

# HOW THE INVESTIGATION OF THE LINK BETWEEN MARINE FOOD WEB AND BIOREMEDIATION WOULD LEAD TO AN IMPROVED HUMAN HEALTH RISK ASSESSMENT

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## Background and Motivation

The **Marine Environment** is a sink of contaminants that, if persistent, sooner or later will be reintroduced in the marine ecosystem which consequently represents also a source of contaminants[1]. This is a **hazard for both humans and wildlife**, which are exposed to the ingestion of contaminated fish [2].

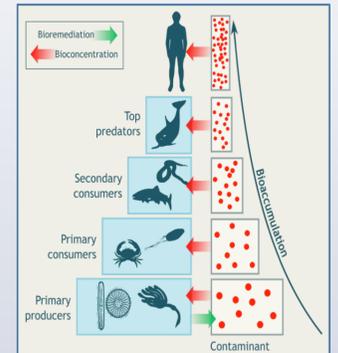
Keeping in mind that the chemical risk cannot be completely avoided, pollutants monitoring and control can represent a strategic and useful tool to assess the risks for the human health coming from a contaminated food chain.

Due to the complexity of the marine ecosystem, it arises the need to study its different sub-ecosystems in a **multiscale approach**, to understand the ecological implications of the **micro-scale** (microorganisms) on the **macro-scale** (food-web), up to the top of the food chain where humans are placed.



**Microorganisms** represent the base of the marine food web and the prominent part of the whole marine environment in terms of biomass and chemical activity. They are the capability to interact with organic contaminants [3] by decreasing their bioavailability and their eco-toxicological effect for both target and no-target organisms. **Microbial ecology** can clarify how the **bioremediation** potential of microorganisms can influence, in polluted environments, the **molecular pathways** that lead to the bio-concentration of the chemicals along the food chain under an **Environmental Health** perspective.

Due to their high persistence, lipophilicity, long-range transport and other chemical and physical properties, **Polychlorinated Biphenyls (PCBs)** are subject to the phenomena of **bio-accumulation** and **bio-magnification**. Considering that PCBs have been extensively used worldwide in hundreds of industrial and commercial applications, they represent a global health concern.



**Aim:** Bringing together the study of molecular, microbial and marine ecology under a Systems Biology perspective, in order to investigate the complex multiscale interactions between the microbial compartment and the marine food web. More importantly, we aim to optimize multiple indicators of environmental health by controlling and tuning the bioremediation pathways of microorganisms with the help of tools from Synthetic Biology.

## Methods

### Mass Balance Analysis

The characteristics of the Northern and Central Adriatic ecosystem in terms of biomass flows and trophodynamic indicators, have been reconstructed from data collected in [4], by using the Ecopath model based on trophic mass-balance analysis.

Figure 1 shows the biomass flow network of our case of study.

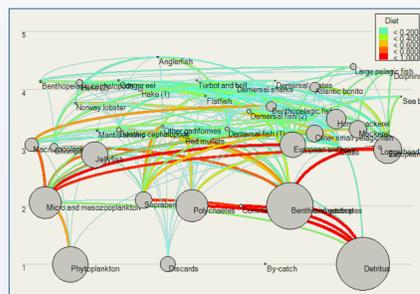


Fig.1 Biomass flow network of the Adriatic Sea reconstructed from [4]. Nodes represent functional groups with radius proportional to their biomass. Edges, and their thickness, represent biomass flows among groups.

### Ecotoxicological Model and Bioremediation Pathways

We defined a toxicokinetic model having a single compartment per functional group. The total contaminant concentration in the biomass of group  $i$  can be estimated as the result of inflows (uptake from seawater and contaminant in immigrating biomass), and outflows (predation, egestion, metabolism, death and emigration).



Fig.2 Microbial dioxin degradation pathways of PCB, PCDD and PCBF. Green boxes highlight those operated by *P. Putida*. Source KEGG PATHWAY database

Several metabolic pathways related to the biodegradation of xenobiotics operated by a large variety of microorganisms, may be taken into account. As an example, Figure 2 shows the dioxin degradation pathway operated by *Pseudomonas Putida*.

### Flux Balance Analysis (FBA)

We apply a computational technique from synthetic biology: Flux Balance Analysis (FBA), which is typically used for genome-scale metabolic network reconstructions, and multi-objective optimization [5].

The main idea behind FBA is to determine the flux through the metabolic network in order to optimize a reaction of interest (e.g., maximization of biomass production). The flux through all of the reactions of the network is estimated at mass balance conditions. In this case, the optimization of the reaction corresponds to a linear programming problem.

In order to integrate biomass and contaminant flows with the bioremediation molecular pathways, we have used the R-package LIM [6] for linear inverse modelling. Starting from a set of data samples and specifying linear equalities and inequalities (constraints) over the flows, LIM allows estimating the space of solutions and optimizing food web flows/microbial reactions, according to a particular objective function.

## Preliminary Results

Starting from the whole Adriatic food web, we have reconstructed a sub-network consisting of five species. We have characterized contaminant flows among species following the biomass flows and based on PCBs concentration data from literature. Flows from/to the detritus have been considered as well.

The radar diagram in figure 3 shows the admissible ranges of contaminant flows between the species considered.

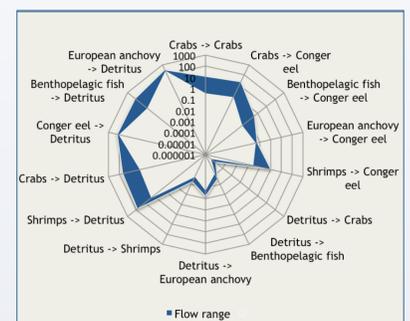


Fig. 3. Radar diagram depicting the admissible flow ranges of PCBs.

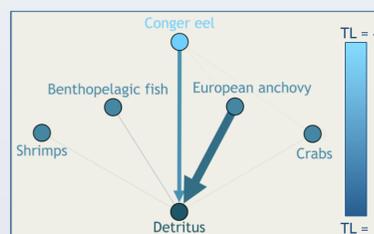


Fig. 4. Network representation of contaminant flows from marine species to detritus. Different colors indicate different trophic levels (TL) and arrow thickness is proportional to the optimal flow values.

Among the possible solutions, the optimal values for biomass and contaminant flows have been computed in order to find the combination that minimizes the environmental availability of contaminants, i.e. the sum of all PCBs flows.

## Conclusion and future work

We report that the application of methods from Computational Systems Biology in the study of the multiscale effects of contaminant bioremediation on the marine food web looks promising.

As future work, we aim at applying multi-objective optimization techniques, which allow finding the best trade-off (Pareto front) among multiple and possibly conflicting functions to optimize.

This would allow us to engineer the microbial metabolic fluxes, in order to optimize multiple high-level environmental indicators, like the minimization of contaminant uptake by species at the higher trophic levels, the maximization of water quality and the effects of the co-bioremediation activity operated by heterogeneous microbial community.



Fig. 4. Example of Pareto optimality between the maximization of water quality and the microbial activity.

## References

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