OcéanIA

AI, Data, and Models for Understanding the Ocean and Climate Change

Inria Challenge Project (2021 – 2025)

Inria
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Preface

There is strong scientific evidence about the effects of climate change on the global ocean. These changes will have a drastic impact on almost all forms of life in the ocean with further consequences on food security, ecosystem services in coastal and inland communities. Despite these impacts, scientific data and infrastructures are still lacking to better understand and quantify the consequence of these perturbations on the marine ecosystem.

This interdisciplinary Inria Challenge project aims at developing new AI and mathematical modeling tools to contribute to the understanding of the structure, functioning, and underlying mechanisms and dynamics of the global ocean symbiome. These actions are essential to gain a better understanding of the oceans and their role in regulating and sustaining the biosphere. This is also an opportunity to structure Inria's contributions to a major topic of AI & Biodiversity, which will be a major achievement for the sustainability of human societies on the blue part of the planet.

Besides the support of Inria, OcéanIA already counts with the support of the French Embassy in Chile through the French Regional Cooperation with South America Program.

The spirit of this document is to serve as a work reference. We expect it to evolve as the work in the project takes place. We also want this communication to facilitate the dissemination of the project focus, goals and scope to potential collaborators.

It is organized in five chapters. The first chapter (Chapter 1) outlines the general principles, motivations and goals that led to the project. After that, Chapter 2 focuses on the particular goals of the project and how the different teams that are taking part of it are expected to contribute to its success. Subsequently, Chapter 3 details the work packages of the project listing the different tasks, expected outcomes and the teams that take part of it. Then, Chapter 4 focuses on how the project is to be organized and the interaction of the work packages and teams. Finally, Chapter 5 outlines some final remarks.

This is a working document. We expect it to change frequently. Check https://oceania.inria.cl for updates.

Introduction | 1

The impact of the ocean in climate change is evident, not only regulating temperature and climate but also absorbing carbon dioxide from the atmosphere, which is one of the main responsible gases for the greenhouse effect. However, oceans already show changes and degradation as a result of climate change, such as acidification, deoxygenation, loss of biodiversity, and a progressive loss of capacity to buffer further increases in CO_2 (Pesant et al., 2015).

Pesant, S., Not, F., Picheral, M., Kandels-Lewis, S., Le Bescot, N., Gorsky, G., … Searson, S. (2015). Open science resources for the discovery and analysis of Tara Oceans data. *Scientific Data*, *2*(1450). doi:10.1038/sdata.2015.23

This situation poses a substantial challenge to humanity as a whole. It is not only an urgent but also a scientifically demanding task. Consequently, it is a problem that must be addressed with a scientific cohort approach, where multi-disciplinary teams collaborate to bring the best of different scientific areas.

This is the spirit of this project: to address state-of-the-art artificial intelligence, machine learning, and modeling topics that will enable us to move forward with the understanding of our oceans and to understand, predict and -hopefully- mitigate the consequences of climate change.

1.1 Motivation

Recent advances in computer sciences and applied mathematics, such as machine learning and numerical simulation, among others, have produced a revolution in our capacity for understanding the emergence of patterns and dynamics in complex systems while at the same time the complexity of these problems poses significant challenges to computer science itself.

The intertwining nature of these two challenges requires that to address the first it is necessary to make progress on the second, that is the state of the art (Rolnick et al., 2019). Also, the explosion in the capacity to gather data in fields like biology or ecology has opened computer sciences to challenging applications. Interestingly, the virtuous relationship between computer science and these new fields needs to go beyond the actual state of the art. A remarkable example is bioinformatics, a scientific field

Rolnick, D., Donti, P. L., Kaack, L. H., Kochanski, K., Lacoste, A., Sankaran, K., … Bengio, Y. (2019). Tackling climate change with machine learning. arXiv: 1906.05433 that emerged prompted by the capacity of processing and analyzing massive datasets of "omics" data using computer methods.

Today, a huge amount of problems posed to computer sciences and applied mathematics arise from environmental challenges caused by climate change, and specifically, those affecting biodiversity. The challenges are two-fold: on the one hand, we must understand the consequences of global warming for ecological systems, and on the other hand, we must be able to predict changes in climate from observations of the same systems, where a key actor is biodiversity. Moreover, our prediction abilities have direct consequences on many economic systems and public policies. Essential to these efforts is our ability to make sense and integrate heterogeneous and cross-scale data, ranging from genomics to satellite images in different environmental settings, tasks for which machine learning and artificial intelligence at large, and mathematical modeling, are especially suited and powerful if a virtuous relationship between them is achieved.

The motivation of this interdisciplinary proposal is to develop new AI and mathematical modeling tools to contribute to the understanding of the structure, functioning, and underlying eco-evolutionary mechanisms and dynamics of plankton in the global ocean. Methods like deep representation learning, causal inference, sequential decision making, transfer learning, multi-criteria optimization are just a few that can be applied to these kinds of complex problems, allowing us to get reliable knowledge from the ocean and its interactions. To do this, we will use the corpus of Tara Océan Expeditions datasets, which is, as far as we know, the most comprehensive case study to develop AI and mathematical modeling methods for studying global ecology along with other related datasets. This fundamental baseline currently makes marine plankton the best-described planetary ecosystem in terms of taxonomic composition, abundance, and genetic diversity, making this project realistic.

Since many years, Inria has a formal commitment to ecology and the environment, an interest that is shared by national, European, and international institutions. This Inria Challenge is a mean of producing tangible results in this direction while also prompting a shift in the current state of the art in the area. In particular, this Inria Challenge proposal is an opportunity to structure Inria contributions to this major topic of ocean-ecology modeling and for developing a quantitative theory of global ecosystem patterning and dynamics.

1.2 Context

There is a clear scientific consensus about the effects of climate change on the global ocean: among others a shift of temperatures, an increase of acidification, deoxygenation of water masses, and perturbations in nutrient availability and biomass productivity. Altogether, these abiotic changes will have a drastic impact on almost all forms of life in the ocean with further consequences on food security, ecosystem services and the well-being of coastal communities. In this regard, Tara Océan has spearheaded the actions directed towards sampling and understanding the different phenomena that are taking place. Despite these numerous impacts, scientific data -even with the import contribution from Tara Océan and infrastructures are not sufficient to adequately understand and quantify the consequence of these perturbations on the marine ecosystem. In particular, critical ecosystems need extensive surveys to characterize the biological acclimation to climate perturbations better. Consequently, it is necessary to not only gather more data but also to develop and apply state-of-the-art mechanisms capable of turning this data into effective knowledge, policies and action. This is where artificial intelligence, machine learning and modeling tools are called for. The application of these methods is not new, however, the inherent complexity of this problem poses important challenges to modern computer science and applied mathematics (Rolnick et al., 2019).

The Patagonian region is a unique ecosystem that represents an open sky laboratory for ecological studies. This pristine region is indeed changing more rapidly under the effects of climate change and describes an oracle of changes to come in the next decades for other parts of the ocean. Patagonia is fundamental to understand the responses of the microbial marine life at the interface between antarctic waters, the coastal ecosystems, and the melting glaciers. This region is also one of the most productive regions in the ocean, accounting for more than 30% of sardines stocks, among other species and one of the most important region in sequestering carbon. Patagonia is also a hot spot of aquaculture, with an intensive salmon production, an ecosystem that is both impacting, and being impacted by, climate changes. In order to understand the functioning of this large scale ecosystem, the Tara Océan Oceans initiative has decided to carry out and intense sampling campaign (see Figure 1.1 for a description). The AtlantEco project was expected to depart from France in Septem-

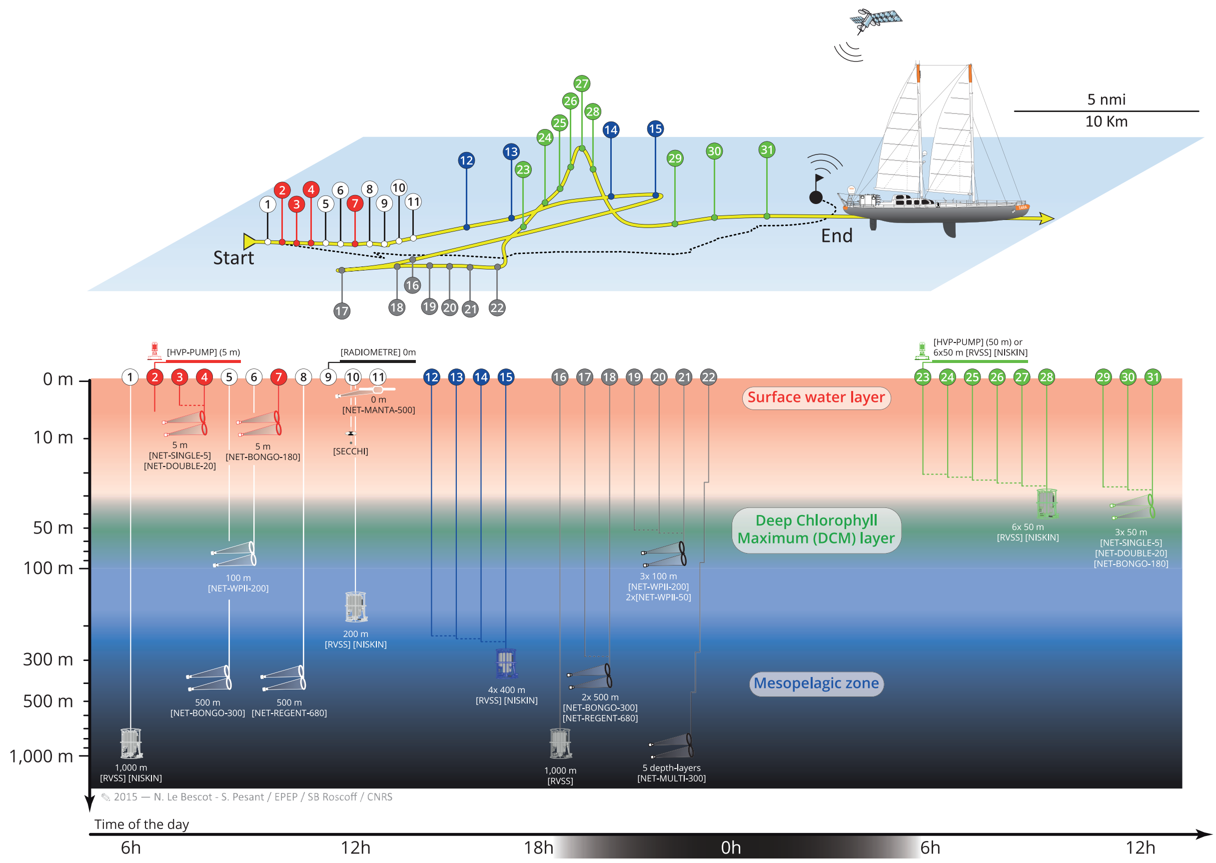

Figure 1.1: Spatial representation and chronology of Tara Océan sampling methodology events during a 24–48 h station. Colored markers along the route of SV Tara Océan (yellow surface track) correspond to sampling events targeting the surface water layer (in red), deep chlorophyll maximum layer (green, here at 50 m), and the mesopelagic zone (blue, here at 400 m). At some stations, an Argo drifter (10 m floating anchor and satellite positioning) was used to follow the water mass during sampling (black surface track). Source: Pesant et al., 2015, shared under a Creative Commons Attribution 4.0 International License.

ber 2020 but because of the COVID-19 pandemic the date has been postponed. It is expected that it transits to the Tara Océan Magallanes expedition in December 2020 and where it will collect data using the Tara Océan protocol in the unique biodiversity of Chile during three months. Inria and its partners are at a strategic and unique position for anticipating these data to come.

The consortium will build a modeling framework dedicated to ocean modeling, contributing to learn causal and explanatory models; fair data models; robust models. This Inria Challenge is an opportunity to contribute key scientific knowledge on a global pressing problem as climate change is, capitalizing on the experience and articulation of the teams involved and the availability of data on a key area, as is the Patagonia, that can provide answers that can be transferred to others parts of the oceans.

Project goals and teams 2

In order to move towards tackling the complex and multi-faceted problem of understanding the role and impact of oceans in climate change, it is necessary to improve the computational and mathematical tools at our disposal and pose a group of domain questions that could be answered using these improved tools.

In recent years, AI -and ML in particular- has been recognized as a broadly powerful tool for technological progress. Despite the growth of research applying ML and AI to problems of societal and global good, there remains the need for a concerted effort to identify how these tools may best be applied to tackle climate change. On the other hand, many computer scientist and practitioners wish to act, but are uncertain how. Similarly, many field experts have begun actively seeking input from the AI, ML and modeling communities. Therefore, this project comes in a timely manner to catalyze these efforts and attempt to create a bridge between the complex problems posed by oceans and climate change and the state of the art of computer science.

2.1 Goals

Although it can be asserted that AI, ML, and modeling tools are key in understanding oceans and climate change, it must also be pointed out that their current limitations pose important hurdles in their application. In the case of ML, only recently it has started to be able to handle structured information, like the one required to understand the networks created by interacting populations of different species. Similarly, in spite of the important efforts on data gathering, the current amount of data available conform to a scenario that can be denominated as small data, that heavily contrasts with the data-hungry methods that conform most of the current state of the art in ML. Yet another important issue lies the black-box approach of many ML methods that do not allow a feasible interpretation or explanation that can be used to articulate a better understanding of the process, which is essential to design new mitigation policies.

Along the same lines, existing modeling tools are hard to apply in biogeophysical contexts like the ones encountered in this project

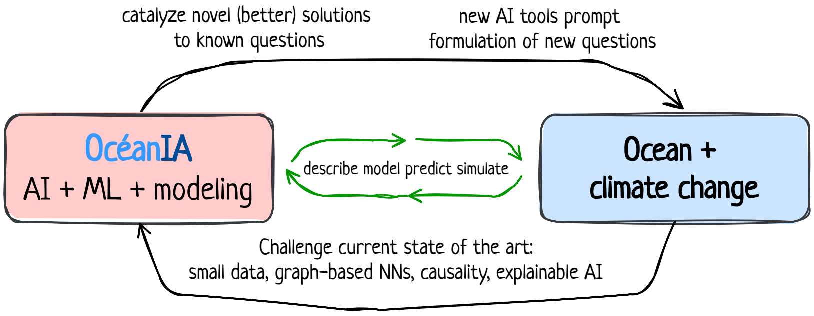

Figure 2.1: The OcéanIA virtuous cycle: AI, ML and applied math should improve the current results and allow oceanographers, marine biologists, and climate change researchers to pose new questions. In return, this application domain constitutes a challenge to the current state of the art and will provide test cases to push that state of the art further ahead.

because of their computational complexity and high processing requirements. This situation could be overcome either by improving the modeling methods themselves or by taking a stab at developing mechanistic approaches that also seem to be capable of complementing AI and ML in the application domain (Baker, Peña, Jayamohan, & Jérusalem, 2018).

Baker, R. E., Peña, J.-M., Jayamohan, J., & Jérusalem, A. (2018). Mechanistic models versus machine learning, a fight worth fighting for the biological community? *Biology Letters*, *14*(5). doi:10.1098/rsbl.2017.0660

This leads us to the core spirit of the project, as illustrated in Figure 2.1. On one hand, AI, ML and applied math should improve the current results and allow oceanographers, marine biologists, and climate change researchers to pose new questions. In return, this application domain constitutes a challenge to the current state of the art and will provide test cases to push that state of the art further ahead.

Consequently, the goals of the project can be stated as two sets as stated by Sánchez-Pi et al., 2020:

Sánchez-Pi, N., Martí, L., Abreu, A., Bernard, O., de Vargas, C., Eveillard, D., … Sebag, M. (2020). Artificial intelligence, machine learning and modeling for understanding the oceans and climate change. In D. Dao, E. Sherwin, P. Donti, L. Kaack, L. Kuntz, Y. Yusuf, … Y. Bengio (Eds.), *Tackling climate change with machine learning workshop at neurips 2020*. url: https://www.climatechange.ai/papers/neurips2020/93

1. address and advance the state of the art in areas like artificial intelligence (AI) —and, more precisely, machine learning (ML)— and mathematical modeling and simulation, and
2. focus on answering the questions from the application domain.

2.1.1 AI, ML and modeling goals

In regard to AI and modeling, our goals are:

1. improve neural network handling of graph-structured information,
2. improve the capacity of ML methods to learn in small data contexts,
3. understand causal relations, interpretability and explainability in AI,
4. integrate model-driven and data-driven approaches, and

5. develop, calibrate and validate existing mechanistic models.

2.1.2 Application domain goals

In the domain application area, the main questions to be addressed are:

1. Which are the major patterns in plankton taxa and functional diversity?
2. Which are the major drivers of patterns and how do they interact?
3. How these patterns and drivers will likely change because of climate change?
4. How will these changes affect the capacity of ocean ecosystems to sequester carbon from the atmosphere, that is the biological carbon pump?
5. What relations bind communities and local conditions?
6. What are the links between biodiversity functioning and structure?
7. How modern AI and computer vision can be applied as research and discovery support tool to understand planktonic communities?

2.2 Participating Inria teams

The team assembled for the project is a balanced and diverse combination of skills, experience, and interests, something that is necessary to address a research-intensive and multi-disciplinary project such as this one.

The Inria project-teams involved and how they contribute to the project are:

- ANGE in modeling, analysis and simulation of geophysical flows and more generally in environmental modeling. The team has been working on the coupling of complex environmental models with observational data (data assimilation) and has gradually oriented part of its research toward the use of environmental data, with or without prior modeling knowledge. ANGE Project-Team has a strong expertise on the models, on the observational data and on the expected forecast performance required in practical applications. It brings applications with real data transfer opportunities through operational actors that use its software daily.

- BIOCORE in modeling ecosystems (from gene to ecosystem) and their adaptation to climate changes, developing strategies for model calibration from available data sets and coupling the models with hydrodynamics. BIOCORE is a joint team with the Laboratory of Oceanography of Villefranche-sur-mer (LOV) joint endeavor between Sorbonne University and CNRS. LOV is a multidisciplinary oceanographic laboratory that studies the role of marine plankton in the functioning of marine ecosystems, the response of biodiversity and biogeochemical cycles to global changes (global warming and acidification). It has a deep expertise for assessing biodiversity by remote sensing calibrated by analytic determination of pigments, which are seen as tracer for phytoplanktonic groups. The PISCO team of the LOV, is associated to BIOCORE has long been specialized in the cultivation and ecophysiological study of phytoplankton (in lab and on site). The LOV is highly involved in the leadership of the Tara Océan project.
- TAU, a joint team between Inria, CNRS and Université Paris-Saclay, working in machine learning and stochastic optimization for 30 years, focusing recently on causal inference and the challenges of the under-specification in big data. In particular, in close relation to the CS questions addressed here, TAU is involved in the Inria Challenge Hybrid Approaches for Interpretable AI (HYAIAI),[1] that started one year ago, and in the European project TRUST-AI,[2] starting next October and devoted to trustworthy AI in small data context.
- Inria Chile was created on 2012 and is the first center of Inria located outside France. It is a driving force for technological innovation and knowledge transfer, collaborating effectively with companies, universities, public institutions, and startups to meet the challenges of the digital revolution. It aims to inspire and educate future generations of scientists and engineers to take the lead in this transformation. Inria Chile is also a means to promote the R&D activities of companies and startups in Chile and Latin America. Inria Chile has expertise in machine learning, evolutionary computing, big data and mastering the connection with the data governance and interpretation and has the engineering know-how to deliver robust software li-

1: https://project.inria.fr/hyaiai/

2: https://cordis.europa.eu/project/id/952060 braries and programs.

2.3 External collaborating partners

Our external partners have developed an important experience in the main subject of the project. They contribute with important methods and experience both in Chile and France. In particular:

- The CMM group led by Alejandro Maass works in understanding biological systems (bioinformatics, genomics and systems biology), and is the Chilean counterpart of the CNRS International Federation Global Ocean Systems Ecology and Evolution (GO-SEE).
- The CNRS laboratory ComBi, at University of Nantes, has produced the main known results relating genomics data with the behavior of the carbon pump and is one of the responsible for handling, analyzing and modeling Tara Océan data since the last decade.
- The project will establish a strategic alliance with the CNRS effort through the GO-SEE Federation, to add into this effort the modernity that AI and Machine learning can propose.
- The group led by Pablo Marquet at PUC is a global leader in metabolic ecology, macroecology, and theoretical ecology and at the forefront of interdisciplinary challenges such as ecological networks reconstruction, invariant distributions of ecological observables, such as species, and gen abundance distributions.
- Tara Océan will allow access to public data and help the consortium defining valid test cases that we will share in this project. For this we will count with the support of André Abreu within Tara Océan.

Also, the resulting resources will be extremely valuable as educational tools, and we may also bring in commercial partners (*e. g.*, "Amazon Sustainability Data Initiative," 2019 or the "Challenge IA-Biodiv – Recherches en Intelligence Artificielle dans le champ de la biodiversité," 2019) who would further support hosting and dissemination of the data and tools.

Amazon Sustainability Data Initiative. (2019). url: https://sustainability.aboutamazon.com/tech-for-good/asdi

Challenge IA-Biodiv – Recherches en Intelligence Artificielle dans le champ de la biodiversité. (2019). url: https://anr.fr/fr/agenda/challenge-ia-biodiv-recherches-en-intelligence-artificielle-dans-le-champ-de-la-biodiversite/

3 Work Packages

Activities on the project are to be organized in three thematic axes that are:

- **Axis I.** enabling activities and shared developments,
- **Axis II.** computer science and applied math objectives, and
- **Axis III.** multi-disciplinary applied objectives.

Work in the axes is organized around work packages. When work inside a work package is best described in smaller units of work, it is then consolidated as tasks. In this chapter we focus on the description of these axes, the work packages that are part of each and the different tasks that we envision that will be carried out. For each work package we provide a (sometimes not so) brief discussion about its motivation and potential impact, the corresponding expected outcomes, in the Inria team in charge of the coordination of the work package and the teams that have manifested interest on collaborating on the work package.

Axis I Enabling activities and shared developments

This axis addresses those tasks that horizontally concern all aspects of the project. In particular, here we meant to create an updated roadmap for the project and a shared lexicon that allows a fluid collaboration. Similarly, we plan to address the technological challenges that involve the access the data and the computing facilities.

WP I.1 State of the art: Paths forward and what should be revisited

A first and very relevant work to do as part of the project is to prepare an updated list of topics worth being revisited using state-of-the-art AI, ML and applied math 'power tools', and what are the limitations that need new developments on the methodological side. In particular, we plan to identify previous works carried out on the Tara Océan data and results that would clearly benefit from an upgrade based on the advanced tools to be developed in Axis II.

For instance, —and just as an illustrative example— Guidi et al., 2016 investigate the carbon pump issue relying on the environmental and metagenomic data gathered by Tara Océan. They have an impressive set of results. Nevertheless, doing a careful read from a AI/ML perspective, it is noticeable that the ML methods applied are rather standard and far from the state of the art. For example, the authors employ partial least square linear regression or the more modern weighted gene correlation network analysis (WGCNA, Horvath, 2011).

Guidi, L., Chaffron, S., Bittner, L., Eveillard, D., Larhlimi, A., Roux, S., ... Gorsky, G. (2016). Plankton networks driving carbon export in the oligotrophic ocean. *Nature*, *532*(7600). doi:10.1038/nature16942

Horvath, S. (2011). *Weighted network analysis: Applications in genomics and systems biology*. Springer Science & Business Media

This opens a broad range of opportunities for applying structure and graph-based ML approaches (WP II.1), causal inference (WP II.3), etc.

The preliminary study carried out for the preparation of this proposal has shown that there is ample space for the application of advanced modeling and learning methods. The results of this updated survey could also be used to update and reshape some future tasks of the project.

Expected outcome(s) of the work package: An survey of the state of the art in the application of mathematical modeling and numerical simulations, and of artificial intelligence and machine learning, in the context of oceanography, marine biology, biodiversity and climate changes. The survey will be a live document to be revised annually and be publicly available.

Coordinating Inria team: Inria Chile

Participating teams: All teams.

WP I.2 Data governance, curation and availability

One of the big technological challenges of the project is to access the available data in a consistent and robust form. It is therefore necessary to govern and curate the data. The need for defining access policies and curation processes has been clearly established on the field (Wackett, 2020), however, it remains an open issue. The result of this process will be curated data hub — or data lake— containing or providing transparent and homogeneous access to diverse set of data sources like Tara Océan data, Copernicus, NASA POWER,[1] NOAA's SeaDataNet,[2] PANGAEA,[3] etc. An important feature here is to offer the possibility of cross-reference

Wackett, L. P. (2020). Web Alert: Marine microbiology databases: An annotated selection of world wide web sites relevant to the topics in environmental microbiology. *Environmental Microbiology*, *22*(5). doi:10.1111/1462-2920.15030

1: https://power.larc.nasa.gov

2: https://www.seadatanet.org

3: https://pangaea.de

and geo-reference this data by providing homogeneous access to all data and capacity of merging with other data sources, either by storing them locally or putting links to external servers. This would be an important asset for the research community globally.

It should be noted that there are lots of metadata standards available, and several initiatives are working on interoperability. The main source of data for the project comes from that produced by Tara Océan Ocean. It follows the M2B3 standard (ten Hoopen et al., 2015) which was developed during H2020 project MicroB3 and authored by EBI, PANGAEA, SeaDataNet and EMODnet. M2B3 is the metadata standard that is most adapted to cross-disciplinary marine science. We will focus as a first step to revise and consolidate these actions.

ten Hoopen, P., Pesant, S., Kottmann, R., Kopf, A., Bicak, M., Claus, S., … Cochrane, G. (2015). Marine microbial biodiversity, bioinformatics and biotechnology (M2B3) data reporting and service standards. *Standards in Genomic Sciences*, *10*(MAY2015). doi:10.1186/s40793-015-0001-5

It is particularly relevant to go beyond regular datasets and also to join other databases that would provide more insight into the Tara Océan database. For example, to ensure access to database gathering hundreds of experiments for the response of phytoplankton to temperature and other environmental conditions.

If possible, we propose to develop an integral science software stack that should be easily deployable, both at local (personal) computers or cloud-provided virtual machines, by making use of modern technological solutions like Docker, Apache Spark, etc. and being as neutral and platform-agnostic as possible.

Inria Chile has an important *a priori* experience on this set of tasks having constructed sophisticated data processing pipelines for astronomy and mining, as well as, in data governance and process mining (Muñoz García, Lamolle, Martinez-Béjar, & Espinal Santana, 2019; Muñoz-García, Del Cioppo, & Bucaram-Leverone, 2017).

Muñoz García, A., Lamolle, M., Martinez-Béjar, R., & Espinal Santana, A. (2019). Learning ecosystem ontology with knowledge management as a service. N. T. Nguyen, R. Chbeir, E. Exposito, P. Aniorté, & B. Trawiński (Eds.), *Computational collective intelligence*, Cham: Springer International Publishing

Muñoz-García, A., Del Cioppo, J., & Bucaram-Leverone, M. (2017). Ontology model for the knowledge management in the agricultural teaching at the UAE. R. Valencia-García, K. Lagos-Ortiz, G. Alcaraz-Mármol, J. Del Cioppo, N. Vera-Lucio, & M. Bucaram-Leverone (Eds.), *Technologies and innovation*, Cham: Springer International Publishing

Other project partners, like CMM and Tara Océan, have ongoing work in these lines. We plan to coordinate with them to generate results that integrate and consolidate the value of current solutions.

Expected outcome(s) of the work package:

- A data governance policy for marine biology and oceanographic data,
- a deployed data lake that consolidates access to the data under the policies devised, and
- a scientific computing software stack.

Coordinating Inria team: Inria Chile

Participating teams: ANGE BIOCORE Tara Océan GO-SEE CMM PUC

Axis II Computer science and applied math objectives

This axis focuses on the computer science topics that we have identified as relevant to the success of the project and where our work will focus.

WP II.1 Structured and graph-based neural networks

Arguably, much of the progress in machine learning in recent years comes from being able to handle more complicated forms of input data than pure tabular data. In particular, with the deep learning revolution, neural networks have become able to grow beyond vectors into n-dimensional tensors (*i. e.* images), graphs, and sequences.

However, there is an increasing number of applications where data are represented in the form of graphs. For example, in e-commerce, a graph-based learning system can exploit the interactions between users and products to make highly accurate recommendations. In chemistry, molecules are modeled as graphs, and their bioactivity needs to be identified for drug discovery. In a citation network, papers are linked to each other via citations, and they need to be categorized into different groups.

The most frequent way to represent biodiversity today is by means of co-ocurrence graphs. These graphs have particular structures that deserve to be analyzed using the presented techniques and its improvements. Comparison of such graphs is a way to see evolution of communities. So having ML methods capable to function on top of this information is essential to understand such dynamics.

The complexity of graph data has imposed significant challenges on existing machine learning algorithms. Recent results have enabled neural networks to handle structured information. The capacity of coupling complex and structured information with powerful machine learning methods that can operate at scale could lead to a shift in the types of problems currently addressable by machine learning. These new results have seen successful applications in the area of natural language processing and have been started to be extrapolated to other domains.

Furthermore, even in contexts like natural language processing (NLP) where the information is structured as a sequence, there is an implicit graphical internal representation, such as a syntactic dependency tree. A syntactic dependency tree defines the syntactic relations among words in a sentence. Similarly, causality and explainability, another important work package of this project rely on dependency graphs.

Structure-based or graph-based neural networks (GNNs) have been proposed and started to be successfully applied in different domains, e.g., in power grid (Donon, Donnot, Guyon, & Marot, 2019) or molecular conformation simulations in TAU. However, there are still questions to be answered to understand how these models can be applied.

A particularly important group of GNNs are focused toward producing metric embeddings from graphs (Narayanan et al., 2017; D. Wang, Cui, & Zhu, 2016) or nodes in graphs (Grover & Leskovec, 2016) that transform them into a lower-dimensional continuous latent space that can be passed through to machine learning model. Walk embedding methods (Perozzi, Al-Rfou, & Skiena, 2014) perform graph traversals to preserve structure and features and aggregates these traversals which can then be passed through a recurrent neural network. Proximity embedding methods use Deep Learning methods and/or proximity loss functions to optimize proximity, such that nodes that are close together in the original graph are likewise in the embedding. Other approaches use methods like graph coarsening to simplify the graph before applying an embedding technique on the graph, reducing complexity while preserving structure and information.

Spatial-temporal graph neural networks (STGNNs) (Jain, Zamir, Savarese, & Saxena, 2016) aim to learn hidden patterns from spatial-temporal graphs, which become increasingly important in a variety of applications such as traffic speed forecasting, driver maneuver anticipation, and human action recognition. The key idea of STGNNs is to consider spatial dependency and temporal dependency at the same time. Potential approaches integrate graph convolutions to capture spatial dependency with RNNs or CNNs to model the temporal dependency.

Donon, B., Donnot, B., Guyon, I., & Marot, A. (2019). Graph neural solver for power systems. *IJCNN 2019 - International Joint Conference on Neural Networks*, Budapest, Hungary. url: https://hal.archives-ouvertes.fr/hal-02175989

Narayanan, A., Chandramohan, M., Venkatesan, R., Chen, L., Liu, Y., & Jaiswal, S. (2017). graph2vec: Learning distributed representations of graphs. arXiv: 1707.05005 [cs.LG]

Wang, D., Cui, P., & Zhu, W. (2016). Structural deep network embedding. *Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining*. doi:10.1145/2939672.2939753

Grover, A., & Leskovec, J. (2016). Node2vec: Scalable feature learning for networks. *Proceedings of the acm sigkdd international conference on knowledge discovery and data mining* (Vol. 13-17-Augu). doi:10.1145/2939672.2939754. arXiv: 1607.00653

Perozzi, B., Al-Rfou, R., & Skiena, S. (2014). DeepWalk: Online learning of social representations. *Proceedings of the acm sigkdd international conference on knowledge discovery and data mining*. doi:10.1145/2623330.2623732. arXiv: 1403.6652

Jain, A., Zamir, A. R., Savarese, S., & Saxena, A. (2016). Structural-RNN: Deep learning on spatio-temporal graphs. *Proceedings of the IEEE conference on computer vision and pattern recognition*

Task II.1.A Model depth

Li, Q., Han, Z., & Wu, X.-m. (2018). Deeper insights into graph convolutional networks for semi-supervised learning. url: https://www.aaai.org/ocs/index.php/AAAI/AAAI18/paper/view/16098

It is an accepted fact that the success of deep learning lies in deep neural architectures. However, Li, Han, and Wu, 2018 showed that the performance of a convolutional GNN drops dramatically with an increase in the number of graph convolutional layers. As graph convolutions push representations of adjacent nodes closer to each other, in theory, with an infinite number of graph convolutional layers, all nodes' representations will converge to a single point. This situation raises the question of whether going deep is still a good strategy for learning graph data.

Task II.1.B Models scalability

So far, the scalability of GNNs is mostly gained at the price of corrupting graph completeness. However, when using sampling or clustering, a model will lose part of the graph information. By sampling, a node may miss its influential neighbors. However, by performing a clustering step, a graph may be deprived of a distinct structural pattern. How to trade-off algorithm scalability and graph integrity is an important research direction. Another research direction is to explore the idea of super-generalization: a GNN is trained on small graphs, and the resulting model is efficient for much larger graphs, as done in TAU (Donon et al., 2019).

Task II.1.C Graph topological heterogeneity

The most current GNNs assume homogeneous graphs. It is difficult to directly apply current GNNs to heterogeneous graphs. These graphs may contain different types of nodes and edges, or different forms of node and edge inputs, such as images, text or other features as the ones to be posed by the scientific challenges of marine biology. Therefore, we plan to develop new methods that would be capable to handle this case of graphs.

Task II.1.D Dynamic graphs

Graphs are in nature dynamic in a way that nodes or edges may appear or disappear, and that node/edge inputs may change time by time. New graph convolution operators are needed to adapt to the dynamics of graphs. Although the dynamics of graphs can be partly addressed by STGNNs, few approaches consider how to perform graph convolutions in the case of dynamic graphs.

Expected outcome(s) of the work package: New models of structure/graph-based neural network that address the challenges posed by the tasks and than can be then used in causality-related problems and/or metabolical structure-related problems. These methods will be contrasted w.r.t. state-of-the-art technique of co-occurrence network that ComBi is currently using, which is based on Markov Blanket (Y. Wang & Wang, 2020). There is also an interest to compare co-occurrence networks. At the moment of writing, ComBi is using graphlet decomposition, that could be used as a 'gold standard' for GNNs.

Wang, Y., & Wang, L. (2020). Causal inference in degenerate systems: An impossibility result. S. Chiappa & R. Calandra (Eds.), *Proceedings of machine learning research*, Online: PMLR. url: http://proceedings.mlr.press/v108/wang20i.html

Coordinating Inria team: Inria Chile

Participating teams: TAU CMM ComBi PUC

WP II.2 Learning and adaptation in small data contexts

Progress in machine learning has made it feasible to address problems in areas of computer vision or natural language processing that only 10 years ago were deemed as intractable of just were not even envision. This raise can be attributed to the progress in three interrelated pillars:

1. the emergence of better hardware substrate to host the operations of neural networks, in particular the emergence of general-purpose computing on graphics processing units (GPGPUs) and tensor processing units (TPUs),
2. the proposal and consolidation of approaches and models like convolutional neural networks, recurrent neural networks, attention mechanisms, transformers, etc., and
3. the creation of datasets that posed important challenges to the state of the art at that time.

However, the need for large annotated datasets suitable for supervised learning limits the applicability and adoption of these recent advances. Furthermore, in many practical scenarios, obtaining such data can be expensive or plainly impossible. Such scenarios are close to the ones we are dealt with in the application context of this project where. Even if the context of marine biology and oceanography Tara Océan has gathered an impressive amount of high-quality data, it is not enough for 'regular' machine learning approaches.

That is why it is crucial to address how machine learning models are trained and adapted to meet this small data scenario. These actions are consolidated as the work in the following directions.

Task II.2.A Transfer learning (TL) and domain adaptation

Here we propose to study how models trained or adjusted for one application and domain can be re-purposed for other applications with minimal impact. In our case, for example, to study how existing models can be applied to new species, other regions, etc. Transfer learning addresses the issue of how to adapt and re-purpose the internal representations of a model that has been trained on a given task to address a similar problem.

On the other hand, domain adaptation is the capacity to cope with changes in the environment because of the natural evolution of the system and/or the need to particularize a general model to a particular instance. For instance, in a previous work (Santana, Martí, & Zhang, 2019) we have addressed how to apply Genetic Programming to adapt general brain-computer interfaces to a particular user.

Santana, R., Martí, L., & Zhang, M. (2019). GP-based methods for domain adaptation: Using brain decoding across subjects as a test-case. *Genetic Programming and Evolvable Machines*. doi:10.1007/s10710-019-09352-6

Task II.2.B Active and few-shot learning

In problems with limited data and/or high uncertainty, like the ones to be dealt here, it is necessary to apply methods that direct the measurements to the areas of the domain where they are most necessary. Guiding sampling using active learning and Bayesian principles. However, due to the limited resources available, few-shot learning methods relying on TL must take care of producing actionable products with minimal data. An alternative, to be explored by TAU in the TRUST-AI European project, is to combine deep learning with stochastic search approaches like Genetic Programming.

Task II.2.C Multi-source and multi-task learning deep neural models

It can be stated that ML methods are about optimizing a model's parameters with regard to a particular metric. This metric can be a score on a certain benchmark or even a business KPI. A process generally denominated as 'training' adjusts a single model or an ensemble of models to perform our desired task. It is then possible to fine-tune and tweak these models until their performance no longer increases.

While these methods generally achieve acceptable performance, by being laser-focused on our single task, sometimes they ignore information that might help the model to do even better on the metric. Specifically, when this information comes from the training signals of related tasks. Sharing representations between related tasks, enable the model to generalize better on the original task. This approach is called multi-source or multi-task learning (MTL).

MTL effectively increases the sample size that is being used for training. MTL also biases the model to prefer representations that are useful for other tasks. This will also help the model to generalize to new tasks in the future (transfer learning) as a hypothesis space that performs well for a sufficiently large number of training tasks will also perform well for learning novel tasks as long as they are from the same environment.

TAU and Inria Chile have been working on this class of problems. For example, TAU has been focusing on a multi-domain adversarial approach (Schoenauer Sebag et al., 2019). On the other hand, Inria Chile has been applying these principles to the prediction of accident risk in mining facilities (Palma, Martí, & Sanchez-Pi, 2021).

Schoenauer Sebag, A., Heinrich, L., Schoenauer, M., Sebag, M., Wu, L., & Altschuler, S. (2019). Multi-domain adversarial learning. T. Sainath (Ed.), *ICLR 2019 - seventh annual international conference on learning representations*, New Orleans, United States. url: https://hal.inria.fr/hal-01968180

Palma, R., Martí, L., & Sanchez-Pi, N. (2021). Predicting mining industry accidents with a multitask learning approach. *Proceedings of the aaai conference on artificial intelligence* (). url: https://ojs.aaai.org/index.php/AAAI/article/view/17805

Expected outcome(s) of the work package: Novel machine learning methods that integrate the results of the previous tasks. These new methods should be made available as open-source tools.

Coordinating team: Inria Chile

Participating teams: TAU CMM

WP II.3 Causality and explainable models in AI

Dramatic success in machine learning has led to a torrent of AI applications. Continued advances promise to produce autonomous systems that will perceive, learn, decide, and act on their own. However, the effectiveness of these systems is limited by the machine's current inability to explain their decisions and actions to human users.

This need has spawned the interest in addressing explainability and causality issues in the context of machine learning and AI.

This task has an additional importance for the context of the project.

Task II.3.A Causal inference

Pearl, J. et al. (2009). Causal inference in statistics: An overview. *Statistics Surveys*, 3

The task of causal inference (Pearl et al., 2009) is to estimate the outcome changes if another *a priori* condition had been applied. For example, suppose two treatments can be applied to patients: Medicine A and Medicine B. When applying Medicine A to the interested patient cohort, the recovery rate is 70%, while applying Medicine B to the same cohort, the recovery rate is 90%. The change of recovery rate is the effect that treatment (*i. e.*, medicine in this example) asserts on the recovery rate. However, randomized control experiments as described above are rarely possible, and the holy grail of causal learning is to infer the causal graph between variables from available data, opening the way to causal inference.

Causal inference has a variety of applications in real-world scenarios. In general, the applications of causal inference can be categorized into three directions:

1. *Decision evaluation.* This is a natural application of treatment effect estimation as it is consistent with the objective.
2. *Counterfactual estimation.* Counterfactual learning (*what-if* scenarios) greatly helps the areas related to decision-making, as it can provide the potential outcomes of different decision choices (or policies).
3. *Dealing with selection bias.* In many real-world applications, records appearing in the collected dataset are not representative of the whole population of interest. Without appropriately handling the selection bias, the generalization of the trained model would be hurt.

The stable unit treatment value assumption (SUTVA) states that the potential outcomes for any unit do not vary with the treatment assigned to other units, and, for each unit, there are no different forms or versions of each treatment level, which lead to different potential outcomes. This assumption mainly focuses on two aspects: (i) units are independent and identically distributed (i.i.d.), and (ii) there only exists a single level for each treatment. An extensive literature exists on making causal inferences under SUTVA, but when considering many real-world situations, it may not always be the case.

The assumption of independent and identically distributed samples is ubiquitous in most causal inference methods, but this assumption cannot hold in many research areas, such as social media analytics (Guo, Li, & Liu, 2019; Shalizi & Thomas, 2011), herd immunity, and signal processing (Sutskever, Vinyals, & Le, 2014). Causal inference in non-i.i.d. contexts is challenging due to the presence of both unobserved confounding and data dependence. For example, in social networks, subjects are connected and influenced by each other.

Guo, R., Li, J., & Liu, H. (2019). Learning individual treatment effects from networked observational data. arXiv: 2004.07511v1 [cs.LG]

Shalizi, C. R., & Thomas, A. C. (2011). Homophily and contagion are generically confounded in observational social network studies. *Sociological Methods & Research*, *40*(2)

Sutskever, I., Vinyals, O., & Le, Q. V. (2014). Sequence to sequence learning with neural networks. *Advances in neural information processing systems*

For such network data, SUTVA cannot hold anymore. Under this situation, instances are inherently interconnected with each other through the network structure and hence their features are not independent identically distributed samples drawn from a certain distribution.

The dependence in data often leads to interference because some subjects' treatments can affect others' outcomes (Hudgens & Halloran, 2008; Ogburn, VanderWeele, et al., 2014). This difficulty can impede the identification of causal parameters of interest. Extensive work has been developed on identification and estimation of causal parameters under interference (i.e. Hudgens and Halloran, 2008; Ogburn, VanderWeele, et al., 2014, Peña, 2018; Tchetgen and VanderWeele, 2012).

Hudgens, M. G., & Halloran, M. E. (2008). Toward causal inference with interference. *Journal of the American Statistical Association*, *103*(482)

Ogburn, E. L., VanderWeele, T. J. et al. (2014). Causal diagrams for interference. *Statistical science*, *29*(4)

Peña, J. M. (2018). Reasoning with alternative acyclic directed mixed graphs. *Behaviormetrika*, *45*(2)

Tchetgen, E. J. T., & VanderWeele, T. J. (2012). On causal inference in the presence of interference. *Statistical Methods in Medical Research*, *21*(1)

For this problem, a strategy proposed by Sherman and Shpitser, 2018 is to use segregated graphs (Shpitser, 2015), a generalization of latent projection mixed graphs (Verma & Pearl, 1991), to represent causal models.

Shpitser, I. (2015). Segregated graphs and marginals of chain graph models. *Advances in neural information processing systems*

Verma, T., & Pearl, J. (1991). *Equivalence and synthesis of causal models*. UCLA, Computer Science Department

Applying graph convolutional networks into a causal inference model is an approach to handle the network-structured data Guo et al., 2019. In particular, the original features of subjects and the network structure are mapped to a representation space, to get the representation of confounders. Furthermore, the potential outcomes could be inferred using treatment assignments and confounder representations.

In a similar line, causal inference can be conceptualized as a multi-task learning problem with a set of shared layers for treated group and control group together, and a set of specific layers for treated group and control group separately. The impact of selection bias in multi-task learning problem can be alleviated via a propensity-dropout regularization scheme, in which the network is thinned for every training example via a dropout probability that depends on the associated propensity score.

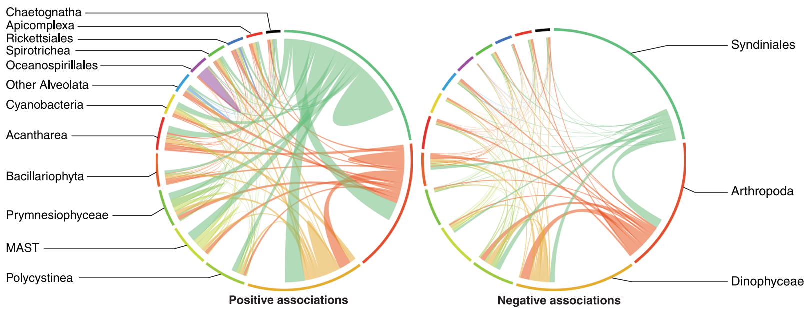

Figure 3.1: Community structure found in photic zone interactome. Top 15 interacting taxon groups are depicted as colored segments in which ribbons connecting two segments indicate co-presence and exclusion. Links are dominated by the obligate parasites syndiniales and by Arthropoda and Dinophyceae. Source: Lima-Mendez et al., 2015.

In the context of the project, there is a particular opportunity for applying causal inference methods in conjunction with the work being carried out in WP II.1 and WP III.1. A particular case are regulatory networks and community structures.

For example, Lima-Mendez et al., 2015 discussed the problem of finding the community structure in the photic zone interactome using environmental factors and organismal abundance profiles relying on Tara Océan data, as illustrated in Figure 3.1. Causality could be used to automatically extract and give a causality direction in the graph at different levels of taxonomic resolution. Work package WP III.1 will centralize and coordinate work in this direction.

Causality has been a long-time research theme at TAU, Isabelle Guyon being a pioneer of the field, in particular through the organization of the cause-effect pair challenges (Kalainathan, Goudet, Sebag, & Guyon, 2019). Other results on this topic include a PhD thesis by Kalainathan, 2019 —along with its corresponding publications (Goudet et al., 2018; Goudet, Kalainathan, Sebag, & Guyon, 2019; Kalainathan, Goudet, Guyon, Lopez-Paz, & Sebag, 2018b)— in which full causal models (and not only pairs of variables) are built using the adversarial principles of deep neural networks.

Inria Chile has also worked on the application of causal inference to the determination of causes of accidents in the petroleum (Martí, Sanchez-Pi, Molina, & Bicharra Garcia, 2014; Sanchez-Pi, Martí, Molina, & Bicharra Garcia, 2014, 2015) and mining industries (Palma et al., 2021) among others.

Kalainathan, D., Goudet, O., Sebag, M., & Guyon, I. (2019). Discriminant Learning Machines. I. Guyon, A. Statnikov, & B. B. Batu (Eds.), *Cause Effect Pairs in Machine Learning*. doi:10.1007/978-3-030-21810-2_4

Kalainathan, D. (2019). *Generative neural networks to infer causal mechanisms: Algorithms and applications* (Theses, Université Paris Sud (Paris 11) - Université Paris Saclay). url: https://hal.inria.fr/tel-02435986

Martí, L., Sanchez-Pi, N., Molina, J. M., & Bicharra Garcia, A. C. (2014). High-level information fusion for risk and accidents prevention in pervasive oil industry environments. *Highlights of practical applications of heterogeneous multi-agent systems — The PAAMS Collection*. doi:10.1007/978-3-319-07767-3_19

Sanchez-Pi, N., Martí, L., Molina, J. M., & Bicharra Garcia, A. C. (2014). An information fusion framework for context-based accidents prevention. *17th International Conference on Information Fusion (FUSION)*. url: http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=6916105&tag=1

Sanchez-Pi, N., Martí, L., Molina, J. M., & Bicharra Garcia, A. C. (2015). Contextual pattern discovery in ambient intelligent application. *International Journal of Imaging and Robotics (IJIR)*, *15*(4)

Palma, R., Martí, L., & Sanchez-Pi, N. (2021). Predicting mining industry accidents with a multitask learning approach. *Proceedings of the aaai conference on artificial intelligence* (). url: https://ojs.aaai.org/index.php/AAAI/article/view/17805

Task II.3.B Explainable AI

In this task we focus on how to address the issue of explainable AI. This task aims to set up a suite of machine learning techniques that:

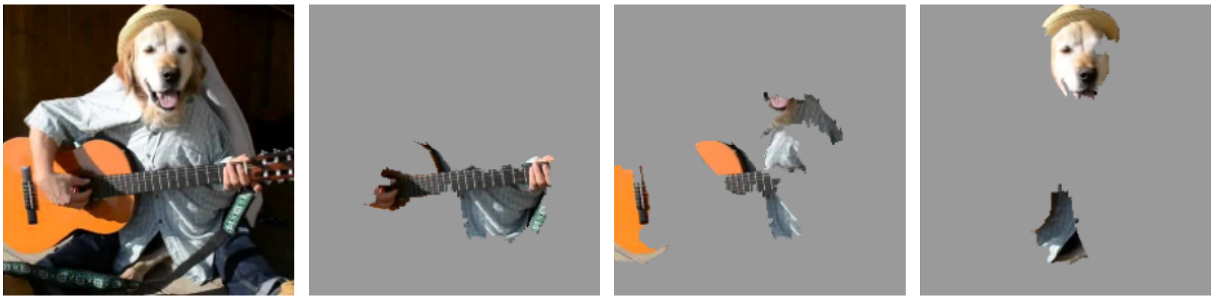

Figure 3.2: How different elements of an image influence each possible classification class. Source: Ribeiro et al., 2016.

- produce more explainable models, while maintaining a high level of learning performance (prediction accuracy),
- create a set of research support tools that combine explainability and causality to cast light into the finding of new scientific discoveries and theories by making surrogate human-readable models, and
- enable human users to understand, appropriately trust, and effectively manage the emerging generation of artificially intelligent partners.

Explainability is a core concern in AI —and computer science, for that matter— at the moment (Barredo Arrieta et al., 2020). It is also an essential component of the challenge as we intend to use the models created to serve as vehicles for understanding nature and at the same time to be a source for new theories.

Barredo Arrieta, A., Díaz-Rodríguez, N., Del Ser, J., Bennetot, A., Tabik, S., Barbado, A., ... Herrera, F. (2020). Explainable artificial intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI. *Information Fusion*, *58*. doi:10.1016/j.inffus.2019.12.012

Current state-of-the-art machine learning methods tend to obfuscate the interpretability of their results. This has been further aggravated by the emergence of highly complex deep learning methods. There has been an important interest on the context of explainablility related to images (Vermeire & Martens, 2020).

Vermeire, T., & Martens, D. (2020, April 16). Explainable image classification with evidence counterfactual. arXiv: 2004.07511v1 [cs.LG]

Images are particularly suitable for the application of these methods and have served to expose many of the drawbacks of current methods. For instance, Figure 3.2 shows some results from Ribeiro, Singh, and Guestrin, 2016 where traced back the parts of the input image (a) that are decisive when trying to classify that image under different classes (b)–(d).

New machine learning systems that will be proposed in this task would have the ability to explain their rationale, characterize their strengths and weaknesses, and convey an understanding of how they will behave in the future. The strategy for achieving that goal is to develop new or modified machine learning techniques that will produce more explainable models. These models will

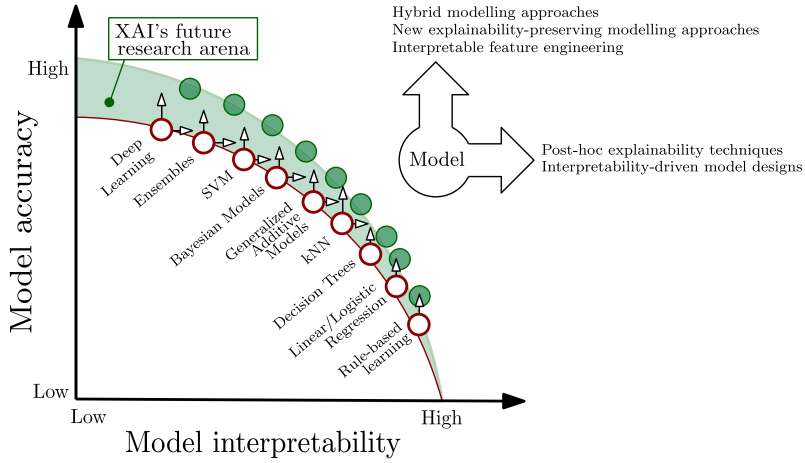

Figure 3.3: Trade-off between accuracy and interpretability of machine learning methods and the area of work of modern explainable AI. Source: Barredo Arrieta et al., 2020.

be combined with state-of-the-art human-computer interface techniques capable of translating models into understandable and useful explanation dialogues for the end user.

Our strategy is to pursue a variety of techniques to generate a portfolio of methods that will provide future developers with a range of design options covering the performance-versus-explainability trade-off space. This trade-off can be appreciated in Figure 3.3.

Here again, there will be cross-fertilization and factorization with the European project TRUST-AI, of which TAU is a partner, adding Genetic Programming in the portfolio, together with other recent or on-going work at TAU that are already disseminated (Escalante et al., 2018; Kalainathan, Goudet, Guyon, Lopez-Paz, & Sebag, 2018a; Tubaro, Casilli, & Coville, 2020).

Escalante, H. J., Escalera, S., Guyon, I., Baró, X., Güçlütürk, Y., Güçlü, U., & van Gerven, M. A. J. (2018). *Explainable and interpretable models in computer vision and machine learning*. doi:10.1007/978-3-319-98131-4

Kalainathan, D., Goudet, O., Guyon, I., Lopez-Paz, D., & Sebag, M. (2018a). *SAM: Structural agnostic model, causal discovery and penalized adversarial learning*. working paper or preprint. url: https://hal.archives-ouvertes.fr/hal-01864239

Tubaro, P., Casilli, A. A., & Coville, M. (2020). The trainer, the verifier, the imitator: Three ways in which human platform workers support artificial intelligence. *Big Data & Society*, *7*(1). doi:10.1177/2053951720919776

Baumgartner, C. F., Koch, L. M., Tezcan, K. C., & Ang, J. X. (2018). Visual feature attribution using Wasserstein GANs. *2018 IEEE/CVF Conference on Computer Vision and Pattern Recognition*

Charte, D., Charte, F., García, S., del Jesus, M. J., & Herrera, F. (2018). A practical tutorial on autoencoders for nonlinear feature fusion: Taxonomy, models, software and guidelines. *Information Fusion*, *44*. doi:10.1016/j.inffus.2017.12.007

Work in this task will be organized in the following directions:

- *Explainable AI and adversarial machine learning*: some recent contributions have capitalized on the possibilities of generative adversarial networks (Baumgartner, Koch, Tezcan, & Ang, 2018), variational autoencoders (Charte, Charte, García, del Jesus, & Herrera, 2018) and other generative models towards explaining data-based decisions. Once trained, generative models can generate instances of what they have learned based on a noise input vector that can be interpreted as a latent representation of the data at hand.
  This is best illustrated in Figure 3.4. In this figure it is illustrated how a neural network trained to classify dogs applies a combined method that segments (b) and then uses this segments to classify the images. When the classifier

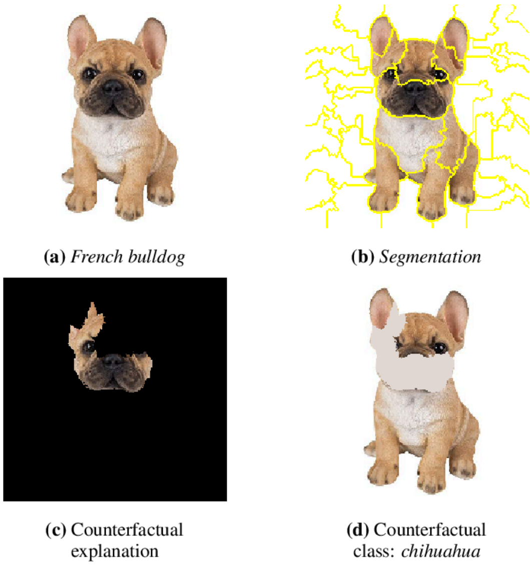

Figure 3.4: Determining key features in image classification using adversarial methods. Source: Vermeire and Martens, 2020.

is confronted with counterfactual examples, it can be appreciated what elements are the determining factors to reach -or reject- a classification, as appreciated in (c) and (d).

- *Interpretable shadow models*: methods like Bayesian networks and, particularly, genetic programming can be constructed to provide human-readable models that can be interpreted, assessed and even lead to new scientific discoveries.
- *Causal inference for understanding internal representations*: representation learning is one of the main results that have lead to the deep learning revolution. It can be hypothesized that causal inference methods can be applied to understand the patterns of those activations and, be used to understand what input and internal features influence the prediction.

Expected outcome(s) of the work package: Outcome of the package will be a toolkit library consisting of machine learning and human-computer interface software modules that could be used to develop future explainable AI systems. We expect this to lead toward the concept of responsible AI, namely, a methodology for the large-scale implementation of AI methods in real organizations with fairness, model explainability and accountability at its core.

Coordinating Inria team: TAU

Participating teams: Inria Chile

WP II.4 Model-driven and data-driven integration and hybrids

Running biogeophysical models (Boittin et al., 2020) can be very CPU time and energy consuming. The idea here is to use deep learning approaches to reproduce the predictions of these resource demanding models. More precisely, to reduce complex models (coupling Navier-Stokes with biochemical source terms) using deep neuronal networks (DNNs).

Boittin, L., Bouchut, F., Bristeau, M.-O., Mangeney, A., Sainte Marie, J., & Souillé, F. (2020). *The Navier-Stokes system with temperature and salinity for free surface flows Part II: Numerical scheme and validation*. working paper or preprint. url: https://hal.inria.fr/hal-02510722

Task II.4.A Learning PDEs from Data

In a first stage, a database of synthetic data coming from the numerical resolution of our PDE-based models will be generated on a broad range of scenarios. These datasets will be used to train deep neural networks (Chen, Rubanova, Bettencourt, & Duvenaud, 2018; Dupont, Doucet, & Teh, 2019). A validation data set will be used to validate and assess the resulting accuracy.

Chen, R. T., Rubanova, Y., Bettencourt, J., & Duvenaud, D. K. (2018). Neural ordinary differential equations. *Advances in neural information processing systems*

Dupont, E., Doucet, A., & Teh, Y. W. (2019). Augmented neural ODEs. H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, & R. Garnett (Eds.), *Advances in neural information processing systems 32*. Curran Associates, Inc. url: http://papers.nips.cc/paper/8577-augmented-neural-odes.pdf

Note that specific stability analysis and dedicated tools like CFL condition, upwinding, etc., are usually required in the numerical processing of transport. In this context, we will build conceptual analogies between DNN architectures (activation functions, number of layers) and our schemes (slope limiters, time discretization). Positivity and energy preservation will be studied as well. In this way, we will generalize our approach to various initial conditions.

Task II.4.B Understanding learning dynamics

There exists a huge literature on model reduction for ODEs and PDEs. However, classical techniques often face difficulties to reduce systems with hyperbolic features. The study of geophysical flows is often associated with advection dominating flows and hence, except for simple/linear systems, there is a lack of efficient model reduction techniques available e.g. for ocean dynamics.

Using simple models: advection equation (2D, with varying advection velocity, etc.), shallow water equations in characteristic regimes, we intend to understand why ML-based techniques give interesting results. In this regard, the work of Rudy, Brunton, Proctor, and Kutz, 2017 and Sirignano and Spiliopoulos, 2018 are good starting points.

Rudy, S. H., Brunton, S. L., Proctor, J. L., & Kutz, J. N. (2017). Data-driven discovery of partial differential equations. *Science Advances*, *3*(4). doi:10.1126/sciadv.1602614

Sirignano, J., & Spiliopoulos, K. (2018). DGM: A deep learning algorithm for solving partial differential equations. *Journal of Computational Physics*, *375*. doi:10.1016/j.jcp.2018.08.029

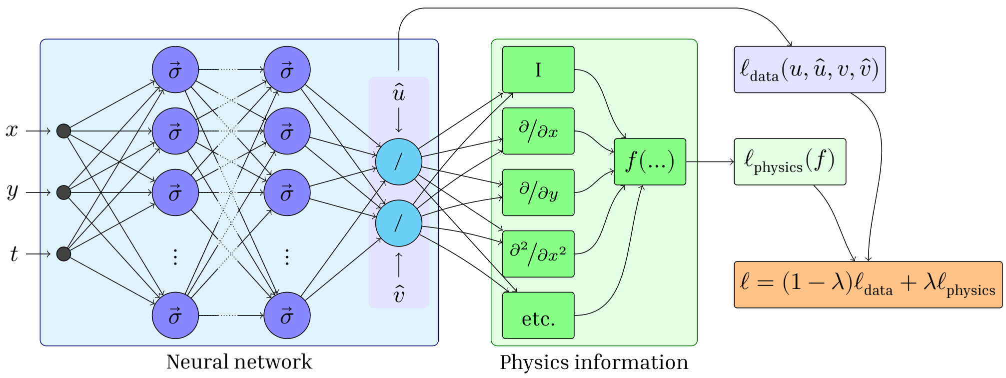

Figure 3.5: Schematic representation of a physics-informed neural network with inputs x, y, and t; outputs $\hat{u}$ and $\hat{v}$. Using automatic gradient calculation we can differentiate the neural network by its input variables and construct a physics error function $f()$. Consequently, the loss function, ℓ, involves a loss term for the data (ℓ_{data}) and a loss term for the physics function (ℓ_{physics}). Source: de Wolff, Carrillo, Martí, and Sanchez-Pi, 2021b.

Task II.4.C Hybrid models: Combining PDE solvers and DNNs

Though remaining in the framework of transport models, we will consider here a general process where a source of physical knowledge under the form of a PDE is available. We will investigate schemes for decomposing a process model into PDE and statistical components which is an open problem. We will analyze for representative cases the properties of such decompositions (existence, unicity, conditions for PDE parameters identification), and propose a formal learning framework. Simple kinetics describing phytoplankton growth as a function of temperature and nutrients will be embedded in the model as a case study to validate the approach and assess its accuracy.

Physics-informed neural networks (PINNs) (Raissi, Perdikaris, & Karniadakis, 2019) are a hybrid approach that take into account a data-based neural network model and a physics-informed mechanistic model which are two different paradigms, as presented in Figure 3.5. They offer a framework where existing knowledge about a physical phenomenon and empirical data gathered about it. This general concept has been previously explored and is known as data assimilation (Vetra-Carvalho et al., 2018), but PINNs bring a novel and sound approach to consolidate the existing models and sampled data.

This feature makes PINNs particularly appealing for the above-described problems and has lead to some preliminary studies by Inria Chile (de Wolff, Carrillo, Martí, & Sanchez-Pi, 2021a, 2021b) and others (Lütjens, Crawford, Veillette, & Newman, 2021).

Recently, this insterest was further verified during the AIMOCC'21

Raissi, M., Perdikaris, P., & Karniadakis, G. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, *378*. doi:10.1016/j.jcp.2018.10.045

Vetra-Carvalho, S., van Leeuwen, P. J., Nerger, L., Barth, A., Altaf, M. U., Brasseur, P., … Beckers, J.-M. (2018). State-of-the-art stochastic data assimilation methods for high-dimensional non-Gaussian problems. *Tellus A: Dynamic Meteorology and Oceanography*, *70*(1). doi:10.1080/16000870.2018.1445364

de Wolff, T., Carrillo, H., Martí, L., & Sanchez-Pi, N. (2021a). Assessing physics informed neural networks in ocean modelling and climate change applications. N. Sanchez-Pi & L. Martí (Eds.), *AI: Modeling Oceans and Climate Change Workshop at ICLR 2021*, Santiago (Virtual), Chile. url: https://hal.inria.fr/hal-03262684

de Wolff, T., Carrillo, H., Martí, L., & Sanchez-Pi, N. (2021b). Towards optimally weighted physics-informed neural networks in ocean modelling. arXiv: 2106.08747. url: https://hal.inria.fr/hal-03260357

Lütjens, B., Crawford, C. H., Veillette, M., & Newman, D. (2021). PCE-PINNs: Physics-informed neural networks for uncertainty propagation in ocean modeling. N. Sanchez-Pi & L. Martí (Eds.), *AI: Modeling Oceans and Climate Change Workshop at ICLR 2021*. arXiv: 2105.02939 [cs.LG]

workshop organized in conjunction with the ICLR 2021 conference (Sanchez-Pi & Martí, 2021).

Sanchez-Pi, N., & Martí, L. (Eds.). (2021). AI: Modeling Oceans and Climate Change Workshop (AIMOCC 2021), Santiago de Chile (Virtual): Tenth International Conference on Learning Representations (ICLR 2021). url: https://oceania.inria.cl/#aimocc

Expected outcome(s) of the work package: This work package will give rise to easier methods to simulate and to handle AI-based models that will allow to more extensively explore different scenearii, including the impact of temperature changes as following IPCC scenarii, in particular in biodiversity along ocean currents.

Coordinating Inria team: ANGE

Participating teams: BIOCORE TAU Inria Chile CMM PUC

WP II.5 Development, calibration and validation of mechanistic models

Task II.5.A Identifiability issues

The high dimension of the biogeochemical models make challenging their calibration and validation from a reduced number of measurements. These nonlinear and dynamical systems often integrate several time scales. It results that the mathematical analysis of these models is challenging. The identifiability of their parameters is often an open question. As a result, identification algorithms based on minimization can converge towards several local minima.

The objective of this work package will be to develop identification strategies tailored to the system to limit the ineffability's issues and eventually to cross validate the models.

Baroukh, C., Muñoz-Tamayo, R., Steyer, J.-P., & Bernard, O. (2015). A state of the art of metabolic networks of unicellular microalgae and cyanobacteria for biofuel production. *Metabolic Engineering*, *30*. doi:10.1016/j.ymben.2015.03.019

Baroukh, C., Muñoz-Tamayo, R., Steyer, J.-P., & Bernard, O. (2014). DRUM: A new framework for metabolic modeling under non-balanced growth. application to the carbon metabolism of unicellular microalgae. *PLoS ONE*, *9*(8). doi:10.1371/journal.pone.0104499

Baroukh, C., Turon, V., & Bernard, O. (2017). Dynamic metabolic modeling of heterotrophic and mixotrophic microalgal growth on fermentative wastes. *PLOS Computational Biology*, *13*(6). doi:10.1371/journal.pcbi.1005590

Task II.5.B Metabolic model reduction

Most of the approaches to reduce metabolic models assume a steady state, where no intracellular compounds can accumulate. In the environment permanently subject to varying signals like light, temperature, pH, etc., such hypothesis reveals to be wrong (Baroukh, Muñoz-Tamayo, Steyer, & Bernard, 2015), and the Dynamic RedUction of Metabolism (DRUM) framework (Baroukh, Muñoz-Tamayo, Steyer, & Bernard, 2014; Baroukh, Turon, & Bernard, 2017) has been proposed accounting for the metabolic dynamics through accumulation and reuse of internal compounds.

More work remains to be done to account for the dilution due to growth or to advection-diffusion in the natural environment and to include the impact of temperature on metabolism.

The mathematical analysis of the metabolic fluxes within the ecosystem still needs developments to understand the key element driving its dynamics. More specifically, methods are lacking to reduce the number of solutions while constrain the metabolic problem. Studying all the possible intracellular fluxes and the dependencies between reactions (Correlation Flux Coupling Analysis) is still an open question.

Task II.5.C Navier-Stokes equation: From Eulerian to Lagrangian

The multidisciplinary approach put forward by ANGE includes hydrodynamic models that enable the simulation of Lagrangian cell trajectories (Demory et al., 2018). In this task, we will tackle the inverse problem using this Lagrangian reconstruction. More precisely, we will build up an inverse problem by comparing the observed trajectories and the simulated to reconstruct the environment parameters. A promising characteristic of this approach is that the number of considered trajectories (observed and computed) can be increased to get a more accurate estimate of the environment parameters.

Demory, D., Combe, C., Hartmann, P., Talec, A., Pruvost, E., Hamouda, R., … Bernard, O. (2018). How do microalgae perceive light in a high-rate pond? Towards more realistic lagrangian experiments. *Royal Society Open Science*, *5*(5). doi:10.1098/rsos.180523

Expected outcome(s) of the work package: Coupling of the Navier-Stokes equations with biological models gives an accurate representation of the hydrodynamics-biology coupling and of the evolution processes but the study of the obtained models is out of reach. Two simplification steps: metabolic reduction and Lagrangian trajectories will give rise to models of reduced complexity over which ML techniques will be applied. The underlying parameter estimation and state reconstruction algorithms will be assessed on these simplified models.

Coordinating Inria team: BIOCORE

Participating teams: ANGE CMM ComBi PUC

Axis III Multi-disciplinary applied objectives

We identified two main “vertical” applied scientific challenges concerning the modeling of the ocean symbiome system and its relation with climate change. All of them have an intrinsic need for the development of computer science and mathematical theories, computational tools and ideas to bring us beyond the state of the art and strengthen the accumulated area of expertise.

WP III.1 Integrating biodiversity community structures and function along the ocean

Task III.1.A Biodiversity and ecosystem functioning

Biodiversity supports important functions, such as primary productivity and carbon fixation and sequestration, that are directly or indirectly used and affected by humans. Understanding the processes driving these functions is fundamental from a basic science and policy perspective. One of the main drivers of changes in ecosystems functions is biodiversity most commonly measured as number of species and mostly in terrestrial and freshwater environments. The most common pattern is an increase in function like productivity and species richness with an eventual ceiling.

In marine environments, these studies are comparatively scarce and most of them restricted to deep sea and benthic ecosystems, for which positive and negative relationships have been reported. Data derived from Tara and other sources would allow for a comprehensive exploration of the relationship between ecosystem functioning and biodiversity, for testing many of the mechanistic hypotheses offered to explain them (*e. g.*, complementarity, selection, and sampling effects). But more importantly, for assessing their relative contribution and testing new ones associated to the integration and variability of these relationships across different levels of biodiversity, from genes to species to traits and functions and their interaction with other driver variables such as temperature that drives both diversity and ecosystems functions, and with different levels of detail. (*e. g.* comparing the relationship between ecosystem functioning and metagenomes with that for meta-transcriptomes). This study will help leverage and overcome important biases such as the underrepresentation of ocean studies with only five reported (van der Plas, 2019).

van der Plas, F. (2019). Biodiversity and ecosystem functioning in naturally assembled communities. *Biological Reviews*, *94*(4). doi:10.1111/brv.12499. eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/brv.12499

The almost non-existence analysis at the levels of metagenomes, meta-transcriptomes, and metabolic trait diversity, which will provide unprecedented evidence linking genes to ecosystem processes. Finally, through AI technique we will be able to understand causality and circular causality among different levels of biodiversity, ecosystem functioning and abiotic variables such as temperature.

Task III.1.B Meta-metabolic modeling

The objective is to develop a metabolic model including the main microbial oceanic compartments, and couple it with physics. Meta-metabolic model is challenging due to variety in the pathways and time scales. The current approaches for metabolic modeling has been developed assuming that the metabolism is at steady state, the DRUM approach (Baroukh et al., 2014) opens new routes to tackle this challenge. It is ambitious to propose a metabolic model of the ocean microbial food web, but with these tools it becomes doable. The model could be calibrated with the Tara Océan Oceans data. This reconstruction of meta-metabolic models for each Tara Océan sample (prokaryiotic fraction) has already been initiated by ComBi, but much remain to be done for the calibration and the validation of such models.

As a main expected result, a notion of ecological niche should be derived from metabolic networks of key organisms (ComBi). CMM and PUC are also active in this context in particular by incorporating regulatory ideas.

Task III.1.C Phytoplankton biodiversity with regard to temperature, present and future

The main purpose is to create a computational modeling framework to properly incorporate plankton complexity into ocean-climate models, assuming the stochastic nature of this system. There area different tasks that can be addressed in this context.

In this case, the objective is to match the V9-18s available in the Tara Océan database and local temperature data, focusing on sentinel genus (i.e. Micromonas or Synecochochocus) for which temperature response model exist (Demory et al., 2019), which have been used to propose phytoplankton biodiversity indexes. These biodiversity models must be improved considering a larger data set encompassing the Tara Océan measurements, especially by

Demory, D., Baudoux, A.-C., Monier, A., Simon, N., Six, C., Ge, P., … Rabouille, S. (2019). Picoeukaryotes of the Micromonas genus: Sentinels of a warming ocean. *The ISME Journal*, *13*(1). doi:10.1038/s41396-018-0248-0

relating local temperature conditions (yearly SST evolution), local nutrient conditions and temperature response: predicting which species can grow in a given environment.

In a first stage, the area where temperature effect is predominated by other factors must be determined and analyzed. For the area whose biodiversity is temperature driven, the future of the local biodiversity must be assessed within the IPCC scenarii.

Task III.1.D Data assimilation in biogeochemical models: Predicting the future

Data assimilation strategies will be developed to calibrate biogeochemical models using the available database. The PISCES biogeophysical model, which is already used by ComBi, will be run for this purpose. Data assimilation with 3D biogeochemical models, including a large number of processes and parameters, is an active subject of research. The tools of AI combined with other approaches from applied mathematics are opportunities for gaining in prediction capability. The idea is to embed key factors affected by global changes such as pH (Carbonate system, including CO_2) and temperature to be able to predict the ecosystem evolution at the end of the century horizon. BIOCORE will focus on the phytoplankton compartment and the primary production.

Surrogate models of the growth rate derived from the other tasks will be used as a proxy within the PISCES model, following the first results within the project Houmus (CNRS Prime) obtained by ComBi.

Expected outcome(s) of the work package: The outcome of this work package can be summarized as:

- conclusive analysis at the levels of metagenomes, metatranscriptomes, and metabolic trait diversity, that provide evidence linking genes to ecosystem processes,
- a notion of ecological niche should be derived from metabolic networks of key organisms,
- original models describing biodiversity in response to temperature,
- enhanced strategies for calibrating biogeochemical models.

Coordinating Inria team: BIOCORE

Participating teams: ANGE Inria Chile ComBi CMM GO-SEE PUC

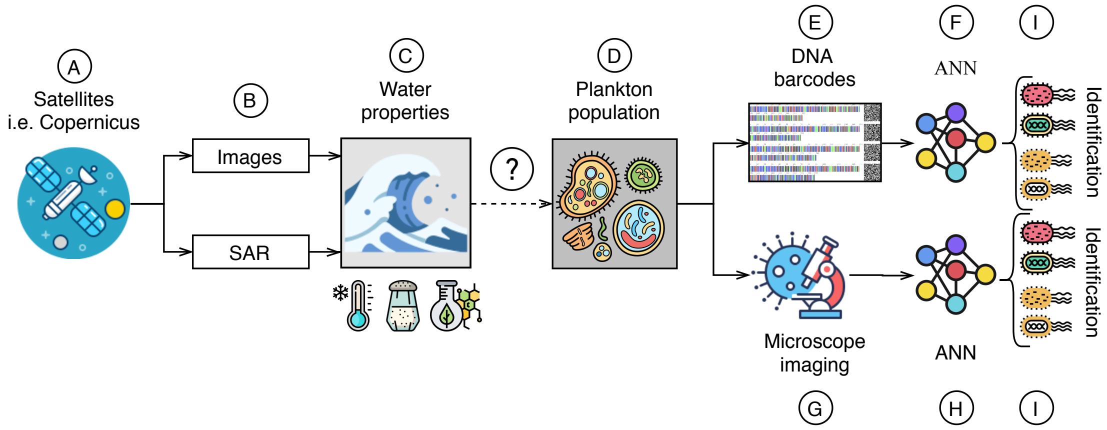

Figure 3.6: Steps or layers for the application of computer vision and machine learning for understanding planktonic populations. From satellites (A) we can obtain images and synthetic aperture radar measurements (SAR) (B). Water properties like temperature, salinity, and presence of chlorophyll (C) may indicate the presence of certain populations (D) but the details can be either appreciated using microscope imagining (G) of DNA barcodes (E). In both cases, AI methods like neural networks can be applied to identify in images or barcodes the presence of organisms: (E)-(F)-(G) and (G)-(H)-(i), respectively.

WP III.2 Understanding plankton communities using AI, ML, and vision

Tara Océan sampling methodology allows for an ample application of computer vision to help the understanding of the characteristics of the biome. This is particularly important as images can be obtained from the samples being extracted but also a camera is submerged as records images of the microscopic organisms found.

Traditionally, plankton is surveyed using either satellite remote sensing, where biomass is inferred indirectly through measurement of total chlorophyll concentration or with large net tows via oceanic vessels like Tara Océan, with subsequent microscopic analysis of the preserved samples.

Satellite imaging methods are extremely accurate in terms of global geographic association and very useful for broad species characterization but may present practical challenges in terms of accuracy of the performed counts, species preservation, and fine-grained characterization.

Clearly, computer vision techniques are called for to help to identify individuals in an automated way. Supervised learning methods, and to a more limited degree, semi-supervised approaches have already been started to be used (Pastore, Zimmerman, Biswas, & Bianco, 2019).

Pastore, V. P., Zimmerman, T. G., Biswas, S., & Bianco, S. (2019). Annotation-free learning of plankton for classification and anomaly detection. *bioRxiv*. doi:10.1101/856815

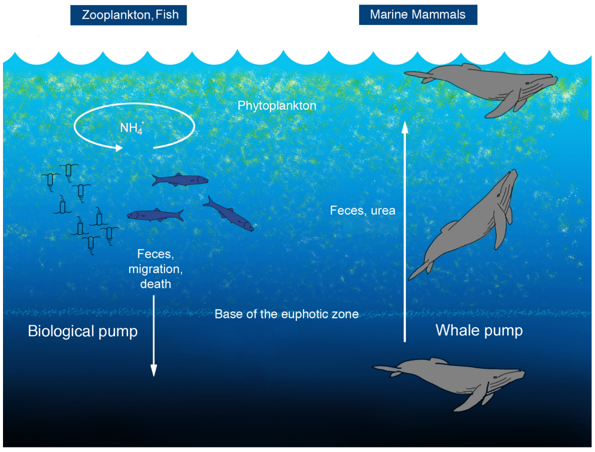

Figure 3.7: Whales movement and feeding across different depths makes them an essential actor in marine biodiversity and a potential key element for carbon capture. Source: Roman and Mccarthy, 2010.

However, there is an important gap to bridge in order to produce useful research tools. Figure 3.6 provides an illustrative outlook of the steps end-to-end that could be addressed, from satellite sensing to *in situ* sampling, etc.

The capacity crossing data from different sources is essential for the success of this work package. Work on WP I.2 is essential to this end. In particular, it should also integrate sources from plankton images *i. e.* Ecotaxa (Picheral, Colin, & J.-O., 2017) and the satellite images stored by the Chilean Data Observatory.[4]

Picheral, M., Colin, S., & J.-O., I. (2017). EcoTaxa, a tool for the taxonomic classification of images. url: http://ecotaxa.obs-vlfr.fr

4: http://dataobservatory.net

Task III.2.A Plankton identification from satellite images

Machine learning techniques will be designed to integrate 'omics' information with high-throughput/high-resolution plankton imaging and environmental data. Our goal here is to address the problem as wide as possible. For example, would it be possible, relying on Tara Océan data, the detected *in situ* populations crossed with satellite images be able to predict the presence of populations and provide tools to authorities and decision-makers. We would like to verify if it is possible to identify the presence of particular organisms based on satellite sensors.

Another approach is to take an indirect approach. Instead of quantifying the presence of different microscopic organisms, it would be possible to detect some large dimension objects that indicate the presence of such organisms. For instance, it has been hypothesized that whales have a big impact on the carbon capture process (Roman & Mccarthy, 2010). Whales cycle energy in the ocean as they feed in deep waters while then leaving their feces and urea at shallow depths (see Figure 3.7). Furthermore, recent studies (Häussermann et al., 2017; León-Muñoz, Urbina,

Roman, J., & Mccarthy, J. J. (2010). The Whale Pump: Marine mammals enhance primary productivity in a coastal basin. *PLoS ONE*, *5*(10). doi:10.1371/journal.pone.0013255

Garreaud, & Iriarte, 2018) that mass mortality events among whales have severe consequences on the balance of ecosystems, leading, for example, to the bloom of highly toxic algae.

Henceforth, the problem would be if it is possible to detect whales from satellite images, something that has been reported to be possible by Guirado, Tabik, Rivas, Alcaraz-Segura, and Herrera, 2019 and Borowicz et al., 2019 although it still requires further study in order to assert the possibility of doing this with minimal supervision.

Häussermann, V., Gutstein, C. S., Bedding-ton, M., Cassis, D., Olavarria, C., Dale, A. C., … Försterra, G. (2017). Largest baleen whale mass mortality during strong El Niño event is likely related to harmful toxic algal bloom. *PeerJ*, *2017*(5). doi:10.7717/peerj.3123

León-Muñoz, J., Urbina, M. A., Garreaud, R., & Iriarte, J. L. (2018). Hydroclimatic conditions trigger record harmful algal bloom in western Patagonia (summer 2016). *Scientific Reports*, *8*(1). doi:10.1038/s41598-018-19461-4

Guirado, E., Tabik, S., Rivas, M. L., Alcaraz-Segura, D., & Herrera, F. (2019). Whale counting in satellite and aerial images with deep learning. *Scientific Reports*, *9*(1). doi:10.1038/s41598-019-50795-9

Borowicz, A., Le, H., Humphries, G., Nehls, G., Höschle, C., Kosarev, V., & Lynch, H. J. (2019). Aerial-trained deep learning networks for surveying cetaceans from satellite imagery. *PLOS ONE*, *14*(10). doi:10.1371/journal.pone.0212532

Task III.2.B Connecting images and genomic features

The Tara Océan dataset provides an extensive overview of plankton images. Both images and genomic provide a lot of diversity to investigate. The connection between these databases via ML techniques could (i) state biogeography of the morphological diversity, and (ii) identify genes responsible for plankton shapes and morphologies.

This topic is mostly new and requires considering raw imaging data. Similarly, ocean images from space will give access in the near future to a lot of content. ML techniques to connect the trait of genomic diversity with the satellite images are required.

Task III.2.C Anomaly detection and explainable AI for automatic plankton discovery

Identifying plankton from microscope images has been already addressed. In this case, what we would like to address is a more general topic of how to identify unknown or out of context species automatically and, at the same time, provide explanations of why that organism represents an interesting specimen (sequence D-G-H-I in Figure 3.6). This would involve the application of transfer learning and domain adaptation in order to adapt to changes in the optics of the sensing equipment and subtle changes in the morphology of the populations.

As part of this task, it will be required to address this problem as object detection and instance segmentation problem. As, in addition to indicating the class of an object as image classification, it is also needed to indicate their location within a bounding box. In this category we find two main families of architectures: region proposals like the regions with CNN features, as for example, R-CNN (Girshick, Donahue, Darrell, & Malik, 2014), Fast R-CNN (Gir-

Girshick, R., Donahue, J., Darrell, T., & Malik, J. (2014). Rich feature hierarchies for accurate object detection and semantic segmentation. *Proceedings of the IEEE conference on computer vision and pattern recognition*

shick, 2015), Faster R-CNN (Ren, He, Girshick, & Sun, 2015), mask R-CNN (He, Gkioxari, Dollár, & Girshick, 2017), and You Only Look Once (YOLO) (Redmon & Farhadi, 2017).

Girshick, R. (2015). Fast R-CNN. *Proceedings of the IEEE international conference on computer vision*

Ren, S., He, K., Girshick, R., & Sun, J. (2015). Faster R-CNN: Towards real-time object detection with region proposal networks. *Advances in neural information processing systems*

He, K., Gkioxari, G., Dollár, P., & Girshick, R. (2017). Mask R-CNN. *Proceedings of the ieee international conference on computer vision*

Redmon, J., & Farhadi, A. (2017). YOLO9000: Better, faster, stronger. *Proceedings of the IEEE conference on computer vision and pattern recognition*

It will require extended use of causal inference to understand the relative unlikeliness of a given observation. Then, the image-based explainable AI method hint what parts of the observed organism that determining its selection. This tool could be potentially be deployed to Tara Océan expeditions to help them assess on-the-fly the populations they are sampling.

Expected outcome(s) of the work package: A new wave of methods that combine causality, explainable AI, computer vision and anomaly detection used to create new research tools for marine biologists.

Coordinating Inria team: Inria Chile

Participating teams: GO-SEE ComBi CMM PUC

4 Interaction and organization

The scientific organization will follow the three axes presented in Chapter 3. Since all the proposed developments can have impact on each other, communication will be a key issue. As for many Inria Challenges, this is the opportunity to spin up fruitful collaborations between teams.

4.1 Work packages interaction and integration

This project has as articulating objective the goal of producing theoretical and practical developments in the intersection of machine learning, artificial intelligence, modeling, simulation, and computational biology while yielding tangible and usable results that could be used in the understanding, prediction, and mitigation of the current global environmental situation. As a strength, external collaborators like CMM have been working for years in collaboration with Inria Chile and, at its time, Inria Chile has started or in already active collaboration with ANGE, BIOCORE, and TAU. It has to be said also that Marc Schoenauer is part of the Scientific Committee of Tara Océan Oceans together with PUC and CMM are two strategic partners of Inria Chile; being CMM the local partner of GO-SEE federation.

A measure of success for the former will be their publication in high-quality journals co-authored by partners. In order to achieve a proper transfer to our external partners for their realistic large-scale applications, this project should provide some mature software along with our methodological developments.

This project will design and consolidate a pipeline of models based on machine learning and probabilistic techniques that will be developed, when possible, using Inria software like scikit-learn (Pedregosa et al., 2011). Table 4.1 shows the scientific intersection domains and where the different teams will collaborate with each other.

Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., ... Duchesnay, E. (2011). Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12

A way to assess the impact and success will be the adoption of the results of OcéanIA as integrated tools to analyze the future Chilean Ocean Data Observatory.

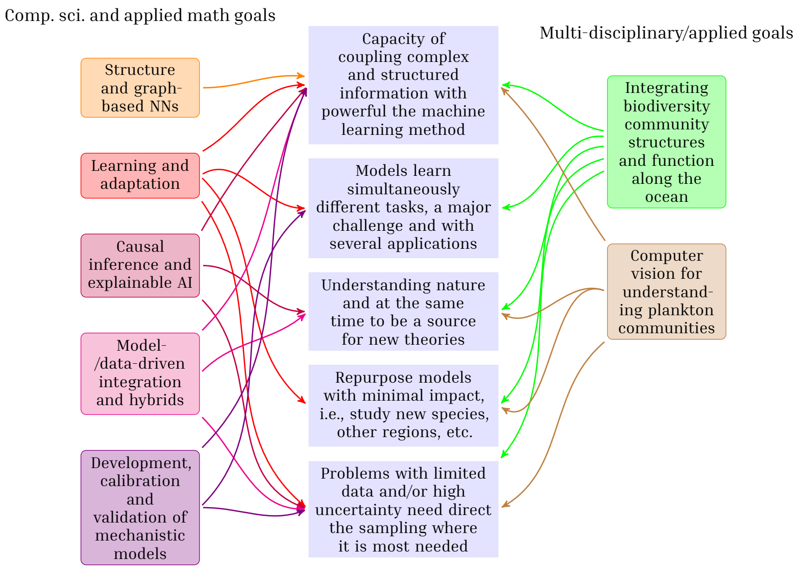

Figure 4.1: Interaction between the basic and applied science axes.

Table 4.1: Projection of work packages in Axis II with respect to the multi-disciplinary science actions (Axis III) expressing how of Inria and external teams will collaborate in them.

	WP III.1 **Integrating biodiversity community structures and function along the ocean** coord: BIOCORE	WP III.2 **Understanding plankton communities using AI, ML and vision** coord: Inria Chile
WP II.1 **Structured and graph-based neural networks** coord: Inria Chile	Inria Chile TAU CMM	Inria Chile TAU CMM ComBi GO-SEE PUC
WP II.2 **Learning and adaptation** coord: Inria Chile	Inria Chile TAU	Inria Chile TAU CMM ComBi GO-SEE PUC
WP II.3 **Causal learning and explainable AI** coord: TAU	Inria Chile TAU PUC	Inria Chile TAU CMM ComBi GO-SEE PUC
WP II.4 **Model-driven and data-driven integration and hybrids** coord: ANGE	ANGE BIOCORE Inria Chile TAU CMM PUC ComBi	N/A
WP II.5 **Development, calibration and validation of mechanistic models** coord: BIOCORE	ANGE BIOCORE Inria Chile CMM ComBi	N/A

4.2 Practical organization

This project is structured with two levels of involvement. The core partners will be actively involved in the proposed research and developments, while the rim members will be invited to general assemblies and targeted meetings and consulted for specific questions (Tara Océan and GO-SEE, but, as was described, some GO-SEE teams are already involved in the research tasks of this project). Note that this division between core and rim partners is not fix and will be reassessed at mid-term of the project. Depending the availability and interested of rim members they would be invited to join a more intense collaboration. In particular, they should provide a diversity of methods and principles that would enrich the project discussion and -if possible- serve to compare our proposals.

Long-distance collaboration is necessary but is not trivial to make it efficient. To ensure an effective collaboration, the project is built on two main practices. First, we will rely on installing a strong collaboration through the co-supervisions of all PhD students and post-doctoral researchers (and hence co-publications) as well as engineers. These co-supervisions will be implemented by regular sojourns of one or more weeks in the different locations (Paris, Saclay, Santiago de Chile, and Sophia-Antipolis). Regular video-conference meetings will also be organized between the teams. Second, we will share the numerical code into common libraries, using Inria collaborative development tools.

This will enforce visibility of each other developments and progress, and encourage interactions. Finally, one general meeting will be organized per year; with the possibility to either invite some other teams to the discussion (in the early stage of the project), or to organize an open workshop the same week (in a second phase). More frequent meetings will be organized on specific topic, only involving the relevant teams.

4.3 Dissemination actions

Dissemination actions, besides the publication of the scientific results in conferences and journals are grouped in three channels:

1. academic/scientific dissemination,
2. general public reach-out, and

3. open-source software contribution and dissemination.

Regarding academic/scientific dissemination, we plan to host workshops and special sessions in reference conferences in the areas of interest of the project. We also plan to organize annual one-week courses by members of the project for PhD students, researchers or engineers under the scope of the Inria Academy and/or the Inria Chile Talks. They could be organized at a different location each year in order to widen the audience and impact. Another possibility would be to organize an international summer school.

Reaching non-academic audiences and the general-public is essential to draw attention to the relevance of oceans, climate change, and science as the means to understand them and address the existing issues. Here we plan to create a reach-out program generating results in a form that is easy to share and modern, like videos and websites.

Finally, we would keep as a general goal to consolidate our work as reusable and redistributable software. Whenever possible, we will contribute with the existing Inria open-source project and, in cases where that option is not possible we will generate our own.

4.4 Intellectual property management

This important aspect has been discussed with the DGD-I and it will be strongly secured and regulated. All libraries developed in this Inria Challenge will be distributed under an open source license, ownership belonging to Inria. Developments of libraries will be under shared intellectual ownership of the original consortium members.

4.5 Attraction of further funding

In addition to the support provided by Inria, the team members will actively seek to attract additional funding to support more challenging activities. We have identified some of these funding sources. In particular, in France and Europe we plan to seek support from:

- Agence française de développement (AFD) / French Facility for Global Environment (FFEM)[1],
- Agence nationale de la recherche (ANR)[2],
- AI plan, and
- ERC H2020 and subsequent plans.

Similarly, in Chile we plan to request support from:

- Agencia Nacional de Investigación y Desarrollo (ANID),[3]
- Instituto Antártico Chileno,[4], and
- Corporación de Fomento de la Producción (Corfo).[5]

1: https://www.ffem.fr/en
2: https://anr.fr/
3: https://www.anid.cl/
4: https://www.inach.cl
5: https://www.corfo.cl

Final remarks | 5

Solving this challenge will enable us to translate biodiversity meta and big data into knowledge, making sense of heterogeneous sets of data. As a consequence, these studies will allow the development of a complete pipeline for the functional analysis of biodiversity and its relation with the environment, particularly in the Ocean but not uniquely. This will lead to the design of different services to the environmental community.

At the oceanic level, there are crucial issues that will be possible to be addressed after this project. In particular to predict biogeochemical cycles from 'omics' knowledge. Indeed, among the more than 150 million genes cataloged by Tara Océan, 30% code for enzymes. These are the components of the global ocean metabolic engine that can potentially be reconstructed and used to go beyond the description of metabolic potential to modeling, from this data, the quantitative metabolic responses of marine plankton in response to environmental variations. Another impact of this project is that it will be the seed to start thinking in next-generation ocean-climate models integrating biocomplexity.

Finally, this project aims to influence politicians and decision-makers with the out-coming new ocean-climate models. As a science-based decision tool, the complexity of the challenge is then to mitigate the risks of the non-adoption.

In the early stage of the project, some additional funding will be requested in local or national programs, as stated in the previous section, to compensate for the extra cost of the proposed long-distance co-supervision. Once mature enough (at the end of the project) our developments will offer us the possibility to launch a wide range of larger-scale projects.

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