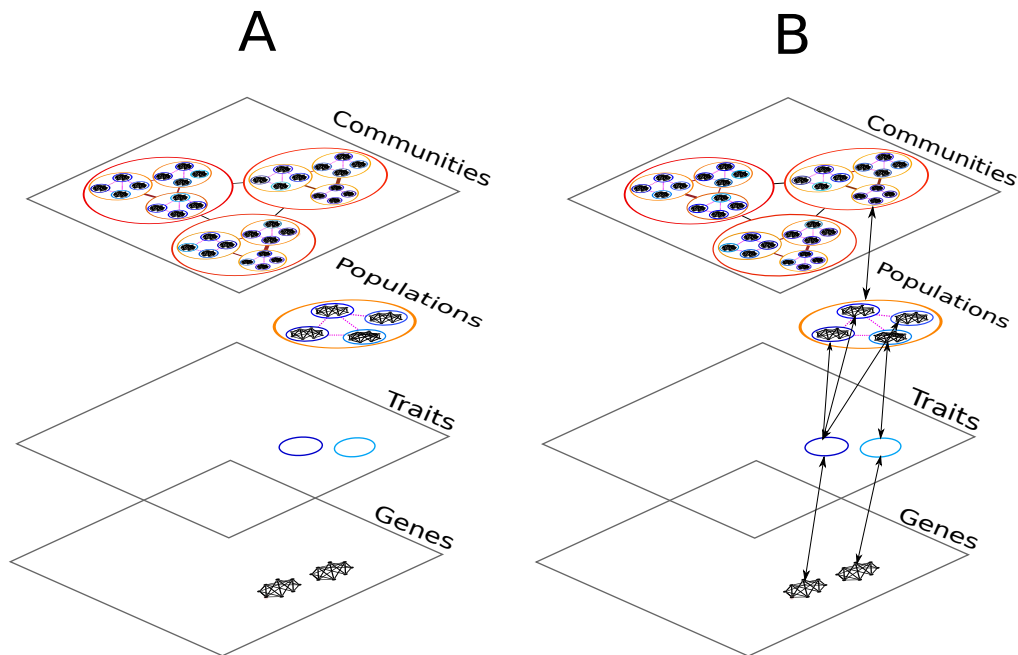
One of the reasons of still being at a very incipient stage is because most methods in data science and Biodiversity research have been considered classically as distinct fields. However, the current scientific ecosystem is at the stage where merging methods from distinct fields is radically transforming the discipline boundaries, the reproducibility of science and our predicting-understanding power<sup>2</sup>. Many of the recent approaches applying deep learning methods in ecology and evolution have mostly focused at one level of biological organization<sup>3</sup>. While this might produce additional gain in detailed knowledge at each level, it remains unknown how many layers are going to be needed for predicting the consequences of feedbacks between the Earth system and Biodiversity.

<sup>1</sup>This is by no means an exhaustive list but it gives an indication of the many projects taking place: NakamotoT, BigQuery, Automated statistician, Modulos, Google AI, Iriseaseml

<sup>2</sup>Reichstein, M., Camps-Valls, G., Stevens, B., Jung, M., Denzler, J., Carvalhais, N., and Prabhat (2019). Deep learning and process understanding for data-driven Earth system science. *Nature*. 566:195-204.

<sup>3</sup>Sheehan, S., Song, Y. S., (2016). Deep learning for population genetic inference. *PLoS Comput. Biol.* 12:e10048452.

The one-level and one-scale approach might be insufficient to understand the consequences of biodiversity decline in predicting the outcome of feedbacks between Earth system and the diversity of life. To gain predictive and understanding power in biodiversity research we are going to need to merge distinct databses into hybrid deep process-based learning methods accounting for many layers and the topology of the interactions within and between the layers<sup>4</sup>. Many methods from data science and biological systems share fundamental properties (i.e., network-like patterns, multiple layers, etc). Yet the full potential of these shared properties have not been sufficiently explored. Biological systems are composed by many layers, and they can contain interdependent hierarchies and feedbacks with interacting learning entities within and between the layers (Figure 2). We will integrate different biological layers into a platform to explore contrasting scenarios of Biodiversity dynamics accounting for interdependencies and feedbacks within and between layers (Box 1 and Figures 3 and 4).



**Figure 2: Biodiversity is hierarchically structured** yet inferring interdependencies among the levels developing hybrid deep-process based learning approaches to predict the consequences of biodiversity decline remains poorly studied. A) Biodiversity has been studied mostly considering independent levels, from genes, traits and populations to communities and ecological networks. B)

<sup>4</sup>Melián, C. J.; Matthews, B.; de Andreazzi, C. S.; Rodríguez, J. P.; Harmon, L. J.; Fortuna, M. A. (2018) Deciphering the interdependence between ecological and evolutionary networks, *Trends in Ecology and Evolution*, 33:504-512.

Biodiversity represented as interdependent levels accounting for feedbacks from genes and traits, and from traits and populations to communities. It remains unknown which of these two scenarios best predict current trends in Biodiversity decline and its consequences for Earth climate, life conditions and the stability of Earth.

### **Box 1. Deep process-based learning networks in Biodiversity research**

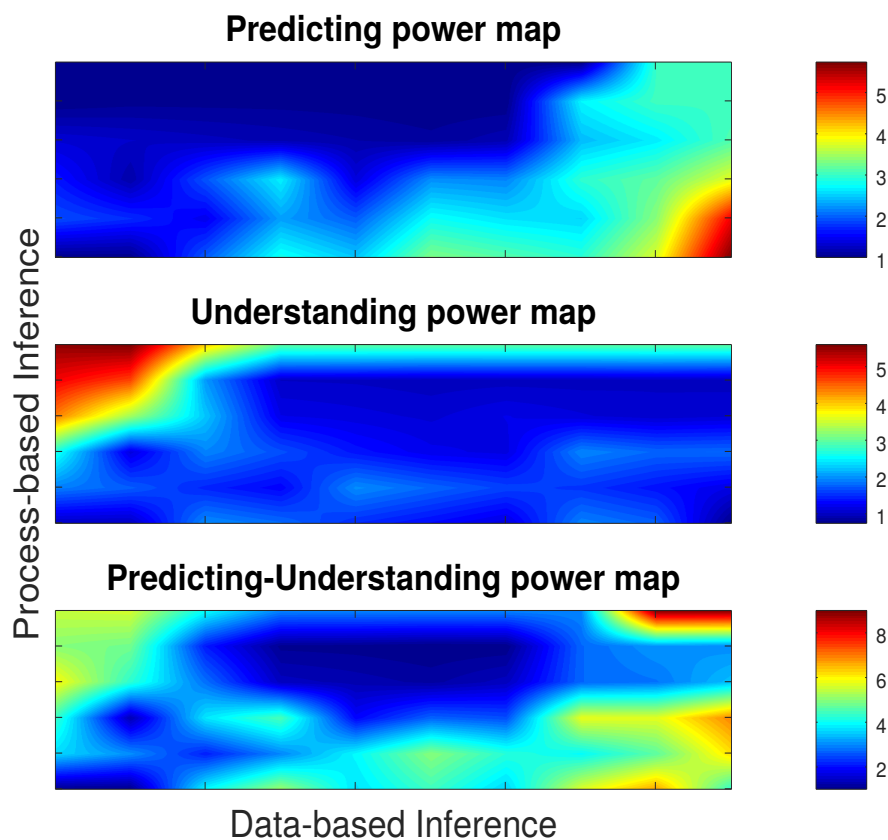
We will implement a multilayer approach to generate process-based species distribution maps accounting for interdependent biological networks. Each layer will be parametrized taking advantage from the integration of biodiversity datasets. Most data in biodiversity are collections of small data. In areas such as species ranges and species interactions, there is a large amount of data, but only a relatively small amount of data for each gene, phenotype, individual or trophic interaction. To customize predictions accounting for interdependent biological levels we will use a formalism considering the heterogeneity at individual level, with its inherent uncertainties, and to couple the individual level together in a hierarchy scaling from genes to phenotypes, populations, communities and species ranges, so that information can be borrowed from other similar levels across the landscape in the absence of empirical estimations. We will implement a multilayer approach using hierarchical Bayesian neural networks<sup>a</sup>. The outputs of the multilayer approach will generate a biodiversity distribution map for many interacting species that can be evaluated against the empirical patterns.

We will contrast two scenarios to explore the best one fitting the empirical patterns. The first scenario will simulate independent levels considering modularity within- and between-layers (i.e., a highly modular pleiotropy matrix determining the genotype-phenotype map and a highly modular within- and between-species interactions with most interactions weak or zero across the landscape.) Such scenario will produce a non- or weakly-interactive species biodiversity map. The second scenario will account for feedbacks among layers. We will explore a range of topologies from bidirectional recurrent neural networks (BRNN) to feedforward neural networks (FNN) and reinforcement learning in unknown and fluctuating environments (RL)<sup>b</sup>. Such scenario will produce an (strongly)-interactive species biodiversity map. We will disturb both scenarios following random and non-random disturbance regimes (i.e., removing specific interactions, abundances and habitats) and will quantify responses to disturbances using a variety of metrics, from biodiversity to functional metrics<sup>c</sup>.

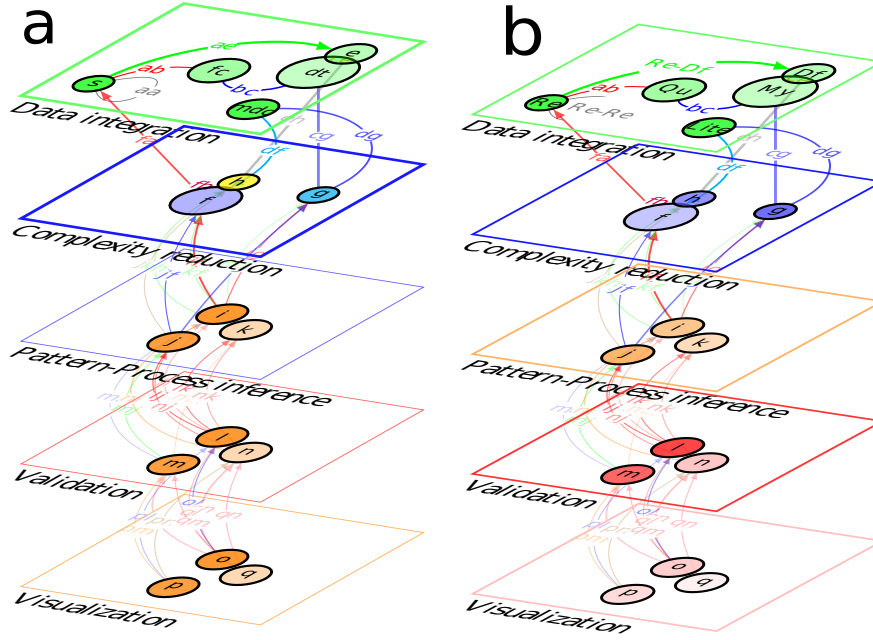
<sup>a</sup>Ghahramani, Z. (2015). Probabilistic machine learning and artificial intelligence. *Nature*. 521:452-459

<sup>b</sup>Schmidhuber, J. (2015). Deep learning in neural networks: An overview. *Neural Networks*, 61:85-117

<sup>c</sup>Melián, C. J.; Matthews, B.; de Andreazzi, C. S.; Rodríguez, J. P.; Harmon, L. J.; Fortuna, M. A. (2018) Deciphering the interdependence between ecological and evolutionary networks, *Trends in Ecology and Evolution*, 33:504-512.



**Figure 3: Prediction and understanding power map.** This figure shows a cartoon of a prediction power map (top), an understanding power map (middle), and a predicting-understanding power map (bottom). x- and y-axis represent data-based inference (i.e., gradient of AI methods from low (left) to high (right) predictive power) and process-based inference (i.e., gradient of process-based methods from low (bottom left) to high (top left) understanding power). The gradient of predicting power map (top) shows a hot spot red area in the bottom right highlighting the region where AI methods best predict the empirical data. The gradient of understanding power map (middle) shows a hot spot red area in the top left highlighting the region where the best mechanistic understanding occurs. The predicting-understanding power map (bottom) shows the sum of the two previous maps highlighting a red hot spot where the best synthesis research joining predicting and understanding power of the empirical data might occur.



**Figure 4: Prototyping a distributed and open automated research platform:** a) Our initial prototype will contain five layers (this is not an exhaustive number. Some might be merged and others, like reporting generation, can be introduced): Data Integration, Complexity reduction, Pattern-process inference, Validation, and Visualization. Nodes and links represent algorithms and interactions between two algorithms, respectively. The inter-layer interactions will be implemented using the Renku-SDSC platform<sup>5</sup>. The intra-layer interactions will be developed initially in julia language (other languages will come into play during the development of each layer). b) A julia-computing-language prototype of an automated research platform. Nodes and links in each layer represent julia packages and interactions between two packages, respectively. The figure shows the julia packages to be used for the Data integration layer containing the packages "Retriever.jl" (**Re**), "Query.jl" (**Qu**), "MySQL.jl" (**My**), "SQLite.jl" (**lite**), and "DataFrames.jl" (**df**). This cartoon representing many intra- and inter-layer connections might be helpful to show the vision of the platform. For example, the path taken to solve a specific intra- or inter-domain (fundamental or applied) question can be quantified by many metrics each producing a distribution of automated solutions across many nodes in a distributed and open network, the Robhoot Open Network (RON). This distribution can be analyzed to quantify properties as robustness, reproducibility and bias of a fundamental or applied solution.

<sup>5</sup>Renku

## **5. Benefits for Eawag and the Biodiversity research community**

My sabbatical period attempts to fill two main gaps in Biodiversity research:

1) developing a platform integrating multiple datasets into process- and ruled-based approaches framing it in multilayer and deep learning networks. The sabbatical will allow me to strengthen international collaborations by submitting a FET-OPEN-EU research grant proposal. The platform, will be fully developed in open source software and coupled to the Renku platform (Swiss data Science Center) and Eawag IT domain. The interactions among different platforms (i.e., Renku, Robhoot and others) will be a collective, multi-institutional networking effort to integrate transdisciplinary, fundamental and applied Biodiversity research. This will help Eawag to strengthen its cooperatiop with international open research platforms by providing expertise and data from Aquatic ecosystems.

2) connecting fundamental and applied research combining open research platforms can provide meaningful for enriching management forums in applied conservation and sustainability centers. Centers that can benefit from such tools in Switzerland and abroad will be the Wyss Centre for Biodiversity, Climate Change and Land use with four planned institutes worldwide, the NCCR centre in Bern and the LifeWatch EU initiative in different parts of Europe. The CEEB could contribute to an emerging network of Swiss synthesis centres with emphasis on distributed and open-data-source driven biodiversity research centers joining fundamental and applied research.