
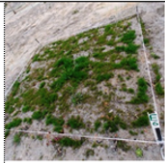

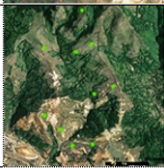


Habilitation Thesis

Contributions to the development of theoretical biology
 and of interdisciplinary directions at the interface
 between life sciences and earth system science

Scale	System	Process	Dependent variables	Independent variables
	Plants in their environment in experimental setting	Plant growth without interspecific relations	Plant traits	N, P, metals, light etc
	Soil - plants - microorganisms system in experimental plots 2 x 2 m	Erosion, percolation	Critical soil share stress, erodibility, hydraulic conductivity	Plant traits , other soil properties
	Field plots, discretization units (DUs) of models 10 x 10 m, 50 x 50 m	Plant growth with interspecific relations	Plant traits Roughness	Soil properties, plant diversity plant traits
	Catchment with soil, plants and water, split in DUs e.g. 10 km ²	Water flow, erosion, sediment transport, sedimentation	Surface water speed Soil detachment rate	Topography, critical soil share stress, erodibility, hydraulic conductivity,

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Thesis summary

The **goal** of this thesis is **to present the foundation, implementation, and future developments of a research program at the interface between biogeochemistry and ecotoxicology of heavy metals.**

The **method** used to structure the thesis **is that of the logic of the scientific discovery.** I have extracted and grouped the contributions or the relevant parts of them into:

- theoretical (provides the general background of empirical investigations, the framework to formulate hypotheses),
- methodological (provides structured approaches for exploratory research and to formulate and test hypotheses),
- field, and experimental research (takes place in the theoretical framework and implements the methodological approach)
- mathematical modeling (allows the investigation of simplified formulations of the natural processes to detect the influence and relative importance of key variables), and
- management and institutional development (whose success depends on all research aspects, from theoretical and methodological background to the soundness of empirical research, and the realism and awareness about the limitations of mathematical modeling).

The presented contributions span from 2005 to 2024. The **originality** of this thesis comes from the method of organization and presentation, underlining the coherence of the research program.

The main theoretical contributions are a reconstruction of the Darwinian law of growth with reproduction, a reconstruction of the potential socio-ecological complexity from the elementary productive processes, a conceptualization of the relationship between multi-scale productive processes at organismal, population and community scale, and the standard nested hierarchy of ecological systems, and a general concept of resilience.

The methodological contributions are an integrated technique for knowledge mapping and conceptual analysis, a framework for integrated modeling of metals biogeochemistry based on the standard nested hierarchy of ecological systems, a highly complex methodology for upscaling ecological processes from a relatively smaller community scale to larger target scale, a simpler complementary framework for integrated modeling based on coupled biological and abiotic processes occurring at different scales, and a methodological framework to study the resilience of biogeochemical services to heavy metals stress.

The empirical contributions published by now are in two directions, one related to scale-dependent patterns of the distribution of organisms in contaminated areas, and one consisting of experimental investigations of biogeochemical processes in soil-plant systems. In the first direction, we found that the decrease of richness in contaminated sites compared to reference sites seemed to be larger as the scale of the organism was smaller, in each site, and a positive correlation between the coefficient of variation of mites' species richness (log-transformed) and the coefficient of variation of the scores extracted by PCA from in situ measurements of geochemical variables on the tailing surface in each station with a plot of 2 m². In the second direction, we investigated the leaching of elements from soil-plant systems, and the control of toxic elements, and P on plant oxidative stress. While these contributions focused on the effects of heavy metals and nutrients in the soil as independent variables, a complementary approach in the field was to look for the effect of morphometric plant traits on the properties of the vegetation cover controlling the water flow on a hillslope. We produced and published a TRL2 custom-oriented integrated tool-box of procedures/workflows and software

modules for extraction of LIDAR metrics describing functional plant cover traits, deterministic models of processes describing the role of plants in the production of target ecosystem services, and coupled experimental and field scale investigations for validations and simulations.

The mathematical modeling started from the problem of including spatially explicit the role of vegetation in erosion models (and associated transport of heavy metals). This led to two complementary problems, one of porting data between scales (different discretization of the model), and one of the deterministic hydrological model with plant variables controlling the flow. We produced a data porting tool and demonstrated it on a model catchment using cellular automata of water flow without vegetation components and a 1D model accounting for the role of plants on the water flowing over hill-slopes, using vegetation porosity as a plant variable.

The environmental management contributions are in a classic nested hierarchy approach (approaches for the integrated monitoring of emergent ecosystem services and restoration of a large alluvial island), and in a multi-scale process approach (triggering an accelerated succession in contaminated areas by inoculation with microorganisms -kind of an eco-remediation technique coupling site scale and landscape scale measures, and a complex approach for catalyzing the development of ecosystems of innovation for environmental services – using bottom-up and top-down measures).

I used the conceptual and methodological results in a simplified form also to organize the teaching, especially by classifying the epistemic strategies reducing the complexity of productive processes in the complementary natural and social domains. At stake was to stimulate interdisciplinarity for solving complex missions instead of competition between experts specializing in various fields and sub-fields.

The future research lines of the research program are also on theoretical, methodological, empirical, mathematical modeling, environmental management, and institutional development directions. In the theoretical direction, we are interested in the comparative ontology of biological and environmental sciences (needed for integration in information systems) and the problem of how different is conceptualized time in different fields and sub-fields of research (with consequences on the up-scaling of complex processes). The methodological direction is coupled with the institutional development of a Critical zone Observatory for catchments with important industrial activity in their structure (including mining). Here we have an already funded Fulbright project and a large-scale project draft for an innovation ecosystem oriented towards the development of a cumulative-impact assessment method in catchments with multiple types of impacts. In this framework, we will implement exploratory projects (for instance one dedicated to the resilience of biogeochemical services to climate change stress, using a stoichiometric approach of elements retention in transversal and longitudinal buffer zones) and projects for technology development (for instance developing to TRL3 the already mentioned LIDAR-based technology).

Rezumatul tezei

Scopul acestei teze este să prezinte fundamentele teoretice, implementarea și dezvoltările viitoare ale unui program de cercetare la interfața dintre biogeochimia și ecotoxicologia metalelor grele.

Metoda folosită pentru a structura teza este cea a logicii descoperirii științifice. Într-o abordare analitică a ceea ce ar putea fi invalidat la niște rezultate științifice am grupat contribuțiile (sau părțile relevante din ele) în următoarele categorii:

- teoretice (furnizează fundalul general al investigațiilor empirice, cadrul în care sunt formulate ipotezele)
- metodologice (furnizează abordări structurate pentru cercetarea exploratorie sau pentru formularea și testarea ipotezelor)
- cercetare în teren și experimentală (are loc în cadrul teoretic adoptat și pune în practică abordările metodologice)
- modelarea matematică (permite investigarea unor formulări simplificate ale proceselor naturale pentru a detecta influența și importanța relativă a unor variabile cheie) și
- managementul și dezvoltarea instituțională (al căror success depinde de toate aspectele cercetării enunțate mai sus).

Contribuțiile sintetizate acoperă perioada dintre 2005 și 2024. Originalitatea tezei este dată de metoda de organizare și prezentare, care subliniază coerența programului de cercetare.

Principalele contribuții teoretice sunt reconstrucția legii de creștere cu reproducere darwinienne, o reconstrucție a complexității potențiale socio-ecologice pornind de la procese productive elementare, o conceptualizare a relației dintre procesele productive organizate la multiple scări ale organismelor, populațiilor și comunităților și ierarhia standard de sisteme ecologice, precum și un concept general de reziliență.

Contribuțiile metodologice sunt o tehnică integrată de cartare a cunoașterii științifice și analiză conceptuală, un cadru pentru modelarea integrată a biogeochimiei metalelor bazată pe ierarhia standard de sisteme ecologice, o metodologie foarte complexă de ridicare la scară a proceselor caracteristice unor comunități de scară relativ mică către o scară țintă (de obicei o zonă de interes managerial), un cadru complementar mai simplu pentru modelarea integrată bazată pe cuplajul unor procese abiotice și biologice care au loc la diferite scări, și un cadru metodologic pentru cercetarea rezilienței serviciilor biogeochimice la stresul datorat metalelor grele.

Contribuțiile empirice publicate până acum sunt pe două direcții, una despre tiparele de distribuție ale organismelor din zone contaminate la scări diferite, iar alta constând în investigații experimentale al unor procese biogeochimice în sisteme sol-plantă. Pe prima direcție, am constatat că scăderea diversității specifice a organismelor în situri contaminate comparativ cu cele de referință este mai mare atunci când scara organismelor este mai mică. De asemenea, există o corelație pozitivă între coeficienții de variație ai bogăției specifice a acarienilor din subrobele luate de pe parcele de 2m² distribuite pe un iaz de decantare și coeficientul de variație al variabilelor geochimice ale substratului în interiorul acelor parcele. Pe direcția experimentală, am investigat percolarea metalelor grele din sisteme sol-plantă și felul cum elementele toxice și fosforul influențează stresul oxidativ al plantelor. Într-o abordare complementară, am investigat și cum anume trăsăturile morfometrice ale plantelor influențează curgerea apei pe pantele cu covor vegetal și indirect modificarea proprietăților chimice ale solului prin transportul dizolvat și particulat al elementelor. Am produs, de asemenea, o procedură la nivel de maturizare tehnologică 2 pentru estimarea trăsăturilor funcționale morfologice ale părții superioare a plantelor și a rugozității și porozității covorului vegetal din date LIDAR.

Problema de la care am început modelarea matematică a fost cea a includerii distribuite spațial a rolului vegetației în modele de eroziune, precum și a transportului asociat de metale grele. Aceasta a condus la două probleme complementare, una de portare a datelor între scări de diferite (între diferite feluri de discretizări spațiale ale modelelor) și una de producere a unui model determinist în care variabile măsurabile ale plantelor să controleze curgerea. Am produs un model de portare a datelor de la grid pătratic la grid hexagonal și l-am aplicat folosind un alt model de curgere a apei (cu automate celulare în rețea hexagonală, dar fără influența plantelor) într-un bazin hidrografic. Apoi am produs și modelul determinist în varianta 1D, rolul plantelor fiind inclus printr-o variabilă de porozitate a covorului vegetal.

Contribuțiile la managementul mediului au folosit inițial abordarea ierarhică standard, apoi cea nouă bazată pe procese cuplate. În varianta clasică am contribuit la proiectarea monitoringului integrat al serviciilor ecosistemice emergente în sisteme fluviale și la proiectarea restaurării unei insule aluviale mari din lunca Dunării. În varianta cu procese cuplate am abordat problema accelerării succesiunii ecologice în zone miniere folosind inocularea cu microorganisme în zonele contaminate în cadrul proiectelor de ecoremediere și măsuri complementare la scări mai mari. O a doua direcție abordată în această variantă a fost catalizarea dezvoltării ecosistemelor de inovare pentru producerea de servicii de mediu.

Pe plan didactic, am folosit rezultatele conceptuale și metodologice pentru a organiza conținuturile disciplinelor făcând apel la o clasificare a strategiilor de reducere a complexității proceselor productive în domeniile științifice biologice/ecologice și sociale. Miza abordării de acest fel a fost de a stimula cooperarea între viitori specialiști din domenii diferite pentru a rezolva probleme complexe.

În ce privește direcțiile de cercetare viitoare, pe plan teoretic voi focaliza pe ontologia comparativă a științelor biologice și ale mediului, care este de interes în proiectarea sistemelor informaționale pentru probleme complexe de monitoring și de cercetare, și pe modul de conceptualizare a timpului în diferite domenii și subdomenii de cercetare, care e o temă foarte importantă pentru ridicarea la scară în timp a proceselor de scări relative temporale mai mici. Direcția de interes metodologic este cuplată cu dezvoltarea instituțională a unui Observator de Zone Critice pentru bazine hidrografice cu activități industriale miniere și de procesare a minereurilor în structura lor. Am obținut un proiect Fulbright pentru transferul cunoașterii necesare în acest sens, este în curs de dezvoltare un proiect pentru crearea unui ecosistem de inovare dedicat în special metodologiilor de evaluare a impactului cumulativ al unor multiple surse de poluare și multiple proiecte de control al poluării în bazine hidrografice, împreună cu alte tehnici și metode necesare în acest scop și sunt aplicate proiecte de cercetare fundamentală și aplicativă.

Part I – Scientific and professional achievements

“Are biogeochemists adequately unified in addressing some of these key global issues in the 21st century? Most biogeochemists would agree that better links are needed with Earth system models, including better links between biogeochemical cycling, organismal traits and their changes, and environmental modeling. This is a major challenge requiring connections between cellular and organismal level systems biology with observational and modeling studies of global biogeochemical cycles. [...] linkages, between biogeochemistry, evolutionary biology, and social sciences, are what we believe to be some key foci for biogeochemists in the coming decades.”

Bianchi et al. (2021)

Introduction, goal, and method

Figure 1 below presents a partial model of the scientific knowledge production system, and figure 2 shows a scheme of how local theories (developed in a disciplinary scientific field or subfield) are related together to reduce the complexity of socio-natural processes (Iordache 2019). The research ecosystems are complex, with many interrelated modules having different functions (figure 1). The coherence of scientific knowledge results from the subtle relationships between the very diverse results of many scientific fields. These facts are highly relevant for any complex interdisciplinary problems, such as environmental problems.

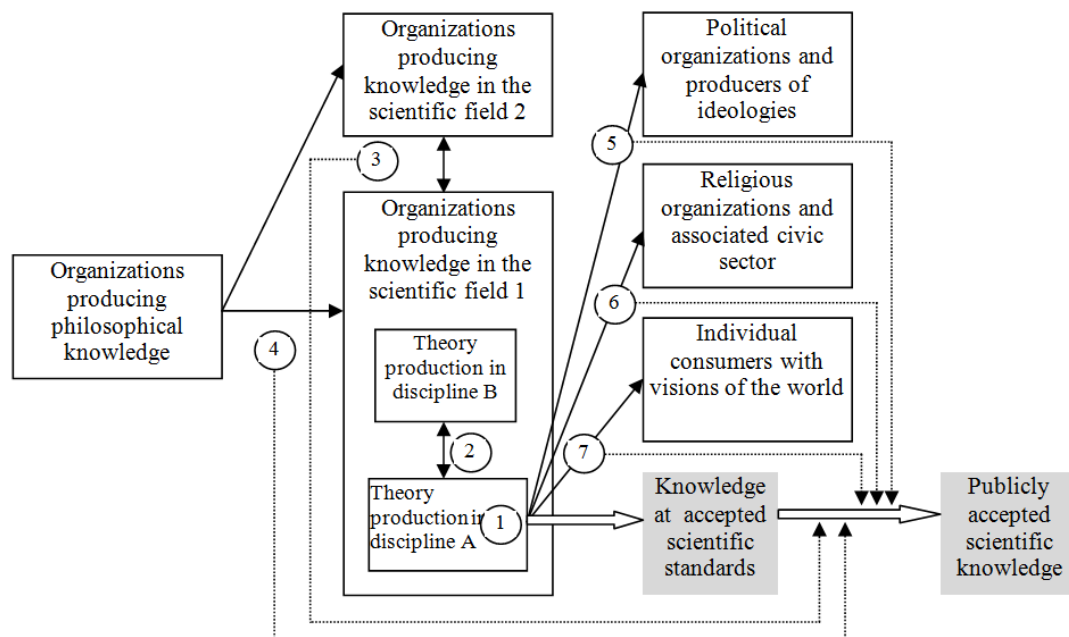


Figure 1 A partial model of the scientific knowledge production system. The technology transfer is not included in the scheme (Iordache 2019). **Legend:** 1 = production processes in disciplinary sub-field (e.g. ecophysiology), 2 = cooperation between sub-fields to solve more complex problems (e.g. ecotoxicological problems). 3 = Interdisciplinary cooperation to solve problems of even larger complexity (e.g. biogeochemical, socio-ecological problems), 4 = theoretical research at the interface between theoretical subdisciplines (e.g. theoretical biology and ecology) and philosophy of science (about assumptions, conditions of possibility, conceptual and theoretical diversity, epistemic standards). 5, 6, 7 = popularization and use/misuse of elements of scientific knowledge.

On a short time scale (a project scale, 3-5 years) the activity of a researcher is either theoretical, methodological, or empirical, and usually will not cover all these topics. The researcher may engage in the mathematical modeling of processes, focus on technology transfer, assist decision-making, or target the development of new institutional frameworks for research and development, but will not do all these things in a single project. However, when the research spans a long time (decades) and is organized in a research program, many, if not all these different dimensions of scientific research are covered.

Figure 2 *Up* Input of notions from common language and formal sciences. *Down* Types of local theories that reduce the complexity of socio-natural processes (adapted from Iordache 2019). The yellow stars indicate the areas of the contributions summarized in this thesis. In red are mentioned the chapters at the interface with the philosophy of science and social sciences. The blue star shows an area with contributions not included in this thesis, although relevant for the management of ecosystem services and the problem of sustainable development¹.

My achievements can be grouped in time into three phases (figure 3): a starting phase (Odum style biogeochemistry), a transition phase, and a phase with coupled abiotic and biotic processes.²

In the holistic phase, the main achievements are 1) a monograph about the ecotoxicology of heavy metals (code F1-Exp.1 in figure 1) 2) an international chapter conceptualizing the structure of larger river systems (TEB1), 3) two articles about restoration and integrated monitoring in a supplement of Archiv fur Hydrobiologie (Mng.1). In the second part of the holistic phase, I acquired formal competence in the philosophy of science.

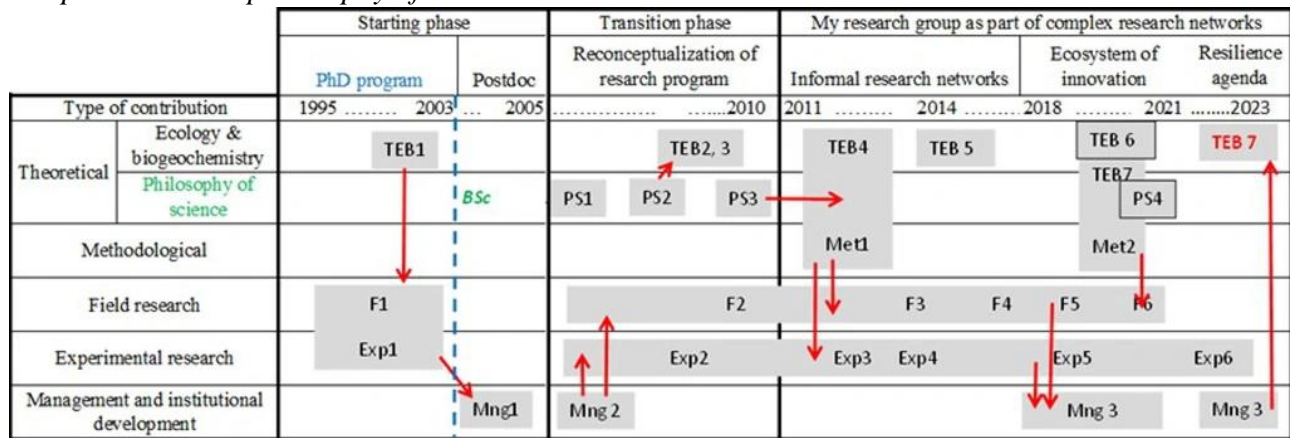


Figure 3 Distribution in time and relations between scientific achievements. Legend: achievements based on field research (F1-F6), on experimental research (Exp.1-Exp.6), achievements in theoretical aspects and biogeochemistry (TEB1-TEB7), achievements in support activities for the main research (management and institutional development, economics – Mng1- Mng4, philosophy of science PS1-PS4).

In the transition phase, I looked for conceptual solutions between full biogeochemical cycles and analytic investigations of separate processes in cooperation with mathematicians (concept of integrated modeling in biogeochemistry PS1), and with experts in soil groups of organisms (structural model of optimized complexity for the role of ectomycorrhizal fungi). I produced a reconstruction of the ecological productive processes in Darwin's "Origin of species" (PS2), which was then used for a Springer chapter about foundations of integrated modeling in biogeochemistry (PS3).

Also, in the transition phase, I coordinated the reintegration of a Marie-Curie Post-Doc from the Friedrich-Schiller University of Jena, with expertise in experiments in mining areas (Mng.2). In 2009, we used budgets of elements and ecological succession in the design and interpretation of lysimeter experiments (Exp2). In our new fieldwork, a milestone related to scales of organisms with their distribution in mining areas (F2). Meanwhile, an article about denitrification at the European scale, including some of the work done in the holistic phase, was published (it will not be reported in this thesis).

In 2010 I became director of our research centre and catalyzed a research network that since 2018 transformed into a formal ecosystem of innovation (Mng.3 with research agenda for 2021-2030). As an informal leader, I have coordinated the literature reviews for interdisciplinary Springer chapters published as main author (role of mineralogy, organic matter, arbuscular mycorrhizal fungi, ectomycorrhizal fungi, TEB4), or single author (succession and biogeochemical processes in mining areas, TEB6). We applied the methodological conclusions of these theoretical contributions in our field and experimental research.

The method used to structure the thesis is that of the logic of the scientific discovery. I have extracted and grouped the contributions or the relevant parts of them into:

- theoretical (provides the general background of empirical investigations, the framework to formulate hypotheses),
- methodological (provides structured approaches for exploratory research and to formulate and test hypotheses),
- field, and experimental research (takes place in the theoretical framework and implements the methodological approach)
- mathematical modeling (allows the investigation of simplified formulations of the natural processes to detect the influence and relative importance of key variables), and
- management and institutional development (whose success depends on all research aspects, from theoretical and methodological background to the soundness of empirical research, and the realism and awareness about the limitations of mathematical modeling).

Thus, I start with theoretical contributions (process 4 in figure 1), continue with methodological contributions for cooperation between scientific fields and sub-fields (processes 2 and 3 in figure 1), with disciplinary and interdisciplinary empirical results (processes 2 and 3 in figure 1), with mathematical modeling (process 2 in figure 1), and finish with the contributions to knowledge transfer for decision making and the development of institutional frameworks for complex environmental problems (involving indirectly, besides institutional channels, also a complex interplay of the processes 5, 6 and 7 in figure 1).

The presented contributions span from 2005 to 2024. The **originality** of this thesis comes from the method of organization and presentation, underlining the coherence of the research program. The new text, written especially for this thesis, is in regular font. The text cited from the contributions is in italics. Besides the major articles and book chapters, I have also used complementary information from several scientific communications, reflecting good quality data sets and important contributions with manuscripts under development.

A. Theoretical contributions

A1. A reconstruction of the Darwinian law of growth with reproduction

A reconstruction of “The Law of Growth with Reproduction” from Darwin’s „Origin of Species” leads to the following result (from Iordache (2010), translated in Iordache et al. (2012)):

A productive process “i” allowing potential natural selection is a system of the following form:

$$(P_i, I_i, G_i, I_j, G_j, M^{rel}_i, M^{rel}_j, S, M^{ob})$$

in which

Properties which should be characterized using an observation model, theoretically independent from the structural model S , are:

P_i , a property or a set of properties describing the biological production of the entity i , with i from 1 to n , where n is the population size and $n \geq 2$ (example: P^g – growth of biomass, or P^r number of descendants by reproduction)

I_i , a set of observable properties at space-time scales smaller than the maximal scale of the organism i (e.g., properties of parts of an organism, genes, etc.)

G_i , a set of properties observable at the maximal scale³ of the organism (e.g., many phenotypic traits)

I_j , are sets of observable properties at space-time scales smaller than the maximal scale of the organisms j , with j from 1 to n excepting for i

G_j , are sets of properties observable at the maximal scale of the organisms j , with j from 1 to n excepting for i

M^{rel}_i , is a set of relational properties between organism i and its environment (the „perceived” environment of organism i)

M^{rel}_j , are sets of relational properties between the organisms j and their environment, with j from 1 to n excepting for i (the “perceived” environment of each organism)

M^{ob} , are intrinsic and relational properties (different from M^{rel}) of the environment coupling the M^{rel} sets and having their distinct lawful dynamics (e.g. the dynamics of the properties in M^{ob} are due to the abiotic transport of resources from areas with large concentrations/densities to areas depleted by the organisms exploring their local environment/home range).

S is the structure of the system of properties described above. S is characterizable by a structural model decomposable into **a production law L** expressed by a mathematical function of the form $P_i = L(I_i, G_i, I_j, G_j, M^{rel}_i, M^{rel}_j)$ (**production model, S_p**) and one or many coupled structural models of environmental entities characterized by the properties M^{rel}_i, M^{rel}_j and M^{ob} (**models of unproductive objects, S_u**). Without competition, the production law reduces to $P_i = L(I_i, G_i, M^{rel}_i)$. The coupling between production sub-models and the models of unproductive objects occurs at the level of M^{rel} . The coupling between productive sub-models takes place at the level of P and M^{rel} (P or a property structurally linked to P – I or G – in a productive sub-model is M^{rel} in another productive sub-model).

The process giving the identity of the potential unit of selection is a system $(P_i, I_i, G_i, M^{rel}_i, S_p)$ describing the development of the organism in the context of competitive organisms.

³ E.g. the spatial limits of a sessile organism give its maximal scale, and the home range gives the maximal scale of an actively mobile organism. The maximal scale is of methodological interest and allows all the traits of an organism to be measured, including for mobile organisms their behavioral traits.

For selection to occur the following conditions should be fulfilled:

The condition of a finite lifetime: the lifetime of the potential units of selection is finite.

The condition of coupling: M^{rel}_i and M^{rel}_j are not fully decoupled in space-time at the existence time scale of the units of selection (i.e. they do not have independent dynamic; either these properties characterize environmental objects which – by M^{ob} – are the same for all organisms, or are parts of a more complex environmental object which are in causal relation at the existence time scale of the units of selection).

The condition of scarcity: to have scarcity in the productive object (it is a condition linked to the functional relationship between P and M^{rel} such as to have the Darwinian „struggle for existence”; when a resource is not a limiting factor, there is no struggle for it).

The condition of variability: to have variability of the values of I_i and/or G_i and/or M^{rel}_i in such a way that P_i would be different because the **fitness** would be different. This condition is needed for sorting the units of selection by P_i . **Fitness** in this reconstructed framework is a measure of the efficiency and effectiveness of the production process and is not defined as the outcome of production P (e.g. number of descendants), which is only an indicator of fitness.

In the absence of the conditions for selection and by eliminating the condition that $n \geq 2$ one has the general form of a productive process.

The distinction between M^{rel} (perceived environment) and the general environment allows not only to specify the local selective environment when the general environment is heterogenous in space but also can be used to account for the development of cognitive systems with different abilities to describe the real general environment, with consequences on the behavioral traits and fitness of the natural or socio-economic productive objects.

A1.1. Reconstruction of the potential socio-ecological complexity from the elementary productive processes

The importance of the reconstruction presented in the previous chapter is that it is general, not dependent on the kind of variables involved in the model. It can be used as a formal template for any production and selection process and can support the formulation of very general problems specific to interdisciplinary research programs.

The model can be used directly or can be used to derive more complex general processes. For instance, one more level of complexity can be obtained by interspecific coupling a productive process characterized by a certain scale (e.g. a plant process) with other productive processes at smaller and larger scales by the M^{rel} (e.g. with microbial processes in the rhizosphere and first-order consumers processes coupled to the aboveground parts of the plant). Another level of complexity can be derived by organizing these coupled processes into autocatalytic processes.

Any of these three general levels of complexity can be specified with variables from the ecological, economic, social, and cultural fields allowing the formulation of operational research programs. Once specified, one can build an extra level of complexity by coupling the specified models. For instance, one can build simple socio-ecological models coupling the productive processes of an organization involved in the management of natural resources with the productive processes of a population of organisms, or more complex ones up to full natural autocatalytic processes coupled to socio-economic autocatalytic processes. Of course, increasing the complexity of the model adds to the already very large cross-scale dimensionality existing in the elementary productive models, which raises the problem of simplifying this to allow operational research. I will explore this problem in the next chapter.

A1.2. Modularization strategies of the complex production processes

Two complementarity strategies present in the “Origin of Species” are to organize the elementary production processes in production systems by nested hierarchies of objects (from parts of organisms to whole organisms, to organisms with their external resources) and to embed such elementary production systems of different species in three-dimensional parts of nature.

The production law $P_i = L(I_i, G_i, M^{rel}_i)$ is modularized (by applying sharp boundaries in the physical space) in a nested hierarchy of objects leading to a developmental system (DS, Iordache 2009, Iordache et al. 2011 as a formal generalization of the homonymous concept of Susan’s Oyama). A development system (DS) is composed of a teleonomic (as if it would have a purpose, for example organisms at Darwin) or teleologic object (TO, having an intentional human purpose, such as farms and projects to obtain new varieties of domestic species, in Darwin’s book) with P_i and G_i as emergent properties, I_i as properties of its structural parts, and the objects with value for it as described by the properties M^{rel}_i located in its environment (Iordache 2009).

Due to the multiscale character of the DS, the discretization of the physical space of the ecosphere in nested three-dimensional units (parts of nature at Darwin, nested hierarchies of ecosystems in current vocabulary) will always cut the continuum of scales in such a way that some of the DS will have parts outside the ecosystem (figure 4). While Darwin communicated the fact that the parts of nature produce new species at various rates (some geographical regions were richer than others), he did not have at the time knowledge about the levels of production complexity supporting this higher productivity (which we currently know that is related to the functioning of the ecological autocatalytic cycles).

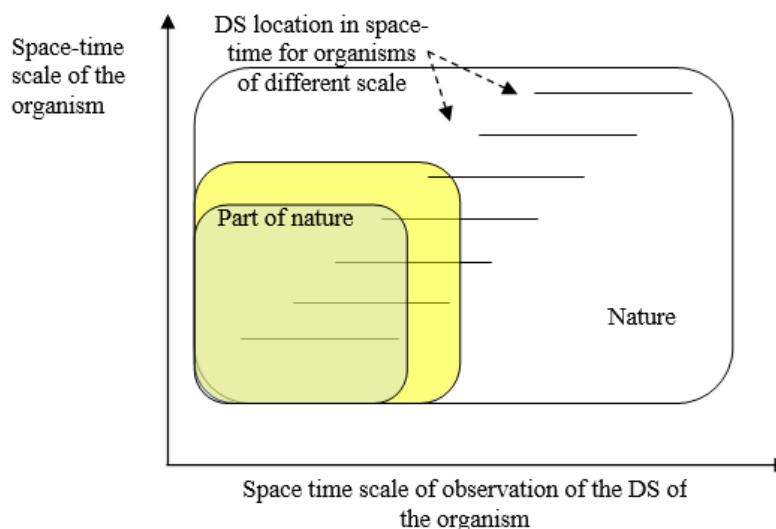


Figure 4 *The space-time location of the Darwinian nature and its parts compared to the scale of the DSs. In contemporary technical language nature and its parts are ecological systems at various hierarchical levels (ecosystems, landscapes, ecoregions, etc) (Iordache et al. 2012).*

Besides these two original strategies, the biology, ecology, and environmental sciences have a large array of approaches to deal with the complexity of nature by simplification. For instance, in evolutionary theory a well-known strategy of the synthetic theory of evolution, which neglects the heterogeneity of the environment and the developmental processes associated with the ontogeny of each organism and produces results explaining the changes in the frequency of genes in populations of organisms. Figure 5 compares the reconstructed entities involved in natural selection in the „Origin of Species” compared to those assumed in the synthetic theory of evolution. Other information about the development of the evolutionary research program with complementary evo-devo and eco-evo-

devo approaches is available in Iordache (2008).

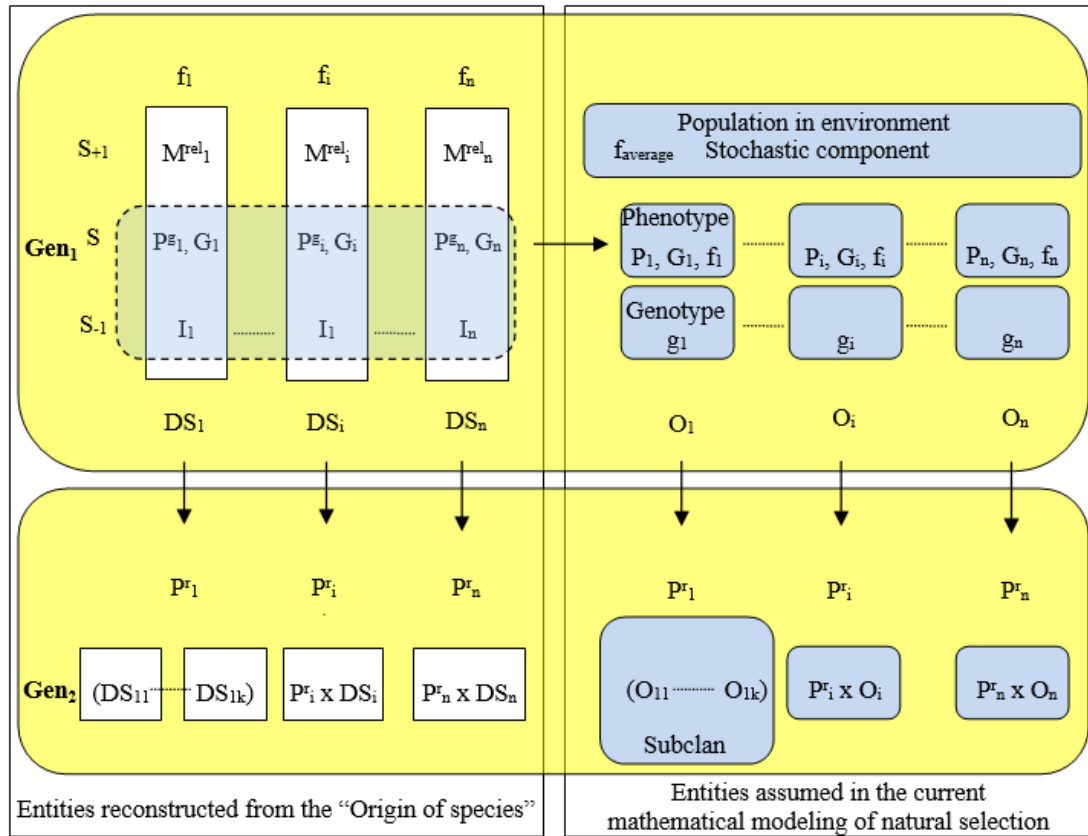


Figure 5 The relationship between reconstructed entities from the „Origin of Species” (developmental systems – DSs) and the entities currently assumed in the mathematical modeling of natural selection. The scale of observation of populations of individuals may be smaller than that needed for observing DSs and that of genes smaller than that of the parts of organisms in Darwin’s work, but for reasons of simplicity they are the same in this diagram. *Legend:* Gen = gen, S = scale of observation of an organism, S-1 = scale of observation of the organism’s parts, S+1 = scale of observation of the DS, P, I, G, M^{rel} as in the general structure of a productive system allowing selection, O = organism, g = gene, f = fitness. F_{average} = average fitness of a population.

A1.2.1. Modularization by functional dynamic modules

In Iordache et al. (2011) I developed an aggregative modularization method by adapting *Pahl-Vostl’s* (1995) *trophic-dynamic concept* in the following way: a functional dynamic module (FDM) is a group of TOs or of parts of TOs having 1) similar rates of TO cycling (inversely correlated with lifetime of the individuals), 2) the same location in space and time, and 3) similar functional niches, i.e. relations with TOs of the same or of different scales. We prefer the term “functional” to the term “trophic” because not only the trophic relations count for the differentiation of functional niches. Another reason is that we wanted this concept to apply to non-biological TOs as well. With this concept, we tackle the TO part of the ecological systems. The abiotic parts (physical solids, liquids, and gases) can be tackled by the standard nested hierarchy approach at the scales resulting from the TO systems modularization.

Specific to this modularization is that the ST scale is not constrained by the manageability of the delineated system. Some populations of TOs can be included in more than one FDM at the same time, because of their internal structural diversity. For instance, populations of deciduous tree DSs have parts with very different rates of biomass cycling, like leaves and wood (criterion 1), as well as parts with different locations in space like below vs. above ground (criterion 2). Thus, the trees will belong

to at least 3 FDMs: 2 above ground and one below ground. The notions of “same order of magnitude”, “same location in space and time”, and “same role in the food web” are to be defined by the researcher, and can be applied more stringently or relaxed, depending on the problem to be solved using this method. The scale of the FDMs varies hugely, which implies that this is not one “true” scale for ecological processes. Rather, the emergence of new structural (e.g. new FDMs) and functional (e.g. increase in overall biological productivity, or changes in the rates of biogeochemical processes) properties should be defined and used to derive the mathematical function that links scale and emergence of new properties in different areas and in different periods (“emergence function”).

As for the functional niche, we must clarify what it can mean in a context where there are interactions with systems of many scales. Luck et al. (2003) introduced the concept of a service production unit (SPU) as a subsystem of or a full biological population directly contributing to the production of a resource or service perceived as such by humans. The concept of SPU can be generalized from the perspective of all other species. For instance, roots can be interpreted as an SPU for fungi, and sporocarps as SPUs for fungivorous mammals. This generalization allows for a precise delineation of what part of an organism located in the perceived environment (M^{rel} , perceived organisms - POs) provides value for a TO organism. For POs with a scale larger than that of the source scale, we answer this question as follows: one has to produce a model linking the POs with the source scale SPU providing direct services (this works for instance for fine roots of plants as SPUs for ectomycorrhizal fungi), or to consider the use of source scale TOs by the large scale entity as a biotic internal control parameter (this could work for consumption of fungal sporocarps by mammals, for instance). We mean by internal control parameters those describing the influence from inside the DS model, but from scales different than the source TO scale; by external control parameters we mean those describing the factors influencing from outside the DS model – e.g. large-scale physical ones, or human action. For entities with a smaller scale than the TO source scale (e.g. in the case of fungi – bacteria, tiny invertebrates) one needs to produce a model linking the source scale individual with small scale organisms through the smaller scale SPU providing direct resources and services (e.g. organic exudates, hyphae) to these smaller scale organisms, and then to up-scale the results of this model to the source scale to form another internal biotic control parameter. The interaction of the source scale individual with each small-scale entity will not count, but the overall pattern resulting from the structural and functional characteristics of these small-scale FDMs. We can now interpret the functional niche of a TO as consisting of variables describing the source scale entities with value for the TO, the source scale SPUs that are part of larger scale entities relevant for the TO, and the internal biotic control parameters. This concept of functional niche is an epistemic one, with no objective reality associated to it. It will not imply that the developmental system of TO will not continue to be spread across scales, but that we must modularize the scale continuum to obtain workable FDMs, which is a strategic part of the epistemic status of the DS. The DS of a TO (the DS’s “world”) will be modeled not only by the TO’s FDMs, but by the entire structural model reflecting also the POs’ direct relevance for the TE, i.e. the epistemic status of a DS is related to the production of a structural model and of the associated mathematical models (and of the hierarchically structured physical abiotic models). An important point is that in a FDM of ecological use the physical environment associated with it is considered homogenous and perceived identically not only by individuals of the same species, but by all individuals of different species grouped in that FDM. This leads to the simplification of the state space used in modeling to make it workable for ecological purposes (where the evolution of the organisms is not considered), and especially for aggregation in view of up-scaling the ecological processes. Another point is that the space-time windows associated to the structural models should be chosen, especially in the case of managerial modularization, such as to be compatible with the human practical possibilities of action.

Based on his technique of modularization a modularized model of a community of ectomycorrhizal fungi DSs is presented in figure 6 (from Iordache et al. 2011).

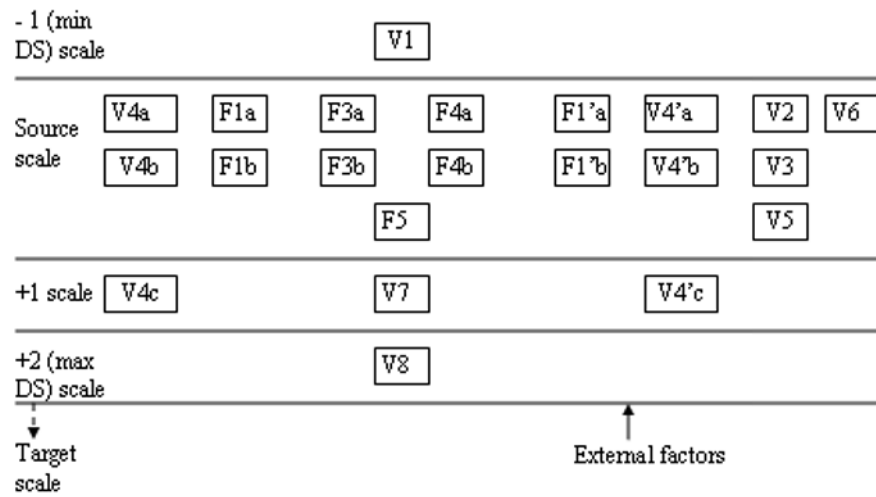


Figure 6 Modularized model of a community of ectomycorrhizal fungi DSs (relationships not represented for the reason of visibility). The scale refers to scale in space, not in time. The physical part is not represented. The part of the model within the source scale (within a stratum) is the structural model for up-scaling under the constraints from FDMs of different scales and external factors. Legend: the TO is noted with F (from fungi), the POs with V (from value); F1a,b = fungi parts (root tips in the case of EMF) in two vertical layers at the roots of tree 1, F1'a,b = fungi parts in two vertical layers at the roots of tree 1', F3a,b = hyphae in the extraradical mycelium in two vertical layers, F4a,b = rhizomorphs in the extraradical mycelium in two vertical layers, F5 = sporocarps, V1 = bacteria, V2 = mineral P and N, V3 = organic P and N, V4 = trees (a, b = roots by layer, c = aboveground parts), V5 = myco-heterotrophic plants, V6 = soil microinvertebrates, V7 = fungivorous invertebrates, V8 = fungivorous mammals.

The extraradical FDMs, located between trees, and the sporocarps' FDMs do not include only the EM fungi (EMF), but also other fungi if present in the same ST location. The root FDMs, as well, may not be limited to the EM fungi present in the rhizosphere, but could also include other fungi (eventually mycorrhizal) along the mutualism-parasitism continuum, if present in the same ST location. To the extent that inter-specific interactions within the fungi species of a FDM are important, they should be taken into consideration when assessing the roles of an individual EMF species, or the EMF community by each FDM.

We need four (apparent) hierarchical levels for understanding the ecological functioning of EMF communities, and one more level eventually for management purposes, if the target scale (of management) is larger than the maximal DS scale (given by the size of fungivorous mammal populations). One more scale should be added if one looks also for speciation processes (which occur at even larger scales, details are provided in Iordache et al. 2011).

A similar method was applied for the DSs of arbuscular mycorrhizal fungi in Neagoe et al. (2013, figure 7).

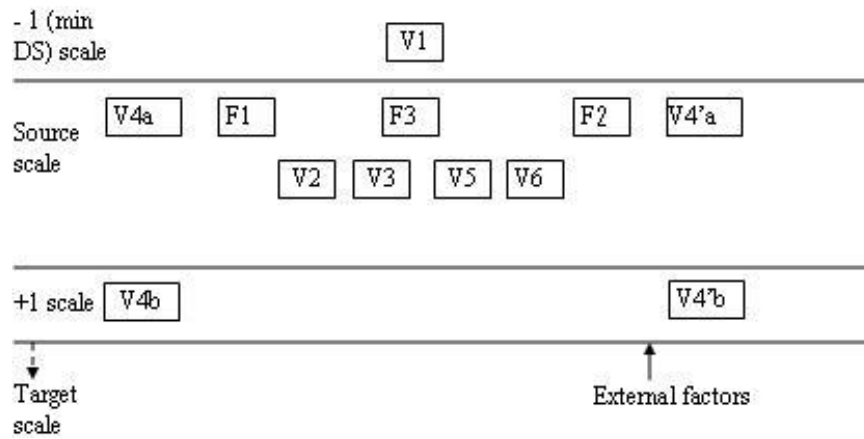


Figure 7 Modularized *model of a community of arbuscular mycorrhizal fungi with the entities with value for them – biotic and abiotic objects influencing them (relationships not represented for the reason of visibility). The scale refers to scale in space, not in time. The physical part is not represented. The part of the model within the source scale (within a stratum) is the structural model for up-scaling under the constraints from organisms of different scales and external factors external to the AM functional dynamic modules. F1, fungal parts on plant roots 1; F2, fungal parts at plant roots 2; F3, hyphae in the extraradical mycelium; V1, bacteria, V2, mineral P, and N; V3, organic P and N; V4, plants (a, belowground; c, aboveground parts), V5, micronutrients, and toxic substances, V6, soil fungi or micro-invertebrates.*

In the end of this part one can conclude that *the models of productive objects implicit in the „Origin of species” cannot be studied operationally as a whole because of their extreme complexity. The multi-scale system of coupled productive systems in the ecosphere can be studied only by disciplinary fragmentation and discretization.* The advantage of knowing the reconstructed law of growth with reproduction is that we can anticipate future research directions needed to fill the gaps in the reconstructed processes both in evolutionary biology and in ecology. In the case of ecology, we have been able to build modularized models of intermediate complexity between that of a community of organisms and a whole ecosystem with autocatalytic cycles. Such optimized models can be used in the design of field investigations for biogeochemical processes and services, and more generally the role of species in the production of ecosystem services.

Overall, DSs reconstructed from the “Origin of Species” have stronger ontological status (as proven by the invariance of the general structure, the larger integrality in systems ecology sense, and relative autonomy of functioning) than those derived by analytical (epistemic) modularization to allow a tractable complexity compatible with the operational research in the current evolutionary and ecological theories. I will illustrate this statement by the situation of the ecological hierarchies in the next chapter.

A2. The nature of the hierarchies of ecological productive systems

The scientific modularization of DSs leads to a nested hierarchy of ecosystems, but not a true one (figure 8). In this framework, it is not the case that the emergent properties at level $n+1$ result only from the interactions between the parts at level n , because besides the n -level entities there are also new larger-scale entities forming the $n+1$ level; each eco-level is characterized by structurally new types of FDMs that are not found at lower hierarchical levels (figure 8). Only the representational three-dimensional physical spaces needed for scientific investigation or management are nested, and not the productive systems analyzed within this three-dimensional space. The standard structural model of an ecological system (including compartments for primary producers, consumers, decomposers, etc) will be then about interactions of different developmental ecosystems of different scales. What is not seen in the standard representation is the large number of smaller-scale populations of Tos compared to the large-scale ones. Many small-scale FDMs are coupled at the same time to a relatively larger FDM (figure 9).

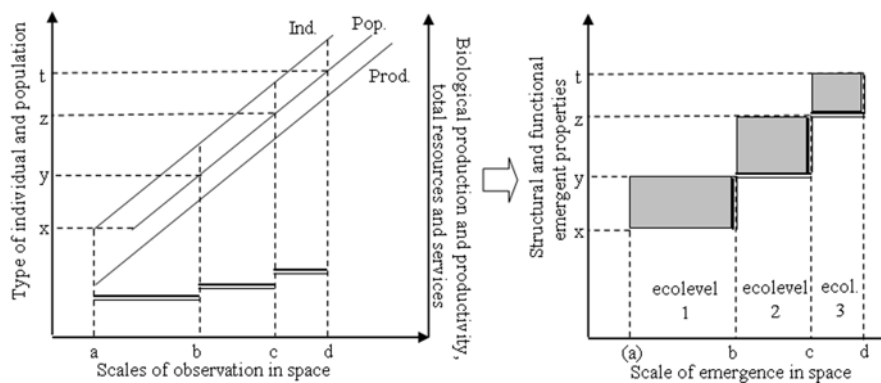


Figure 8 The relationship between the scale of biological structural elements and processes (individuals, populations, left graph – left axes, production and productivity, left graph – right axes) and the hierarchical structure of ecosystems (right graph). At scales of observation from a to b (corresponding to ecological level 1) one can perceive all types of individuals (and their populations) from x to y , but only some of the individual types from y to z (and not their populations). The FDMs including populations of type y to z are said to “emerge” at higher hierarchical ecological level 2. Grey areas on the right graph suggest the multidimensional spaces characterizing each ecological level in which the processes supporting the productivity of each level can be conceptualized. Note that the simplistic linear models (emergence functions) from the left graph can be cut in a different way leading to alternative hierarchies. The real forms of the emergence functions are not linear and depend on the starting point of observation in space (initially published in Iordache et al. 2009a, b).

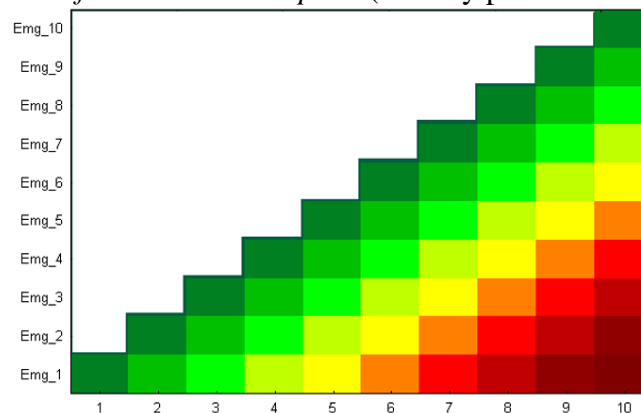


Figure 9 Theoretical relationships between the number of eco-levels and the number of emergent FDMs (communities) of each type (Emg_1 to 10) within an eco-level (1 to 10). The color change from green to red indicates an increase. Biodiversity of the overall biocenoses (system of communities) is related to the number of FDM types and instances, and to the species diversity inside each FDM.

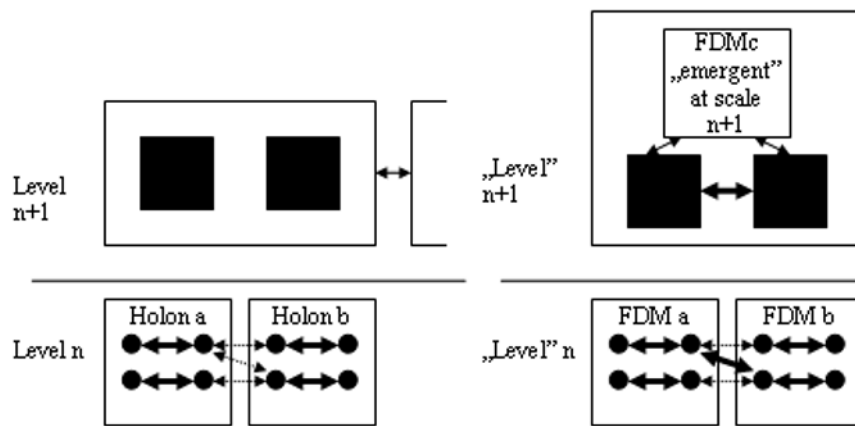


Figure 9 Simplified representation of a true nested hierarchy (left, applicable, for instance, to molecules – level n, and cells level n+1) and apparent hierarchy of system (right, resulted from the epistemic modularization of ecological systems). In the apparent hierarchy, (abiotic physical parts not represented) the holon at n+1 level includes subsystems that are not present at n level, which is not the case for true hierarchies. In the true hierarchy the interaction within the subsystems of a holon is strong and between holons is weak, while in the apparent hierarchy, they may be very strong between holons (when for instance the FDMs include parts of the same population of DSs with different functional niches, or parts of the same DSs with different location in space and time, or different turnover rates).

To make compatible the standard hierarchy of natural capital with the much more complex pseudo-hierarchy of ecological systems reconstructed above, here we separate the scientific use of the term ecosystem from the applied, managerial use, by the additional term natural capital. An ecosystem is natural capital when the modularization of the emergence function is done for management goals, i.e. of interest is the value of the ecosystem for humans. For a modularization in the interest of management, leading to a theoretical hierarchy of the natural capital, one has to use only scales appropriate for the coupling of natural DSs with human developmental systems (organizations, management projects) by natural resources and services relevant to humans. The theoretical natural capital hierarchy resulting from a managerial modularization of the emergence function is a hierarchy of the natural capital, with specific natural resources and services produced at each level (Iordache and Bodescu 2005), and with specific managerial organizations created for (“emergent at”) each level. An emergence function for human developmental systems (organizations) can be constructed and modularized leading to a hierarchy of socio-economic systems, with an important difference being that this modularization is no longer at the latitude of the researcher, but imposed by national and international institutional reality. The theoretical natural capital hierarchy may follow the socio-economic current hierarchy for reasons of manageability of the natural modularized entities.

What is interesting in real management is how particular organizations and projects deal with the ecological system, what they perceive as valuable, and how they interact when they want to maximize their separately perceived values (when they are in a conflict of interests, leading eventually to an environmental crisis).

Another important distinction to make is between production and management of natural resources and services. The production takes place at all scales of the ecological emergence function, but the management can occur only at the human-relevant scales. One problem is how to take into account the contribution of small-scale organisms (like EMF) to the overall natural resources and services production at the management scale. This can be done through the SPU concept. From a managerial perspective, the TOs’ populations of the same species (or fragments of such populations) found in an FDM are SPUs. The SPU concept allows the identification of each species’ contribution to the overall

theoretical or real natural capital value (using modularized models of the type presented in figures 6 and 7), and on this basis, the design of targeted management measures.

A3. A general concept of resilience

In Aligică and Iordache (2022) I contributed an analysis of the concept of resilience in natural, biological, and environmental science. *Resilience in physics, biology, and environmental sciences describes aspects of the process resulting from a **temporary stressor acting on an entity**. The **entity** can be an **object** (e.g., material, network, biomolecule, cell, tissue, organism, population, soil, river basin, water drainage system, socio-ecological system) or a **process** (e.g., molecular clock, network of cooperation within a species, interaction between species, ecosystem process, natural resource management process). The objects can be static (without change independent of the stressor) or dynamic (changing without stressor at one- or several-time scales). The **stressor** is conceptualized in the local ontology of each scientific discipline, for instance as a force, a disease, a removal of species, or as climate change. The stressor is either an **external driving factor** of the entity (most often) or an **internal driving factor** (for instance human action in the holistic socio-ecological approach). The driving factors act most often at the spatial scale of the target entity, but there are cases in biology and environmental sciences when upscaling and downscaling of effects occur (for instance, the effect of a toxic substance will propagate from the scale of cells to that of organisms, and even to ecosystems). The time scale of action is smaller than the lifetime of the target entity and can have various forms (e.g., pulse, ramp, press), durations, and frequencies. The **stress** is described as **changes of the state** of the entity, with the state described in terms of one or more **response variables**. The resilience is explained by **mechanisms** relating to the stressor and the changes of state/response variables. Knowledge about mechanisms is useful to control/manage the resilience of the target objects and processes with respect to the driving factors and is delivered to the organizations managing the biological and environmental entities.*

There are five properties relevant for the discussion about resilience in physics, biology and environmental sciences. Definitions of resilience vary between scientific disciplines, and within the same field, but all refer to one or several of these properties: resistance (continuation with unchanged identity), elastic deformation (rebound, restoration of reference identity); plastic deformation with or without loss of functions and extension to new ones (extensibility, reconfiguration, state transition, recovery and extension of functions), adaptability (transformability, evolution with change of identity) and preparedness (intentional).

These notions have been used later to develop a conceptual methodological framework for the resilience of biogeochemical services (chapter B3).

B. Methodological contributions

The role of the methodology is to operationalize the theoretical framework. If the theoretical framework has weaknesses, the methodology cannot solve them. However, without operationalization, these weaknesses cannot be revealed by the lack of sound scientific results and there are no incentives for the evolution of the theoretical framework. Thus, methodology has a key contribution to the evolution of research programs.

B1 Conceptual analysis and knowledge mapping

Conceptual analysis is usually used in analytical philosophy, and knowledge mapping in bibliometric studies. The first one is relevant in science for the detection of theoretical assumptions in scientific text, while the second allows faster detection of the main clusters of scientific knowledge when the literature body is very large. I have applied innovatively a combination of textual and conceptual

analysis to reconstruct structural invariances of productive systems from the “Origins of Species” as described in Iordache (2009) and innovatively used knowledge mapping to organize the literature for the conceptual methodological framework presented in chapter B3 (Iordache and Neagoe 2023).

What is relevant methodologically for scientists from the conceptual analysis is that the border between the philosophy of biology and ecology and the theoretical biology and ecology is currently blurred, most of the journals in this field host articles from both areas, and many authors work in both areas. This is not something new. The role of this kind of method in contemporary science is to catalyze the development of new research programs. Figure 11 shows an excerpt from a poster communicating this approach at an international conference in 2007.

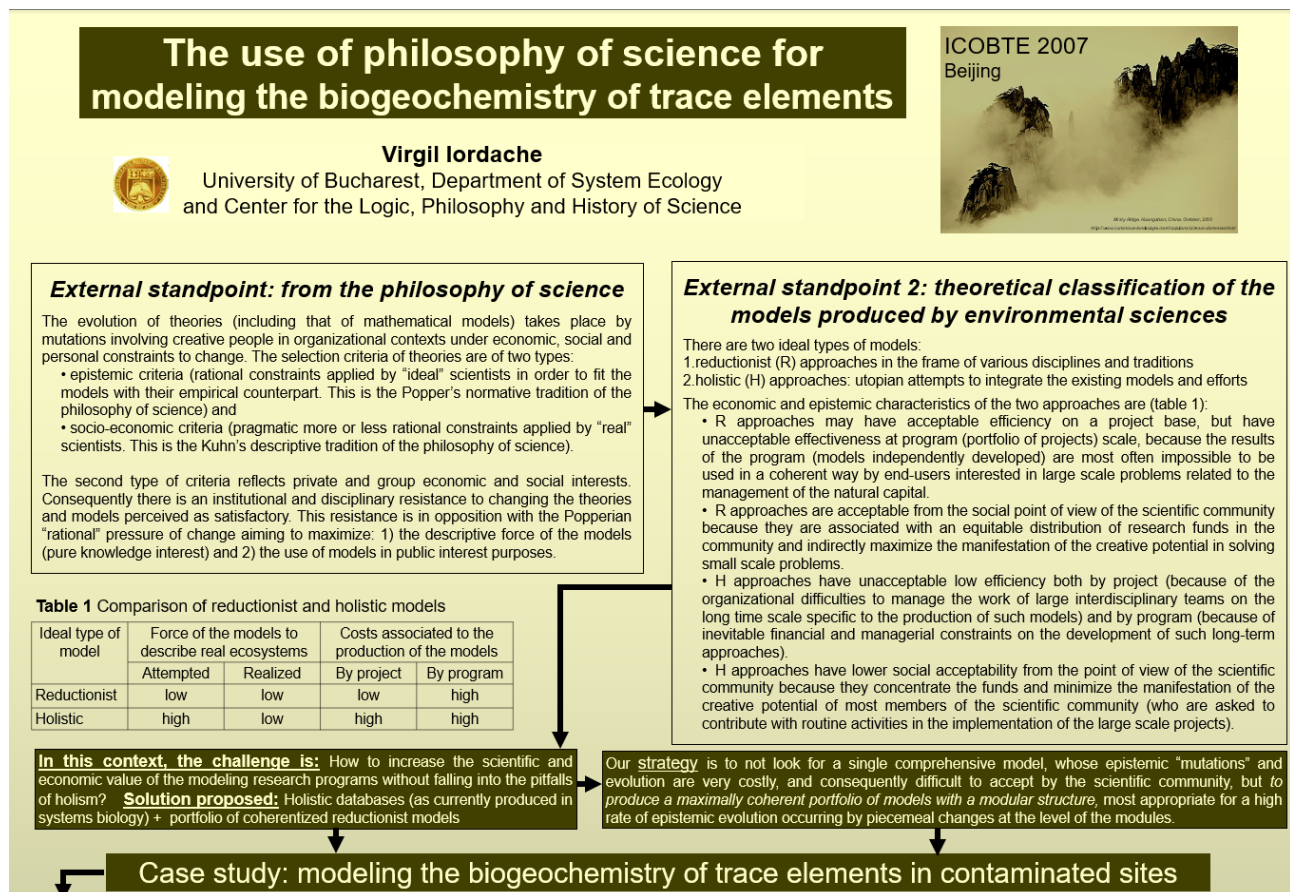


Figure 11 An excerpt from a poster communicating an approach using elements from the philosophy of science to catalyze the development of new methodologies in the biogeochemistry of trace elements (Iordache 2007).

For knowledge mapping in short, a core set of publications is selected using keywords by search in the topics of the articles, this set is expanded to all articles citing those from the core set, and the expanded set is exported from Web of Science as a plain text file, with full record and cited references. Finally, the exported data are filtered to remove duplicates and keep the desired category of the article. What was innovative was that the data were organized in a nested form, as presented in table 1 below, which allowed us to detect which research clusters about biological diversity and ecosystem services are overlapped, and which are distinct. Data were processed with the software Citespace.

A combination of the two methods can be useful to map the diversity of key concepts in any scientific field and detect the lines and gaps allowing new research directions. Such combinations have been used for instance to organize the new research directions communicated in part G of this text.

B1. Integrated modeling of metals biogeochemistry: Potential and limits

In the review with the title of this chapter (Iordache et al. 2009) *we performed an analysis of a family of models relevant to the integrated modeling in metals biogeochemistry by two approaches: a hierarchical one, and a disciplinary one. The hierarchical approach was done in a theoretical framework accepting the existence of a hierarchy of ecological systems and splitting the population of analyzed models into classes based on their relevance for various biological and ecological hierarchical levels. We identified two types of integrated models: between abiotic and biotic components at the same levels, and between biotic components across hierarchical levels. The complementary, disciplinary approach, focused on bioremediation models, to assess the potential of technological transfer based on modeling of heavy metals biogeochemistry.*

Table 1 *Results of the interrogation of the Web of Science (WoS) database (August 2022) for the effects of heavy metals (HMs) on ecosystem services (ES), biodiversity, resilience to HMs stress, and the elements of a conceptual, methodological model (presented in chapter B3). The grayscale suggests the relevance of the returns for three complementary approaches (black box, gray box, and white box models of ES production). Italics indicate the merged sets of data.*

Keywords	Core publications found in WoS	Primary articles in the extended set	Primary articles in two merged sets	Primary articles in four merged sets
Black box approach: “HM” AND “ES” “HMs” AND “ES”	334	5955	6931 (178 duplicates removed)	16176 (1283 duplicates removed)
Grey box approach: “HM” AND “biological diversity” “HM” AND biodiversity “HMs” AND “biological diversity” “HMs” AND biodiversity	1295	12431 (From 2012 to 2022)*		
White box approach: “HM” AND resilience “HMs” AND resilience	271	5161	10528	
Complex interrogation for the conceptual, methodological model	60 reviews	4173	(247 duplicates removed)	
	121 primary articles	1441		

* The total for all years was higher than 40000, more than the processing capacity of CiteSpace.

At the time of this research, we were working in the standard ecosystem ecology paradigm of biogeochemistry and proposed a methodology for linking the biogeochemical properties between ecological levels using a combination of statistical and deterministic modeling (figures 12 and 13). At the same time, aware of the potential difficulties related to the pseudo-hierarchical character of the ecological hierarchical levels (as shown in figure 10 above) we also devised a first method to operationalize the DS approach by looking at the scale-specific heterogeneity in space of the distribution of heavy metals, from the scale of fungi to the scale of trees, to the scale of the discretization units of heavy metals transport models by surface water (figure 14). A key element of the approach presented in figure 14 is the internal feedback loop allowing the potential adjustment of the starting theoretical framework depending on the results of its implementation. However, it was not yet technically possible to describe these scale-specific patterns of heavy metals distribution in soil and sediment, because the measurement methods were prohibitive at the time (expensive analytical methods and geospatial location limiting the maximal number of measurements). We implemented the approach from figures 12 and 13 in a contaminated area and the main limitation for conclusive results was the very large heterogeneity in space of heavy metals at the meter scale, which precluded the upscaling of the experimental results based on local soil samples. Fortunately, the prices of GPS systems and field XRF spectrometers became affordable and we were able to change towards the approach based on DS, multiple scales of processes, explicit spatial structure of the abiotic variables controlling the development of organisms, and structural models of the kind presented in figures 6 and 7. Empirical results will be presented in chapter C1.

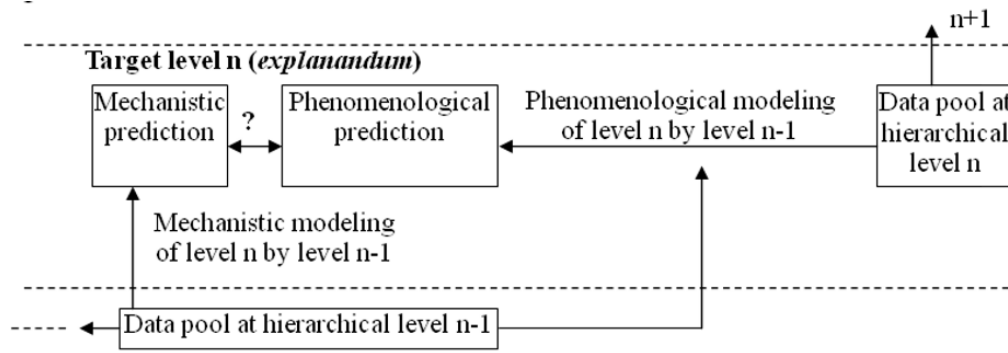


Figure 12 Overall structure of a modeling approach in the hierarchical paradigm. Each level is characterized by specific, emergent properties, which when measured lead to specific data sets. Phenomenological models are 1) those describing patterns of variation and correlation (laws) of the properties characterizing a certain level 2) those correlating statistically (or by other methods without explanatory power, such as neural networks) the properties at lower levels and higher levels. Mechanistic models are those linking deterministically (assuming causal effect) the properties specific to lower levels with those specific to the integrating level (Iordache et al. 2009).

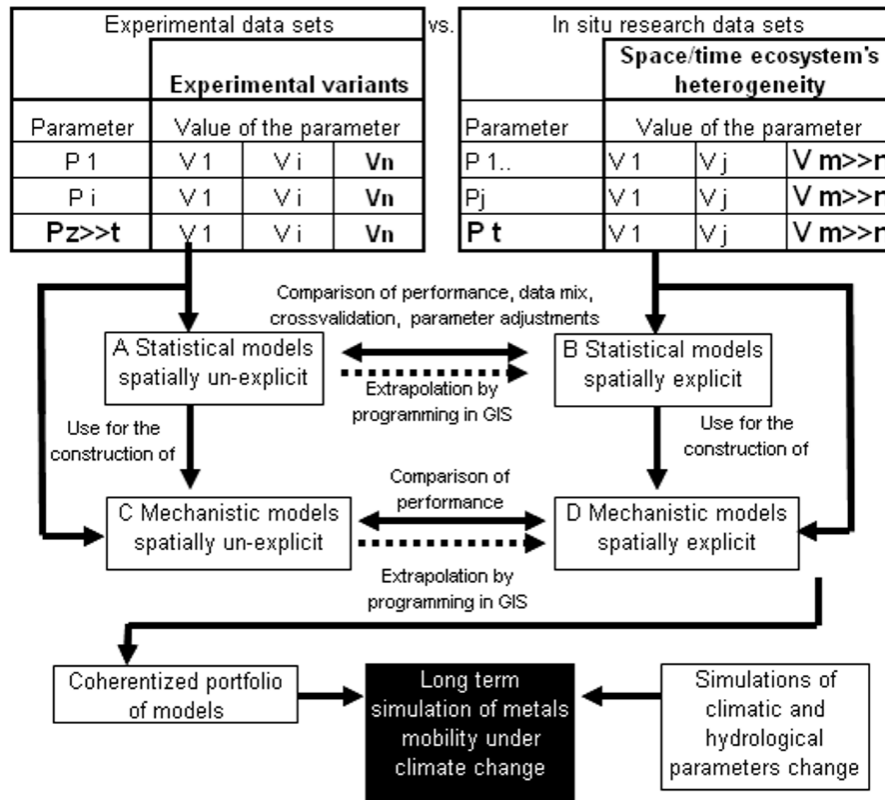


Figure 13 Diagram showing the detailed structure of the modeling approach for developing a coherent portfolio of models in the hierarchical paradigm. One can notice the combination of field and experimental investigation, which remained a constant of our approach (Iordache et al. 2009).

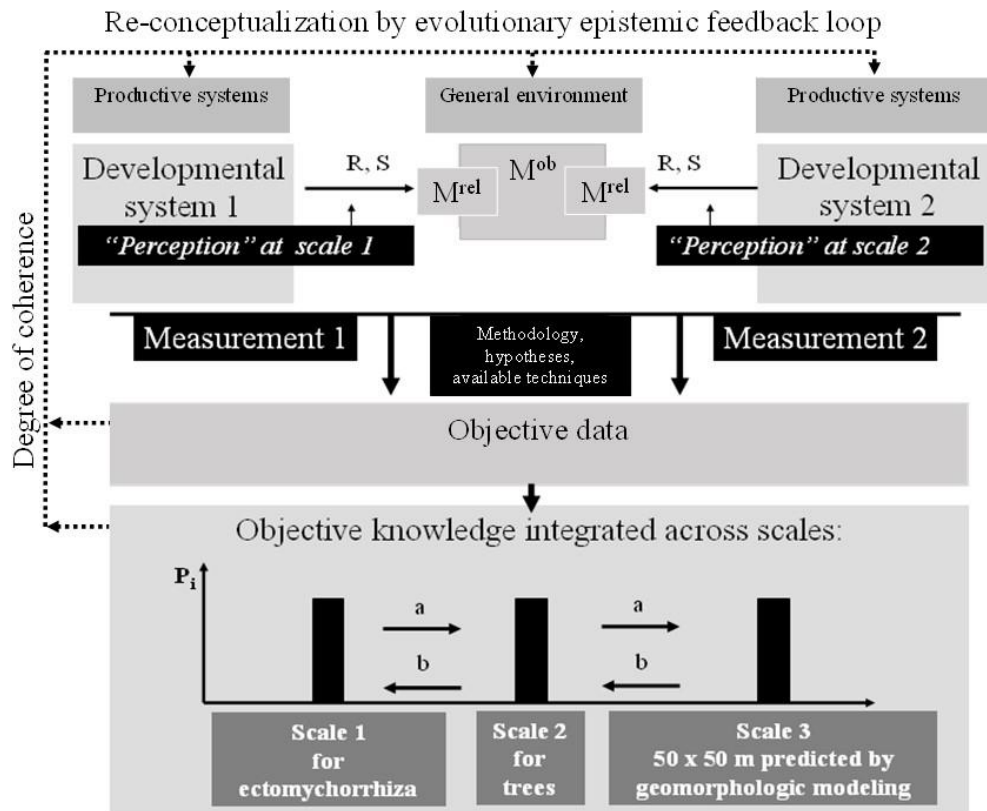


Figure 14 The developmental systems of different types “perceive” objective entities (which provide resources *R* and services *S*) at different scales. To model the behavior of DSs we need to measure the relevant variables at space-time scales specific to the teleonomic objects from their structure. If the same variable (or a set of variables) is measured at different scales and one obtains the same value (suggested by the equal stick of the inserted graph), one cannot simply extrapolate across scales. This is because of the formally irreducible heterogeneity of the environment. One needs specific empirical research to establish the conditions for upscaling (or bottom-up modeling of other variables, “*a*” on the inserted graph) and downscaling (or top-down modeling of other variables, “*b*” on the inserted graph). These conditions will be investigated to produce multi-scale data sets, and the degree of coherence of the integrated knowledge, and its coherence with the starting concept model, can lead to adjustment of the initial concept model (evolutionary epistemic feedback loop). (adapted from Iordache et al. 2009).

B2. A general methodology for upscaling ecological processes in the DS approach

In the same chapter where we introduced the functional dynamic module (chapter A2 here, Iordache et al. 2011) we proposed a methodology for upscaling the biomass production from the scale of a DS to larger scales, and then applied it to ectomycorrhizal fungi in the same chapter and to arbuscular mycorrhizal fungi in Neagoe et al. (2013).

Up-scaling the biomass production function from the original DSs of scale 1 to a larger target scale 2 is not a simple physical space-time (ST) procedure because it involves an increase in the complexity of the state space from the original to the target system. The scale issues are related to the position in space-time (ST) of the original TOs as grouped in FDMs, of their internal and external resources, of DSs of larger scale to which they are directly connected, and to the ST patterns of physical processes of larger scale controlling the value of abiotic parameters relevant for the original and large scale TEs.

Up-scaling the biomass production function from the FDMs of the source scale to the target scale

may involve the previous down-scaling of other processes. One of these situations occurs when the source scale DSs use as a resource an organism of larger scale (for instance as a carbon source). In this case, one needs a model down-scaling the biomass production of that organism to the specific portion of biomass/carbon made available for source-scale organisms, which is different from the model describing the overall biomass production of that large-scale organism. Another situation is connected to the pattern (perceived at large scale) of distribution in space of the biomass of source scale FDMs, a pattern controlling the choice of mathematical tools for up-scaling. This pattern may depend in time on external control parameters that can be modeled in space and time only at a large, target scale. For instance, if one predicts with hydro-geomorphological models the dispersion of a toxic pollutant with a resolution of 50x50m, this information should be down-scaled if the DSs controlled by this pollutant, whose up-scaling we are looking for, have a much smaller scale. The distribution at a small scale can be influenced by the external control parameters, by changing the species' location in space, changing the species' location in time, or changing the turn-over rate of the biomass, with overall consequences on the FDMs structure and associated productivity.

The steps for up-scaling the biomass production (and related biogeochemical processes) from the original (source) DS systems could be based on **structural aspects** like (1) ST location and turn-over rate of the source TOs (characterizing biomass turn-over and position in ST of the TOs by one or several modules reflecting their life cycle and morphological properties), (2) entities providing resources and services to the original TOs (identifying the resources relevant for each TO type by module and characterizing their ST position), (3) entities using resources and services of the original TOs (identifying the use of source TO modules as resources by developmental systems centered on types of TO of larger scales, and identifying the position of these large scale DSs in the system of target scale), (4) external control factors (identifying the large scale abiotic factors, described as external parameters, influencing the DS of the original scale and identified above) and (5) the homomorphic model of the system of DSs and of its integrating system (identifying the overall ST scale of the system of FDMs characterizing the source DS, the relationships of these FDMs with larger scale ones and the external control parameters). In addition, **functional aspects** include (6) biomass production functions at source scale (characterization of the production functions at DS, populations of DSs, and FDMs of the source TOs at the original scale in the field, i.e. implicitly taking into account the influence of smaller scale DSs), (7) large scale DS's influence on the production function (characterizing the mathematical functions describing the influence of large scale DSs on the productivity of the original DSs), (8) large scale abiotic factor's influence on the production function (characterizing the mathematical relationships underlying the influence of large scale abiotic parameters on DSs at the original scale, the space distribution of the abiotic parameters in the system of target scale with a resolution of original scale, and the mathematical functions predicting their space-time dynamic and the abiotic processes involved at the target scales) and (9) large scale abiotic factor's influence on large scale DSs connected to the source scale (the same as in point 6 done for the large scale FDMs mentioned at point 3 keeping into account only the abiotic processes influencing all DSs whatever the scale). The **integration** relies on (10) stratification (stratifying the system of target scale into strata having the scale of the system of FDMs characterizing the original DS as identified), (11) production function by strata as controlled by large-scale DSs and abiotic factors (assessment of the productivity or other associated processes of interest of original DSs by types of strata, as modeled by the system of FDMs developed within stratum under the control of larger scale DSs and abiotic parameters, providing the possibility to correct for results obtained in later hierarchical levels) and (12) model up-scaling (extrapolation of production function to the target area of interest by types of strata).

While this holistic methodology may be more adapted to the reality of ecological processes than that based on the standard hierarchical model of ecological systems (nested hierarchies) it is too data-intensive and not operationalizable with the current techniques of measuring and estimating biological and abiotic variables. It may have a heuristic value for the research on the role of groups of organisms in ecological production, but for biogeochemical research one needs simpler approaches, like the one presented in the next part.

B3. Contributions to the theoretical foundations of integrated modeling in biogeochemistry and their application in contaminated areas

In this chapter of a book dealing with bio-geo interactions in contaminated soils (Iordache et al. 2012) we moved from thinking biogeochemistry by ecological systems (in terms of full local biogeochemical cycles) to an approach based on coupled processes of different scales towards a model with smaller complexity.

As a first step, we make an inventory of *the processes of metal mobility by various pathways potentially existing in a site (from the smallest scale environmental process up to 10^5 m^2) and a region (10^5 - 10^{10} m^2) (table 2 and table 3). Site and region roughly correspond to the ecosystems and regional landscape from the standard ecological hierarchy, and are management units.*

Table 2 Site-specific processes involved in metals mobility. Shaded areas indicate processes crossing the site-region scale boundary. (from Iordache et al. 2012).

Scale	Transport pathway of metals	Mechanism
Part of soil column 10^{-8} - 10^{-4} m^2	Various	Chemical and microbiological weathering
Part of soil column 10^{-4} m^3	Biological	Microbiological direct and indirect (by organic carbon) immobilization / mobilization for hydrological fluxes
Rhizosphere	Biological	Microbiological direct and indirect (by organic carbon) immobilization / mobilization for plants
Soil column 10^{-8} - 10^0 m^2	Hydrological	Diffusion and dispersion
Soil column 10^0 m^2	Various	Other biological weathering (by plants, invertebrates)
Soil column 10^0 m^2	Hydrological	Colloidal transport
Soil column 10^0 m^2	Hydrological	Soluble transport
Soil column 10^0 m^2	Hydrological	Soluble complexes transport
Soil column 10^0 m^2	Hydrological	Preferential flow (vertical)
Soil column 10^0 m^2	Biological	Bioaccumulation in soil invertebrates with low mobility
Bioaccumulation area 10^{-2} - 10^4 m^2	Biological	Plant up-take (bioaccumulation in plants)
Field 10^3 - 10^4 m^2	Hydrological	Unsaturated (preferential) flow (to groundwater)
Slope area 10^2 - 10^4 m^2	Hydrological	Infiltration excess overland flow (dissolved and particulate)
Slope area 10^3 - 10^5 m^2	Hydrological	Retention in and remobilization from transversal buffer zones
Bioaccumulation area 10^3 - 10^5 m^2	Biological	Bioaccumulation in mobile epigeous invertebrates
Large slope area 10^3 - 10^6 m^2	Hydrological	Saturation excess overland flow (dissolved and particulate)
Large slope area 10^4 - 10^8 m^2	Hydrological	Sub-surface storm flow (lateral flow)

These processes generate patterns in metal distribution at different scales, and what we have to do is to separate by modeling and in situ observation the patterns generated by the processes of interest from the patterns generated by other processes. For instance, the contamination of the floodplain in the vicinity of a smelter can occur both by hydrological processes and by atmospheric deposition, and we must separate the effect of sedimentation during floods from the effect of particle deposition.

The field research of selected processes of interest, depending on the research question and practical problems to be solved is complemented by experiments at several scales (table 4). The experimental

results can then be upscaled to a scale relevant to the site or regional scale and using the spatial structure of the variables relevant to the modeled processes at the experimental scales.

Table 3 *Region-specific processes involved in metals mobility. Shaded areas indicate processes crossing the upper-scale boundary of regions.* (from Iordache et al. 2012).

Scale	Transport pathway of metals	Mechanism
Region 10^4 - 10^{10} m ²	Hydrological	Groundwater flow in different types of aquifers
Region 10^4 - 10^8 m ²	Atmospheric	Dry and wet deposition from local sources
Bioaccumulation area 10^4 - 10^8 m ²	Biological	Bioaccumulation in mammals and in non-migratory birds
1 st order catchment 10^5 - 10^6 m ²	Hydrological	Retention in and remobilization from transversal buffer zones
2 nd -6 th order catchment 10^6 - 10^8 m ²	Hydrological	Interactions between types of hydrological flows
Region of 10^6 - 10^7 m ²	Various	Soil catena formation
Large order catchment 10^7 - 10^9 m ²	Hydrological	Retention in and remobilization from longitudinal buffer zones (floodplains)
Region of 10^6 - 10^7 m ²	Atmospheric	Volatilization
Bioaccumulation area 10^5 - 10^{12} m ²	Biological	Bioaccumulation in migratory birds
Region 10^8 - 10^{11} m ²	Various	Zonal soil formation
Region 10^9 - 10^{12} m ²	Atmospheric	Dry and wet deposition from distant sources

Table 4 *Processes involved in metals mobility investigated in experiments at different scales* (from Iordache et al. 2012).

Name of the system and usual scales	Environmental complex system studied at these scales	Processes, fluxes, effects studied / control variables
Pot 10^{-2} m ²	Soil + plants	Exploration by root, bioaccumulation / microorganisms, organic carbon, level and spatial structure of amendments
Lysimeter 10^{-1} - 10^0 m ²	Soil + plants + small scale hydro-system	Same as in pots + leaching, internal redistribution, net outputs / same as in pots + soil structure, hydraulic conductivity, humidity, redox potential on profile
Plot 4×10^0 - 10^2 m ²	Soil + plants + larger scale hydro-system + other organisms	Same as in pots + effects of heterogeneity in space, margin effects, other processes due to external entities (consumers, runoff, etc) / same as in pots + variables for external entities.

Figure 15 provides an example of how one can use processes occurring only at three scales to predict the effects of local impacts on the transport of heavy metals at large distances (Iordache et al. 2012), and table 5 provides examples of hotspots of pollution with heavy metals to illustrate the approach (Iordache et al. 2011b). What is critical for the success of such an approach are up-scaling and downscaling methodologies of some variables of interest (for instance concentrations of pollutants) using geostatistics and methodological models coupling biotic and abiotic variables, such as vegetation properties with hydrological flow properties.

From this perspective, biogeochemistry becomes strongly interdisciplinary, uses theoretical resources from many scientific fields (ecology, soil science, hydrology, other environmental sciences), and deals with the mobility of elements in three-dimensional (physical) volumes (sites, regions, etc.) hosting complex systems formed by coupled entities fully or partially located in that physical volume. Such spatially well-delineated entities are management units providing local

resources and services and having large distance effects on the local resources and services production in other sites. The processes specific to this approach result from the multiple coupling between entities occurring in a three-dimensional physical space volume. Each simple couple of entities supports phase-specific and multiphase abiotic or biological processes. Thus, what is specific to this interdisciplinary biogeochemistry is the complexity of the processes and not the scale of the management unit (site or region), which is only the starting point for formulating the scientific problem and is also considered in the communication and interpretation of results for management purposes.

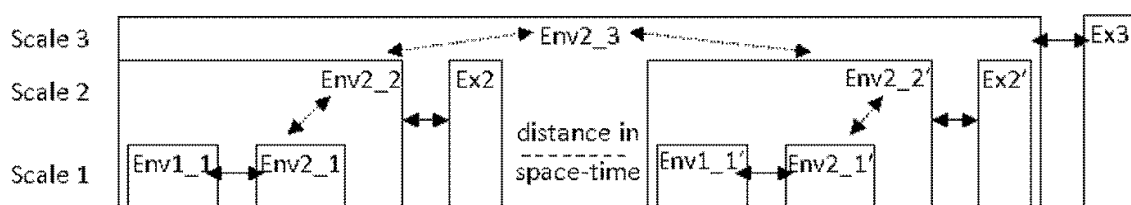


Figure 15 General representation of the structure of a model in an integrated approach to assess the effects of local processes involving metals at one space-time location on other local processes at a large distance in space-time (designate by '). Env1_1 can be a tailing-dam or a mining dump or polluted soil, or a complex soil-vegetation entity, Env2 (scale 1 to 3) can be hydro-systems, Ex2 can be geo-morphological, pedologic, and microclimatic entities in the landscape, Ex3 geologic and regional climatic features of a larger catchment, and the model could attempt to predict the effects of local phyto-remediation of a contaminated site in the slope area of a small catchment on late and distant bioaccumulation of metals in crops in an agricultural floodplain site. The coupling at the same scale and between scales is based on variables characterizing the coupled entities and a methodological coupling model. Successive up-scaling and downscaling of some variables are needed to predict ST large-distance effects of local changes. (Iordache et al. 2012).

Table 5 Examples of distant pollution hot-spot resulted from the coupling of local scale and large-scale processes (Iordache et al. 2011b).

Source of metals	Large scale process	Distance to "hot spot"	Local scale process at distance (in "receptor area")		Location in Romania
			1	2	
Batteries factory	Atmosferic dispersion	2-3 km	forest barrier effect	-	Pantelimon (NEFERAL/ Acumulatorul)
Smelter		2-5 km	runoff	transversal particles buffering (geomorphology + plants)	Ampoi - Zlatna
Smelter		2-4 km	runoff	longitudinal particles buffering (geomorphology + plants)	Ampoi - Zlatna
Smelter		4-5 km	runoff	longitudinal buffering	V. Viilor - Copsa Mica
Mining dump	Surface water transport	12 km	longitudinal buffering	-	Ampoi - Hg mining dumps to floodplain
Mining dump + tailing dams + polluted soil		25 - 40 km	longitudinal buffering	-	Ampoi - various sources to floodplain
Acid mine drainage		10-15 km	groundwater recharge in karstic NATURA 2000 area	-	Geoagiu - mine to downstream groundwater Ardeu

To make fully operational this general framework for contaminated sites management one needs to compare the ontologies of soil science, hydrology, and population ecology, to identify scale-specific patterns of metals distribution reported in each discipline, and infer the coupling mechanisms between disciplinary entities in the cases where one or more variables explicitly or implicitly common are reported to be involved in the generation of the patterns. This was initiated, as reported in

Iordache et al. (2012) and its completion is a research direction.

One can conclude that *metal biogeochemistry is only one side of the research of productive systems. There is an optimal complexity of the integrated models in metal biogeochemistry. A minimally complex structural model can be built according to the structure of the developmental systems included in the productive entity, allowing for the structural integration of several environmental entities. A complementary functional integration results from the observation that it makes little sense to study the circulation of one element (e.g., a heavy metal) in the population of developmental systems (DSs) identified by the structural model separately from the circulation of other elements playing the role of resources or toxicants (e.g., macronutrients), because all of them influence the productivity of the DSs.* This idea of looking at the same time for the circulation and effects of many elements will be further developed in the B3 chapter, as well as in the empirical contributions (chapter C).

Other more specific methodological considerations related to the role of mineralogy and the hazard assessment of sources of pollution in mining areas have been published by Jianu et al. (2011), and related to the role of organic carbon in influencing heavy metals mobility by Neagoe et al. (2011). They are the results of comprehensive reviews of the role of these variables at all scales, without methodological innovations besides pointing out the connections between processes at various scales and the need to consider the scale specificity of each process.

B4. A conceptual methodological framework for the resilience of biogeochemical services to heavy metals stress

After twelve years of field research, experimental research (roughly from 2009 to 2021), and mathematical modeling of ecohydrological processes in the framework presented in chapter B3 we moved one step further by accounting for the functional (traits) diversity inside the SPU of plants, besides the structural (species) diversity in Iordache and Neagoe (2023). This was needed because the species diversity could not explain the difference in the erosion control and biogeochemical services resulting from our research and was convergent with other findings reported in the literature.

Figure 16 presents a scheme for studying biogeochemical services and their effects in areas contaminated with heavy metals (HMs). The role of the scheme is to provide the conceptual model needed for an integrative literature review. One can notice the long-term feedback loop of the ecotoxicological effects of HMs on the stress factors themselves by the processes involved in ES production, including the management reactions (and converging with the DPSIR model).

To point out its novelty, we compared in table 6 the approach schematized in figure 16 with two mainstream methodological approaches. The simplest way to evaluate the effect of stressors on the production of ES is to consider that the stressor will change the land cover (ecosystem) types in the affected area without interest in the detailed processes leading to this result (black box approach). By mapping the ecosystems and ranking them concerning the production of specific ES, one can assess the changes due to stress at the landscape scale. A more complex approach is to use abiotic and biotic ecosystem variables as indicators of the production of ES, in particular the structural and functional biodiversity, without accounting for mechanisms coupling the indicators and the rates of ES production (gray box approach). For some hydrological or biogeochemical ES it is possible to model deterministically the effects of stressors on the coupled biological and abiotic processes involved in their production. Until now, this has not been done for HMs as stressors, although there are large bodies of knowledge about their effects on biological diversity and ES. The three approaches described in table 6 are complementary and can be applied in a tiered system.

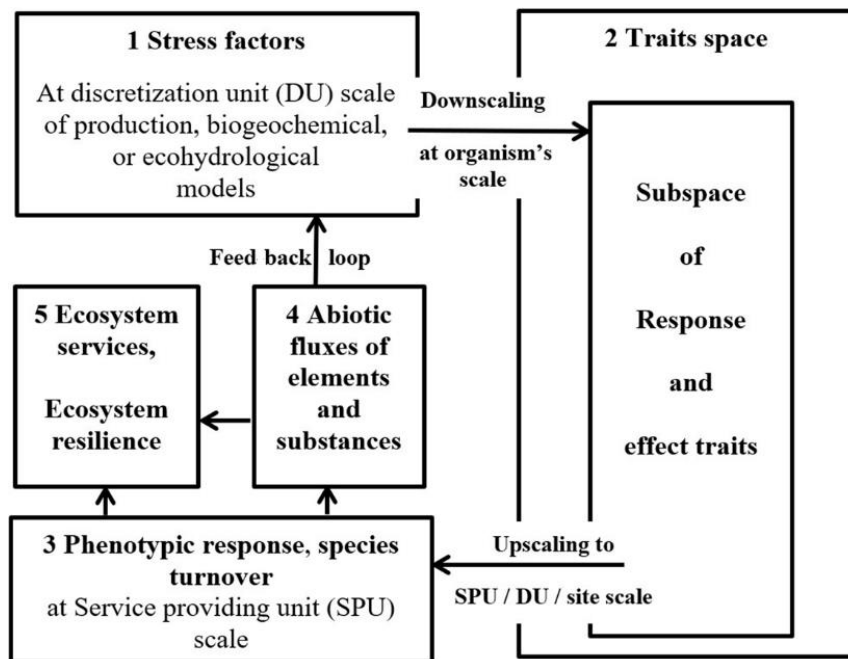


Figure 16 Conceptual model of the effects of HMs and other stressors on processes involved in producing biogeochemical and other regulating services in areas contaminated with HMs. The structure follows the cause-effect chain from stress factors as primary independent variables to the same stress factors as final dependent variables in the long term. The response traits include stoichiometric traits, accounting for the circulation of many toxic elements, macronutrients, and micronutrients at the same time. There is feedback on stress factors from SPUs by the functional traits and their consequences on ecosystem processes. This feedback is relevant for understanding environmental resistance and resilience to stress. One can notice two operations not usually included in other methodological frameworks: the downscaling of stress factors to the organismal scale and the upscaling of functional traits from the organismal to the SPU scale.

Long-term research networks of areas contaminated with HMs embedded in their larger socio-ecological context can tackle the complexity and time scales of the processes referred to in figure 16. One can decompose the complex problem of describing the integrated chain of processes into fundamental research and applied research priorities. The novelty of the approach comes from the complementarity of the deterministic approach of HMs impact on biogeochemical services (“white box”) with other methods, from an innovative conceptualization of the resilience of biogeochemical services to HMs stress (see table 6), and the potential of catalyzing long-term research networks of contaminated areas.

Table 7 presents a hierarchical structure of a heuristic concept of the resilience of biogeochemical services to HMs stress used for methodological purposes in this article. One can notice it is cross-scale and capitalizes on the existing simple concepts at the scale of the service-providing units, on more complex ones at the scale of ecohydrological and biogeochemical processes, and very complex ones at the scale of socio-natural processes. The same table shows how the SPUs are included in integrating larger-scale studies. The relevant aggregated functional traits of each SPU control the rates of processes at a larger scale. Characterizing the resilience of the entire system depends on the availability of integrated models and databases across scales. These data and knowledge depend on portfolios of projects organized in the frame of coherent research programs, which rely on institutions stimulating interdisciplinary cooperation (contributions to institutional development are presented in chapter E of this text). Details about how to organize research programs and projects in this framework are presented comprehensively in Iordache and Neagoe (2023).

Table 6 The “white box” approach developed in this article compared to more traditional ones (simplified from Iordache and Neagoe 2023).

	Approach 1 Black box	Approach 2 Grey box	Approach 3 White box
	The stressors lead to changes in land cover/ecosystem diversity. By correlating ecosystem types/diversity and ESs production, one infers the effect of stressors on ESs.	The stressors lead to a change in biological diversity inside ecosystems or other indicators. By correlations between structural and functional biological diversity and ES production, one knows the effect of stressors on ESs.	The stressors lead to changes in particular populations and communities producing a specific ES. One can model the production change by the causal effects of SPU functional properties on other processes supporting the production of a particular ES.
Advantages	Low costs of assessments, fast application, easy to be institutionalized.	Medium costs. Allow the connection between biodiversity management and management plans for contaminated areas. Relatively simple interdisciplinary approach.	Allow prioritization of actions for species management in the contaminated area and the quantification of the positive externalities by simulating the processes involved in producing an ES.
Disadvantages	No connection with the ecotoxicology agenda. Not informative concerning the management of species in the contaminated area, the space-time distribution of the positive externalities due to ES is unknown.	Weak connection with the ecotoxicology agenda. Not informative for the prioritization of species management actions in the contaminated areas, the space-time distribution of the positive externalities is not known.	Comparatively higher costs for the knowledge production and monitoring of remediation actions. More complex institutions are needed for implementation, with high transaction costs.
Useful especially	In the screening phase at a large decisional scale, when low budgets are available for contaminated site management or when there is high resistance to cross-sectoral cooperation	In classic ecological restoration / gentle remediation approaches, social climates are open to cooperation between the managers of contaminated lands and biodiversity managers.	When the beneficiaries of the positive externalities due to a specific class of ES are economically strong, there is a social climate favorable to institutional innovation.

Table 7 Structure of the cross-scale heuristic concept of the resilience of biogeochemical services to HMs stress, organization of the integrated modeling for its operationalization, and needed institutions for implementation.

Resilience of entities and processes involved in the production of biogeochemical services	Exo(endogenous) stressor, mechanism of resilience	Measurable properties for resilience estimation					Variables for cross-scale integrated modeling		Institutions needed
		R	ED	PD	A	P	Independent	Dependent	
SPUs	External HM stressor, ecophysiological, populational, and community mechanisms	x	x	x			HM, other abiotic variables, SPU species abundances, and other species variables.	Functional traits (FT) of SPU species, aggregated FT at the SPU scale	Research projects, integrated monitoring systems
Coupled SPU-abiotic processes	External or internal HM stressors depending on the scale of the system (ecosystems, landscapes, catchments), ecohydrological and biogeochemical mechanisms			x			Variables at the DU scale controlled by aggregated FT at the SPU scale (e.g., Hydraulic conductivity, critical soil share stress, surface roughness, vegetation porosity), other abiotic variables	Variables directly relevant for the production of biogeochemical services (e.g., surface water speed, soil detachment rate, infiltration rate, fluxes of elements, the retention time of elements)	Inter-disciplinary research programs, long-term research, and monitoring sites (LTRMS)
Socio-natural processes	Internal HM stressors, organizational and institutional mechanisms			x	x	x	Rates of biogeochemical services externalized from the contaminated areas and internalized in other organizations or action arenas; other natural, social, and economic variables.	Production variables at micro (organizational) scale, macro (socio-economic) variables at action arena/community scale	Local inter-disciplinary ecosystems of innovation, international networks of LTRMS, and large-scale institutions catalyzing cooperation

C. Empirical contributions

C1. Scale-dependent patterns of the distribution of organisms in contaminated areas

The point of this line of research is that the organisms will respond to the concentrations of toxic elements integrated at their maximal scale. Due to the spatial heterogeneity of concentrations measured at different scales (figure 14), one cannot simply use an average concentration at the site scale to understand the stress on all organisms but would need a mapping of toxic elements at the right resolution.

The first suggestion that this hypothesis might be confirmed was reported by Iordache et al. (2010). *We investigated the structure of biological communities at the ecosystem and landscape scale in four small catchments including in their structure contaminated areas resulting from mining and processing of heavy metals ores. The contaminated hot spots (ecosystems) were mining dumps, tailing dams, and areas polluted by atmospheric deposition around a smelter. The groups of organisms have been selected such as to reflect information about the properties of the biotope from small scale (soil microorganisms, oribatid mites), to average scale (plants, thysanoptera, carabid beetles), and large scale (birds). The objectives of the research have been to characterize the secondary succession in heavy metals contaminated ecosystems of different types and ages and to characterize the potential of each group of organisms as a bio-indicator of the ecosystem state. The overall structure of the community was a result of sub-ecosystem, ecosystem, and landscape scale structural characteristics. Soil microorganisms and oribatid mites were useful indicators of the heterogeneity of the abiotic conditions within the investigated ecosystems, but less for comparison with surrounding reference systems. Plants, thysanoptera, and carabid beetles were good indicators of the ecosystem state as compared to the reference ecosystems from the surrounding landscape. Birds were not sensitive to the state of the contaminated ecosystems, but rather to the structure of the integrating landscape (figure 17).*

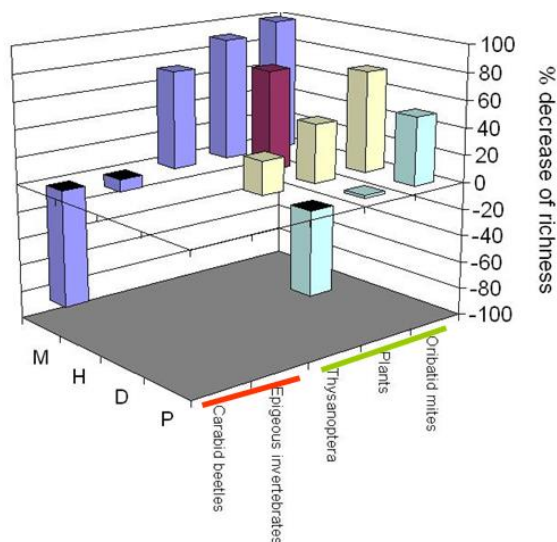


Figure 17 The percentage of the decrease of the richness of different groups in the contaminated area compared to the nearby reference ecosystem in four mining sites (coded as M – tailing dam, H and D – mining dumps, P – catchment contaminated from by smelter). *The decrease of richness in contaminated sites compared to reference sites seemed to be larger as the scale of the organism was smaller, in each site (no statistics were performed in this preliminary research). For organisms with scales smaller than the size of the site (signaled by the green line in the figure) the difference in richness was smaller a) in sites in a later primary succession phase compared to an earlier phase and b) in sites in secondary succession compared to primary succession phases (Iordache et al. 2010).*

For more insights, we used field X-ray fluorescence to map the distribution of toxic elements in contaminated catchments and field plots, which involved building preliminary relationships of these measurements with standard methods of heavy metals analysis by wet digestion and ICP-MS. The results, not presented here for the reason of space, are families of regression curves F-XRF – ICP-MS for a family of contaminated sites from Romania. After having such maps at the needed resolutions, we performed a sampling of the mites as the target group in contaminated catchments and tailing dams leading to several publications that point out the details of the species and community response (Manu et al. 2016, 2017, 2019). I will not insist on the details of this taxonomic group, which will be presented in another habilitation thesis dedicated to populational and community issues, but will only illustrate the findings relevant to my general hypothesis in figure 18 (from Manu et al. 2019).

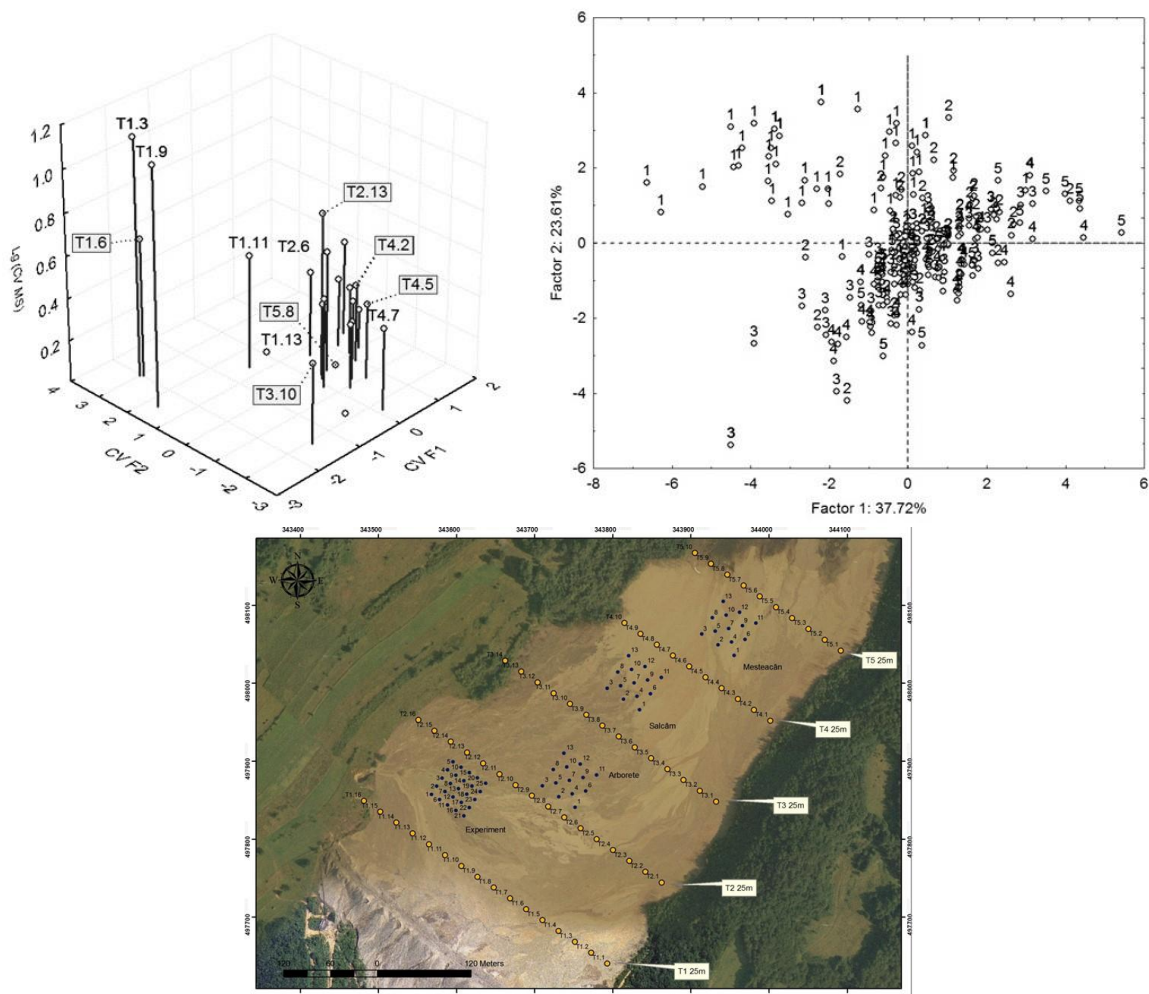


Figure 18 Left: Correlation between the coefficient of variation of mites' species richness (log-transformed) and the coefficient of variation of the scores extracted by PCA from in situ measurements of geochemical variables on the tailing surface in each station with a plot of 2 m². Codes indicate examples of stations on the five transects (e.g. T1.3 = transect 1 station 3); Right: biplot of the samples scores on the factors 1 and 2 extracted by PCA from in situ geochemical measurements. Numbers indicate that the measurements belong to the same transect, from 1 to 5 (graphs are from Manu et al. 2019, the map is from Iordache et al. 2015).

While correlations of species abundances with the concentrations of toxic elements at their scale were highly variable, showing that the toxic elements are not in all cases an important control factor of mites distribution in contaminated areas, the coefficient of variations of species richness in each station from transects across a tailing dam (log-transformed) was correlated with the coefficients of variation (CVs) of the scores of in situ geochemical measurements extracted by principal component

analyses (PCA) on the first two factors (figure 18). Both correlations with the CVs computed for the first ($R = -0.63$) and second ($R = 0.52$) PCA factors were statistically significant ($p < 0.05$). This means that at the community level, the spatial heterogeneity of toxic elements distribution at the mites' scale is an important driver of the community structure.

Other results describing the control of fine-scale heterogeneity of heavy metals in a contaminated catchment on the distribution of grassland plants at the scale of 5x5 m resolution will be published. The raw data are available at <https://aspabir.biogeochemistry.ro/>, and figure 19 shows the sampling approach in our model catchment. This model catchment was used also for modeling the role of plants in hydrological processes (chapter D2).

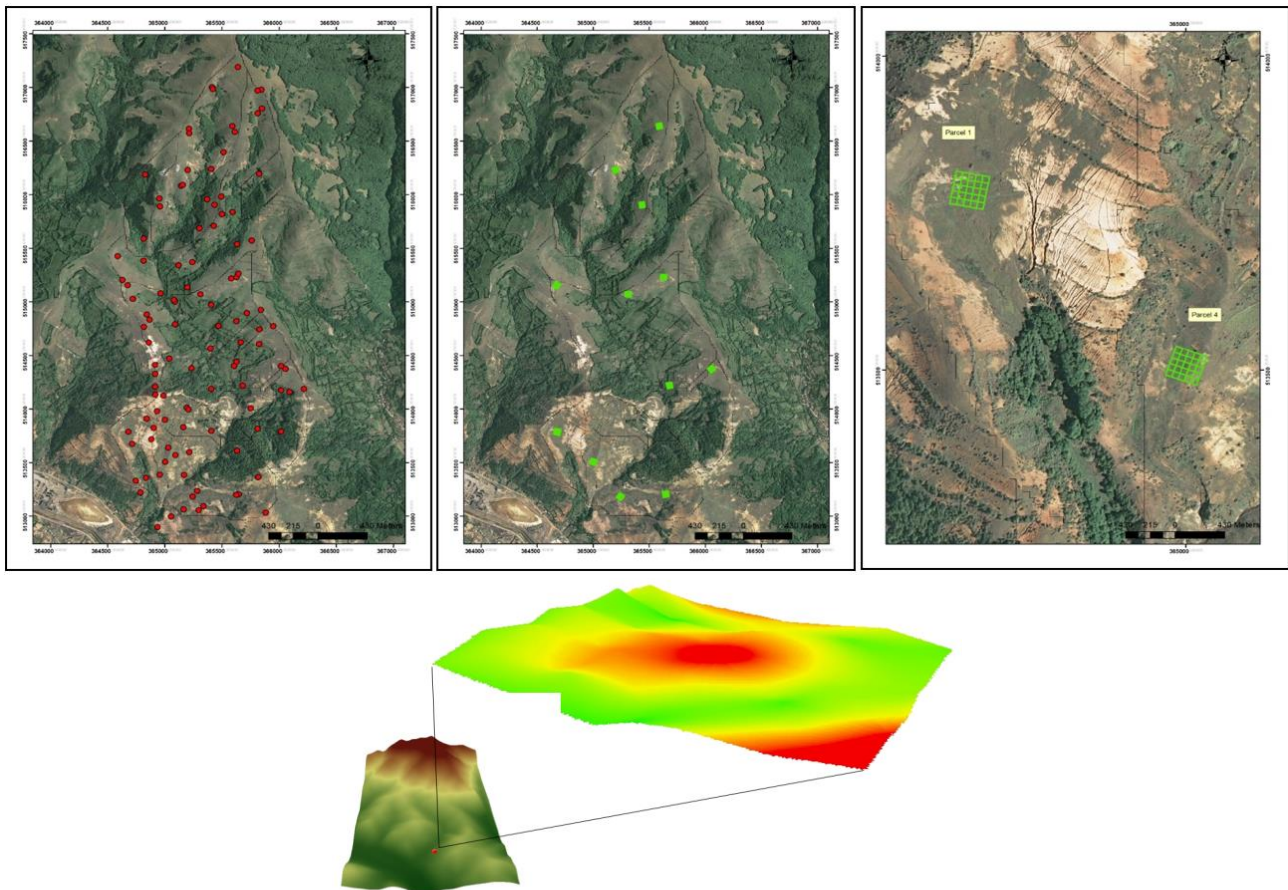


Figure 19 The sampling approach in a contaminated catchment (up) and the map of Pb in plot number 3 (down). 113 points were used for the basin scale interpolation of different variables, and twelve 50x50 m plots for downscaling at the plant ecophysiological scale. The larger concentration of Pb in plot 3, for instance, is associated with a horizontal area in the center of the plot, resulting probably from the buffering of the particulate flux of Pb transported by runoff (Iordache et al. 2015, Căldăruș et al. 2014).

C2. Experimental investigations of biogeochemical processes in soil-plant systems

The pot, lysimeter, and field plot experiments allow the investigation of partly overlapped sets of variables and hypotheses, partly different ones, and can also be used in a complementary way. Overlapped sets of hypotheses can be about the same plant and soil variables and processes at increasing spatial scales, leading to sometimes different results due to substrate/soil heterogeneity and the influence of interactions between individual plants. Typical new hypotheses tested with lysimeter experiments are those about vertical fluxes of elements by water. Typical new hypotheses at the field plot scale are those about the effect of sampling time (plant age) on the variables and relationships in between (because in pots and lysimeters usually all plants are sampled at one moment). The three types of experiments can be used in a complementary way for methodological purposes (pots are cheaper than larger-scale experiments and allow the screening of more experimental variants), for basic science purposes (for instance to look for the effects of plant age and substrate heterogeneity), or for phytoremediation purposes (screening many variants at pot scale before investing in large scale field experiment, see for these aspect the complementary habilitation theses of Dr. Aurora Neagoe).

Because of their complexity, the experiments are teamwork, and the main authorship can be shared with other authors. In our team, the tactic was to share the responsibility in the following way:

- phenomenological hypotheses related to plants and soil (rejection of null hypotheses for all the differences between directly measured variables in the experiments are allocated to my colleague Dr. Aurora Neagoe, who specializes in ecophysiology and phytoremediation.
- phenomenological hypotheses related to fluxes of elements by water and plants and the integrated control of toxic elements and nutrients on oxidative stress of plants (tested by statistical models) were my responsibility, as processes useful for building a biogeochemical and ecotoxicological image later at a larger field scale.

In table 8 below I summarized several findings. In the next part of this subchapter, I give details for each finding.

Table 8 Summary of the experimental results presented in this chapter.

Experiments		Main findings	Publication
Scale	Design		
The leaching of elements from soil-plant systems			
Lysimeter	Two-way design, disturbed and undisturbed mining dump inoculated in two variants and control. The independent variable included the export of elements by water and plants	Inoculation changes the export of elements by water and plants and their relative importance.	Neagoe et al. (2009)
Pot	Two-way design, mining dump with four plant species with and without inoculation. The independent variables included the export of elements by plants.	Inoculation decreases the export of metals by plants although increases the biomass, depending also on the plant species.	Neagoe et al. (2013)
Pot and lysimeter scale	One-way design, tailings material with inoculation. The independent variables included the export of elements by water/	The inoculation decreased the concentrations of elements in leachate.	Nicoară et al. (2014)

Table 8 Continued.

The control of toxic elements, and P on plant oxidative stress			
Pot	Two-way design, mining dump with four plant species with and without inoculation. The independent variables included chemical traits and oxidative stress variables	P and toxic elements co-control oxidative stress.	Neagoe et al. (2013)
Pot and lysimeter scale	One-way design, tailings material with inoculation. The independent variables included chemical traits and oxidative stress variables.	The control of the toxic elements on the oxidative stress depends on the depends on the age of the plants and the scale of the experiment.	Nicoară et al. (2014)
Lysimeter and field plot	One-way design, tailings material with inoculation in two concentrations.	The control of P and toxic elements on oxidative stress depends on the age of the plants and the scale of the experiment.	Neagoe et al. (2014).
Pots, lysimeter, and field plots	One-way design, tailings material with amendments. The independent variables included chemical traits and oxidative stress variables.		Constantinescu et al. (2019)
Experiments coupled with field studies		Main findings	Publication
Scale	Design		
The control of N and P on the accumulation of toxic elements and oxidative stress in plants			
Pots and small catchment	A sampling along contamination gradients was repeated to validate statistical models. Two-way design with N and P added on the most contaminated soil. The independent variables included chemical traits and oxidative stress variables	Nitrogen, phosphorus, and organic carbon in the soil were predictors of toxic elements accumulation in plants at the catchment scale. The oxidative stress of <i>Agrostis capillaris</i> in the field was controlled by N and P but differently than at the pot scale.	Iordache et al. (2022)

C2.1. The leaching of elements from soil-plant systems

In a bivariate experiment with lysimeters, we looked for the effects of disturbance (undisturbed with and without amendments of uncontaminated soil TS (top soil) or compost K vs. repacked mining dump substrate) and inoculation with vesicular-arbuscular mycorrhizal fungi (M variants) and plant-growth-promoting bacteria (MS variants) *on the dynamics of metal concentrations in the upper soil horizon and the relative importance of the export of metals by plants compared with the export by leachate* (Neagoe et al. 2009). The idea was a classic biogeochemical one, namely that the higher the disturbance of the system, the higher the export of elements from the system. On the other hand, the inoculation with fungi and bacteria would facilitate the succession and close the system from the point of view of the fluxes of elements (towards more internal cycling).

Figure 20 shows the relationship for treatments using disturbed lysimeters between the ratio of the metal export by plants/export by leachate and the ratio of the metal concentration in topsoil after the experiment/before the experiment. It can be observed that when plants played a more important role than the leachate in the export of metals, those metals also tended to accumulate in the topsoil. In contrast, when the water was more important in facilitating the export of metals, the concentration

of those metals in the topsoil tended to decrease. This pattern, although present, was not as clear in the undisturbed treatments.

As mentioned, the experimental treatments were characterized by different degrees of soil disturbance. The control (C) was the least disturbed, the treatments mixed with expanded clay were the most disturbed (CB), and those amended or mixed with inoculated expanded clay were in between (CBM and CBMS). In this context, one could predict that the C variant would have the lowest relative export of metals compared to the stock of metals in the soil. At the other extreme, the CB, CBM, and CBMS treatments would have the highest export of metals compared with the stock of metal in the soil. This prediction was confirmed except for U and Cu. The general picture described by these data is depicted in figure 21.

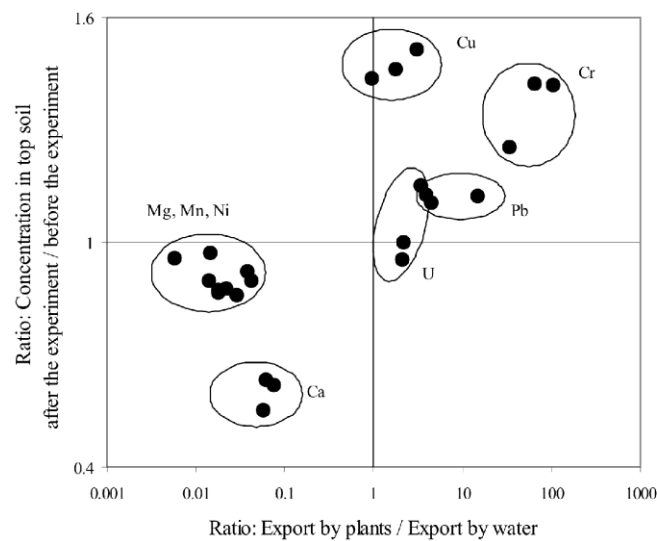


Figure 20 Relationship between the ratio of the export by plants/export by percolated water and ratio of the concentration in top soil after the experiment / before the experiment, for the repacked variants.

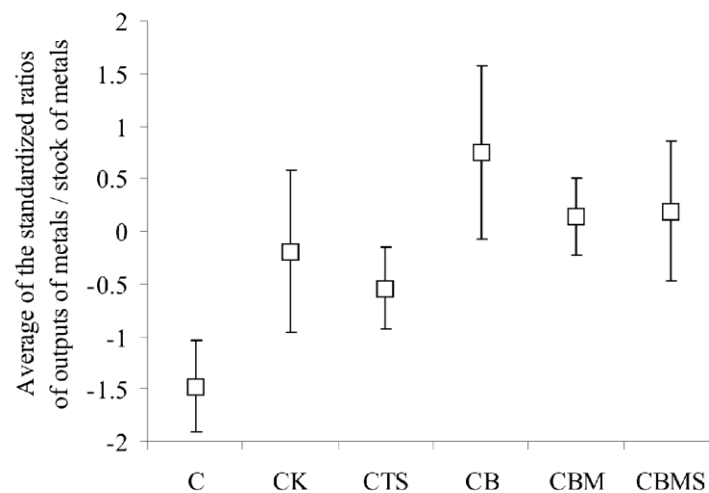


Figure 20 The ratio between the total export of metals from the lysimeters and the stock of metals in soil (average for the studied metals and S.D.). To ensure an equal influence of each metal on the final pattern the ratios of a metal in an experimental variant have been standardized using the mean of the ratios of that metal in all variants. C = undisturbed control, CK = control amended with compost, CTS = control amended with uncontaminated soil, CB = control mixed with expanded clay, CBM = control mixed with expanded clay inoculated with fungi, CBMS = control mixed with expanded clay inoculated with fungi and plant-growth-promoting bacteria.

Plant species also play a role in the output of elements from the contaminated substrate/soil, as demonstrated by another experiment in which we compared four species, namely phacelia (*Phacelia tanacetifolia*), mustard (*Sinapis alba*), clover (*Trifolium pratense*) and sunflower (*Helianthus annuus*) (in the experiment of Neagoe et al. 2009 presented above we worked with a mixture of *Festuca rubra* and *Melilotus albus*). *The variations of metal concentrations as a result of inoculation do not simply follow the changes in the biomass of the plants, as shown by the percent variation of the stocks of metals (table 9). At least in the case of phacelia and clover, while the biomass increased, the stocks of many of the metals had an inverse trend, underlining changes in the bioaccumulation factor as a result of inoculation.*

Table 9 *Percent variation of the stocks of selected toxic elements in plants from contaminated to contaminated and inoculated variant (CI). The sign + or - near the plant name indicates the variation of total plant biomass in the case of each species. One can see that the variation in plant biomass is not always the same as the variation in the stock of metals, which underlines the metal and species-specific influence of inoculation on the bioaccumulation factor.*

Plant species	Elements						
	As	Cd	Co	Cu	Pb	U	Zn
Phacelia +	-31	-10	-32	-10	-23	-20	21
Clover +	-18	-11	-19	80	20	63	9
Sunflower -	-34	-12	-20	-27	-8	-29	-1
Mustard +	34	17	29	5	7	-4	11

Another proof that the inoculation with bacteria, this time without fungi, decreases the leaching of elements in different ways depending also of the plant species was published by Nicoară et al. (2014). *A general pattern of elements' concentrations decrease occurred, with many significant differences (figure 22). For instance, following inoculation As in the leachate of pot experiment with A. capillaries decreased by three-quarters, Ni by almost two-thirds, while Cu and Mn were down by half. Pb could not be detected in the leachate of the inoculated pots. Zn also showed a decrease in average concentration but this was not statistically significant. As, Cu, Ni, and Zn concentrations decreased in the leachate from F. rubra pots. In the lysimeter experiment, metals in leachate also showed a decrease in concentration as a result of inoculation but manifested great heterogeneity, leading to fewer statistically significant differences (Mn and Zn).*

The inoculation did not have a statistically significant effect on the concentration of toxic elements in easily available fractions from the amended mining substrate. However, there was a statistically significant decrease in concentrations at the end of the experiments both for pots (Cu, Ni, Pb, Zn, inoculated and not inoculated) and for lysimeters (As, Cu, Ni, Pb, Zn, inoculated, and not inoculated).

Recently (Neagoe and Iordache 2023), we found that the response of usually non-mycorrhizal plant species such as *Lupinus angustifolius* to the inoculation of the mining-dump substrate with arbuscular mycorrhizal fungi (AMF) commercial inoculum had a positive effect on the plant development, with consequences on the fluxes of elements from the soil-plant system. *The fact that a species classified as non-host hypothetically had ecological relations (other than symbiotic) with AMF when the physiological adaptations of the non-host plant were no longer efficient, like in acid mining dump conditions, raised the questions of the potential mechanisms. We reviewed the literature allowing a comparison between the interaction mechanisms of AMF with host and non-host plants and summed up the knowledge in figure 23.*

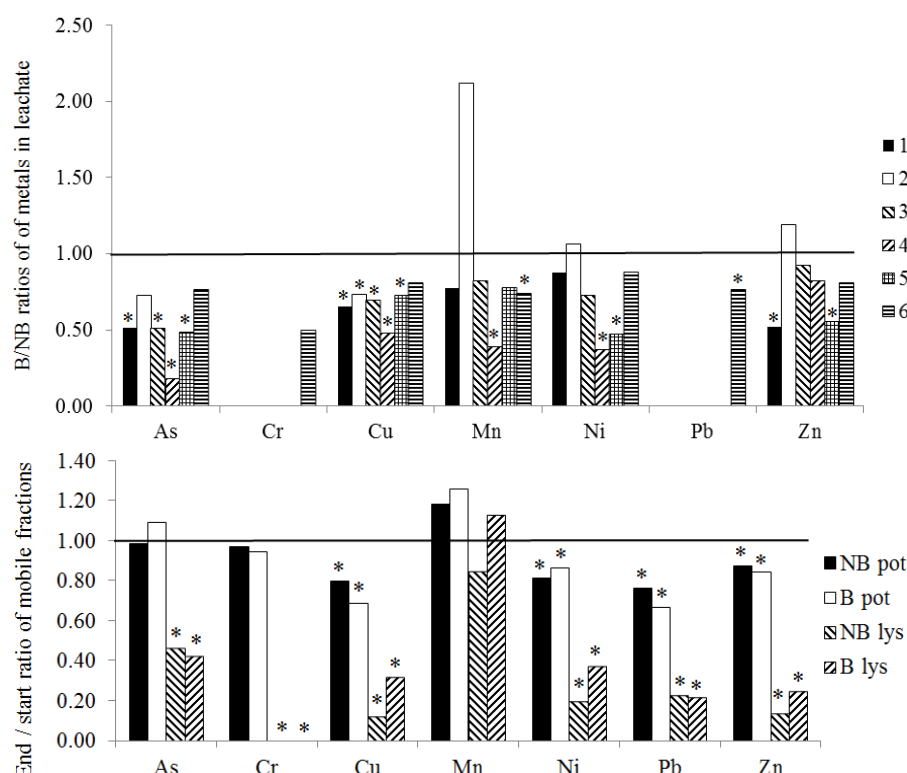


Figure 22 Patterns of element distribution in leachate and mobile soil fractions ((F1+F2, extraction agent 1 M NH_4NO_3 for F1 and 1M $\text{CH}_3\text{COONH}_4$ for F2). **Above:** the ratio between element concentration in leachate from inoculated (B) and not inoculated (NB) treatments at pot (treatment 1-5 in the legend) and lysimeter (treatment 6 in the legend) scale. **Below:** the ratio between the mobile fractions at the end of the experiment and at the start of the experiment. Cr concentrations in the mobile fractions at the lysimeter scale were detectable at the start of the experiment, and below the detection limit at the end of the experiment (ratio assumed to be zero on the graph). Legend: 1 = *Helianthus annuus*, 2 = *Verbascum thapsus*, 3 = *Deschampsia flexuosa*, 4 = *Agrostis capillaris* at pot scale, 5 = *Festuca rubra*, 6 = *A. capillaris* at lysimeter scale, * = significant change because of inoculation (above) and between the end and the start of the experiment (below) (Mann-Whitney U test).

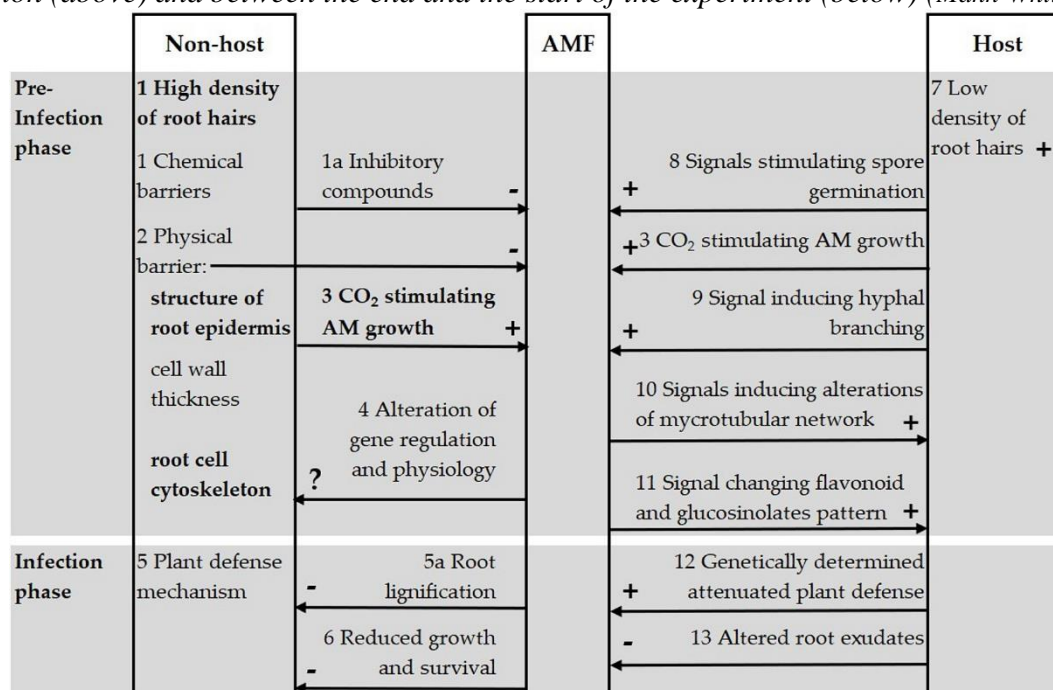


Figure 23 Interaction mechanisms of AMF with host and non-host plants (Neagoe and Iordache 2023).

From an ecological and evolutionary standpoint, there are ‘continuums of associations’ in the development of saprophytic fungi of the rhizosphere to mutualistic mycorrhizal fungus. Every interaction depends on the dispositions and developmental stages of the plant and fungi partners as well as on environmental factors. It became clear that there are no neutral interactions between fungal endophytes and plants but a balance of antagonism. The ecological relationships between AMF and their host plants are known to range from mutualism (++) to parasitism (+-), depending on the plant genotype, developmental phase, and environmental conditions (Neagoe and Iordache 2023).

We have also worked on the problem of leaching in floodplains contaminated by tailings and nutrients, using undisturbed cores (Iordache et al. 2022a). *One could expect that the order of new reactions during floods is important for the fluxes of elements. In this context we tested the following hypothesis: the order of percolations with water having different pH and chemistry changes the export of elements by leaching from small columns of contaminated floodplain sediments. To test the hypothesis, we sampled 24 columns of sediments from two locations in the Arieş floodplain, Romania. Two columns from each site were used to characterize the initial chemistry and mineralogy of the sediments, and 5 columns were percolated with water having different pH and chemistry. In the first variant, the order of floods (six percolations for each type of water) was from neutral water to technological basic water (sampled downstream of an active tailing dam), to technological acid water (sampled upstream of an active tailing dam). In the second variant, the order was from acid technological water to basic technological water and neutral water. We measured in the percolated water the pH, conductivity, heavy metals, and total phosphorus, ammonium, nitrate, nitrite, and phosphate. After the 18 percolations, we cut the columns longitudinally and made the chemical and mineralogical characterization of the sediment. We computed the total fluxes of elements exported from each sediment type in each order of hydro-chemical events, tested by bivariate ANOVA the hypothesis, and interpreted the results in function of fine structure of the exports of elements in time, and the differences between the initial and final chemistry and mineralogy of the sediments. The conclusion was that the order of the floods with neutral, “basic” and “acid” technological water changed the patterns of the export of elements (fluxes, stoichiometry, figure 24), but also that the spatial heterogeneity of sediment geochemistry interferes with the effect of timing. The experiments with undisturbed field sediment and water from streams and technological sources are not strictly replicable because of the uniqueness of their properties. The findings from this experiment stimulated our interest in the stoichiometrical approach of element retention in floodplains (Part II of this thesis).*

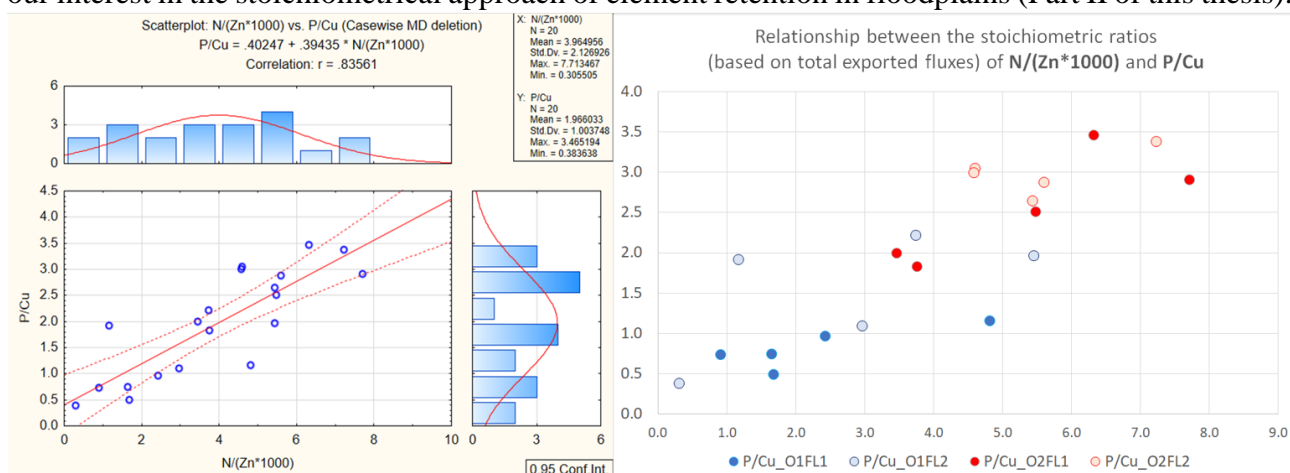


Figure 24 Patterns of the ratios of total fluxes of P/Cu and N/Zn (18 floods). O1 = order 1 of flood (neutral-basic-acid, O2 = order 2 of floods (acid-basic-neutral), FL1 = floodplain 1, FL2 = floodplain 2. (Iordache et al. 2022a).

C2.2. The control of toxic elements, and P on plant oxidative stress

This line of research was innovative because the effects of toxic elements were usually studied separately from the effects of macronutrients. We arrived at the integrated research of these control factors by noticing the improvements in plants' state as a result of inoculation with mycorrhizal fungi when grown on substrates or soils contaminated with toxic elements (sampled from mining dumps, tailing dams, or around smelters).

Figure 25 from Neagoe et al. (2013) shows that in roots there were almost no correlations between the variation of oxidative stress parameters and metals, but there was an important correlation between SOD, POD, and proteins, on the one hand, and P on the other. Larger concentrations of P in roots tend to be associated with lower SOD activity, more clear in the contaminated soil (C and I variants), than in the uncontaminated soil. A larger increase in P concentration in roots from one variant to another is associated with a larger decrease in SOD activity when computed based on total protein, but not when computed based on dry biomass. Other correlations in shoots and leaves are presented in table 10. In shoots, the variation of SOD is positively correlated with that of some metals (Zn), negatively correlated with Fe, and positively with P. The variation of POD in leaves is positively correlated with that of Fe. In leaves, the variation of SOD is positively correlated with that of Cu, Fe, and P, while that of the LP is negatively correlated with the variation of Cu and P. In leaves and shoots, there is no statistically significant relationship between the raw values of SOD and P.

In Nicoară et al. (2014) we inspected the correlations between elements and biochemical variables in the case of the pooled set of data for *A. capillaris* (pot and lysimeter) to detect patterns. There is a cluster of significantly inter-correlated elements in roots, and this cluster is also correlated with the lipids peroxidation. In aboveground parts, a similar cluster includes As, Mn, Pb, Cu, and Zn, which is correlated with lipids peroxidation and assimilating pigments (table 11). However, as illustrated in figure 26, all these correlations are because the samples at pot and lysimeter scale are grouped in separate clusters, and not the effect of inoculation on elements content and biochemical variables (within each cluster of data there is no correlation, but due to the location of the cluster in the variable space there is an overall correlation). Once noticed that the scale of the experiment influences the effect of toxic elements and nutrition improvement (by inoculation) we wondered if this was not due to some extent to the age of the plant at the sampling time, and not only the different plant growth conditions as the dimension of the experiments growth from microcosm to mesocosm.

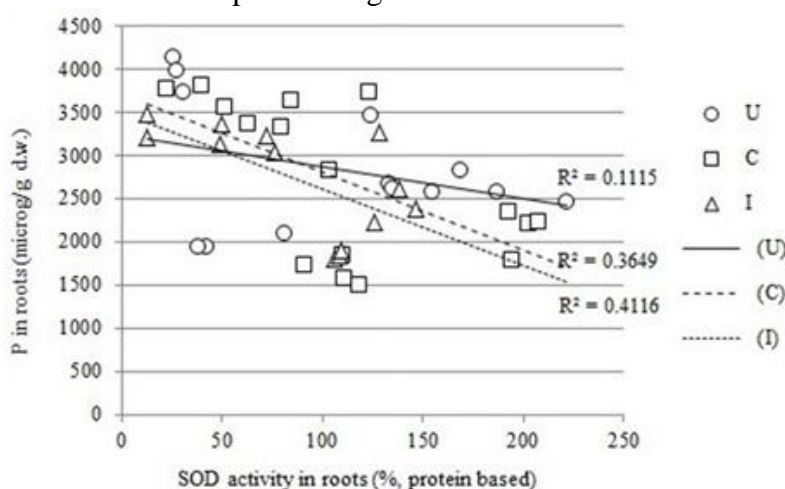


Figure 25 Relationship between SOD activity in roots and phosphorous concentration in roots based on all replicates data (U = reference soil, C = contaminated soil, I = contaminated and inoculated soil). Larger P concentrations tend to be associated with lower SOD activity, especially in the contaminated soil (C and I variants). (Neagoe et al. 2013).

Table 10 Significant correlation coefficients between the percent variation of biochemical parameters, P, and selected metals. Blank spaces refer to non-significant correlations. (Neagoe et al. 2013).

Parameters	Element				
	Cu	Fe	Mn	P	Zn
Roots (N = 8)					
Proteins				0.80 p=.018	
SOD (protein-based)				-0.73 p=.041	
SOD (biomass-based)					0.78 p=.021
POD (biomass-based)				0.89 p=.003	
LP			0.79 p=.020		
Shoots (N=6)					
Proteins			0.83 p=.043		0.83 p=.040
SOD (biomass-based)		-0.90 p=.014		0.89 p=.017	0.85 p=.030
POD (biomass-based)		0.95 p=.003			
Leaves (N = 8, and for Mo 7)					
SOD (protein-based)	0.84 p=.009	0.95 p=.000		0.83 p=.010	
SOD (biomass-based)	0.93 p=.001	0.92 p=.001		0.88 p=.004	
LP	-0.83 p=.011			-0.76 p=.028	

Table 11 Statistically significant coefficients of correlations (at $p < 0.05$) between toxic elements in *Agrostis capillaris* plant parts and biochemical plant variables.

		Roots							Plant variables aboveground			
		As	Cr	Cu	Mn	Ni	Pb	Zn	LP	Chl a	Chl b	Carotenoids
Aboveground	As		NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
	Cr	NS		-0.46	0.46	NS	NS	-0.53	NS	NS	NS	NS
	Cu	NS	NS		NS	NS	0.50	0.73	-0.55	0.87	0.88	0.88
	Mn	0.51	NS	-0.80		NS	NS	NS	NS	-0.76	-0.78	-0.77
	Ni	NS	NS	NS	NS		NS	NS	NS	NS	NS	NS
	Pb	0.65	NS	NS	NS	NS		0.65	NS	NS	NS	NS
	Zn	NS	NS	0.66	-0.51	NS	NS		-0.75	0.84	0.83	0.84
LP roots		NS	-0.66	0.62	NS	NS	NS	0.84	not applicable			

Correlation coefficients above the black diagonal characterize elements in roots and those below the elements in shoots

Legend: NS = not significant, LP = lipids peroxidation.

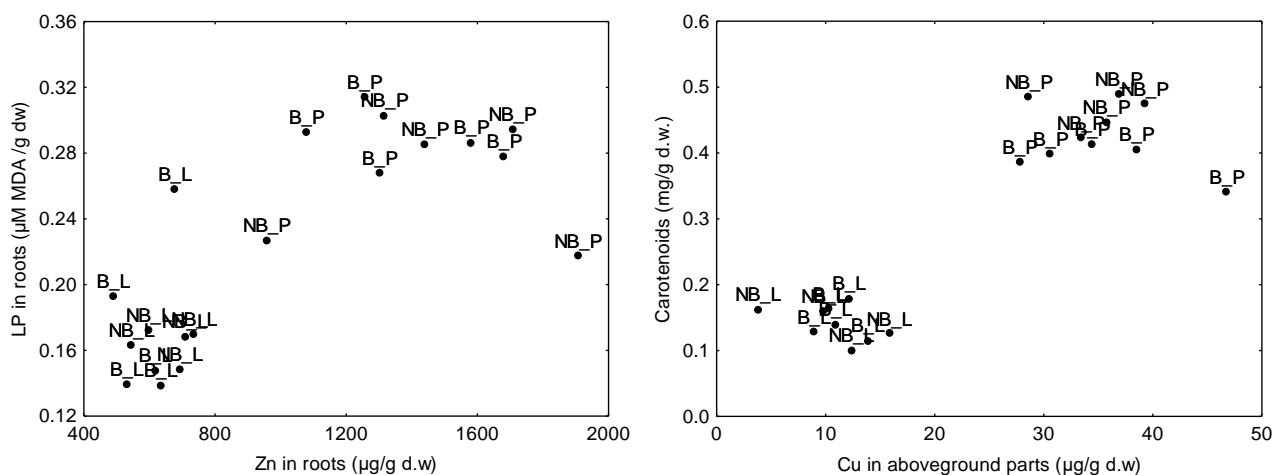


Figure 26 Examples of correlations between metals in plants and biochemical variables. One can notice that the pattern is due to the clustered distribution of samples at pot and lysimeter scales. Legend: LP = lipids peroxidation, B_L = inoculated with bacteria at lysimeter scale, B_P = inoculated with bacteria at pot scale NB_L = not inoculated with bacteria at lysimeter scale, NB_P = not inoculated with bacteria at pot scale.

In Neagoe et al. (2014) we coupled experiments in lysimeters and field plots. When analyzed by experiment we found that there are statistically significant positive correlations between P and protein concentrations when computed based on the replicates of the treatments in several subsets of data ($R = 0.63$ with $p=0.028$ in roots at month 10, $R = 0.642$ with $p = 0.024$ in above-ground parts at month 3.5, and $R = 0.67$ with $p=0.018$ in above-ground parts at month 10). Negative correlations between protein concentrations and SOD activity are statistically significant in all plant parts and data subsets (figure 27).

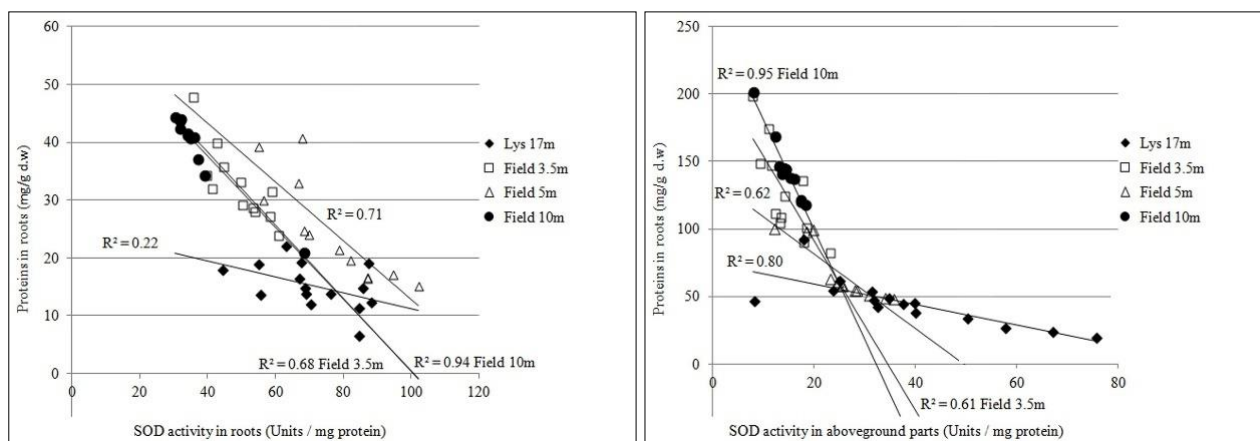


Figure 27 Relationships between proteins and SOD activity, with linear correlations computed for each data subset. All correlations are statistically significant. Legend: C = control, F7% = treatment with 7% inoculum, F1% = treatment with 1% inoculum, m = months, Lys = data subset at lysimeter scale, Field = data subset at field scale. (Neagoe et al. 2014)

There are also few statistically significant correlations between biochemical variables and several toxic elements (table 12): for Mn and Ni at the lysimeter scale, for As, Cu, and Zn at field scale month 3.5, for Mn at field scale month 5, and As and Cu at field scale month 10. The correlations existing at field scale month 3.5 occur because of inoculation, the smaller concentrations of metals, larger concentrations of proteins, and lower SOD and POD activity being characteristic to the 7% (statistically not significant) and especially the 1% treatment (statistically significant).

Table 12 Correlations between several plant variables and metals in roots and shoots for each data subset (type of experiment and moment of sampling). Legend: *, **, and *** indicate the degree of statistical significance (0.05, 0.01, and 0.001), NS = not significant for any metal. (Neagoe et al. 2014).

	Lysimeter, 17m		Field, 3.5m		Field, 5m	Field, 10m
	Roots	Shoots	Roots	Shoots	Shoots	Shoots
P [µg/g dw]	Mn* 0.55	Mn* 0.54, Ni** 0.69	NS	NS	NS	As* -0.61 Cu* 0.70
Proteins [mg/g dw]	NS	NS	As*** -0.88, Cu*** -0.81 Zn* -0.62	Cu* 0.67 Pb* 0.63 Zn* 0.60	Mn* -0.68	NS
SOD [U/mg prot.]	As* -0.62	NS	As** 0.80, Cu* 0.64, Zn* 0.47	NS	Mn* 0.66	NS
POD [U/mg prot.]	NS	Mn* 0.59	As*** 0.86 Cu* 0.65	NS	NS	NS

To prepare the exploration at the whole data set scale we first investigated the correlation between metal in plants. The analysis of the whole data set shows that the concentrations of elements are strongly inter-correlated (table 13). Principal component analysis (PCA) allowed the extraction of two factors summarizing about 70% of the variability of toxic elements in roots and above-ground parts.

Table 13 Correlations matrix for the concentrations of metals in plants and loadings of the elements for the factors extracted by PCA (varimax normalization, percents indicate the part of data variability explained by each factor, values in bold are factor loadings of metals strongly contributing to the extracted factor) (Neagoe et al. 2014).

		R, above ground parts, n = 49							Factor loadings	
		As	Cr	Cu	Mn	Ni	Pb	Zn	F1 31.84%	F2 28.61%
R, roots, n=51	As		NS	0.42 p=.003	-0.30 p=.039	NS	NS	NS	0.28	0.66
	Cr	NS		NS	0.40 p=.005	0.29 p=.044	NS	0.50 p=.000	0.68	-0.32
	Cu	0.88 p=.000	-0.292 p=.038			-0.33 p=.019	NS	0.41 p=.003	0.30	0.80
	Mn	0.46 p=.001	NS	0.34 p=.013		NS	NS	0.32 p=.027	0.47	-0.64
	Ni	0.53 p=.000	NS	0.59 p=.000	0.41 p=.003		NS	NS	0.24	-0.60
	Pb	0.67 p=.000	NS	0.71 p=.000	NS	0.48 p=.000		0.58 p=.000	0.71	0.15
	Zn	0.33 p=.017	0.30 p=.032	0.35 p=.011	NS	0.37 p=.007	0.52 p=.000		0.90	0.17
Factor loadings	F1 48.89 %	0.91	-0.13	0.93	0.51	0.73	0.81	0.52		
	F2 19.86 %	-0.17	0.92	-0.23	0.20	0.24	0.13	0.59		

The inspection of the correlations between biochemical variables and toxic elements at the scale of the whole data set has been performed using the coefficients of the factors extracted by PCA (which are correlated with several elements, table 14). There are many correlations at this scale (table 14), but looking in detail shows that they are due to the clustered distribution of the data subsets (figure 28 with an example for proteins in roots and above-ground parts), and not correlations manifesting at the scale of each data-subset.

Table 14 Correlation coefficients between plant variables and coefficients of the factors extracted by PCA from metals concentrations in plants. NS = not significant (Neagoe et. al 2014).

	Roots		Above ground parts	
	F1	F2	F1	F2
SOD lg(U/mg prot.+1)	0.34 p=.014	NS	NS	-0.64 p=.000
POD lg(U/mg prot.+1)	NS	0.31 p=.029	NS	-0.63 p=.000
Proteins mg/g dw	-0.62 p=.000	NS	NS	0.77 p=.000

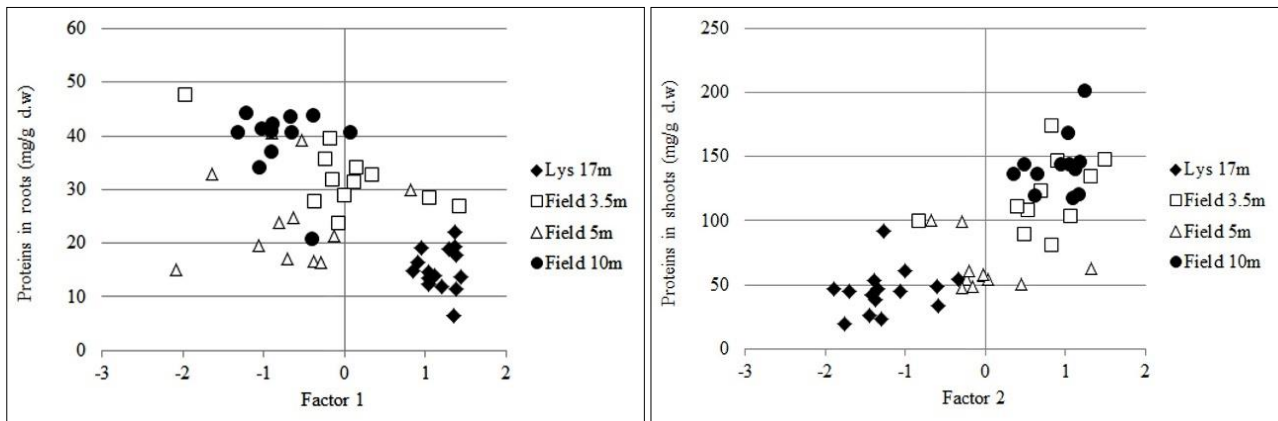


Figure 28 Graph of the protein concentration in roots and shoots in function of the coefficients of factors extracted by PCA from concentrations of metals (presented in table 13). Legend as in figure 27 (Neagoe et al. 2014).

The most complex published experiment looking for the effect of time on sampling was by Constantinescu et al. (2019, with the design presented in figure 29 to make it easier to understand the results). The tailing materials originated from the surface of a single tailing dam but were from different surface locations. The method of sampling and homogenization was, for each experiment, the approach usually reported in articles dealing with single-scale experiments, but a geochemical heterogeneity of the substrate persisted from one experiment to another, as illustrated by the principal component analysis for all sampled substrates at all sampling times and scales (figure 30).

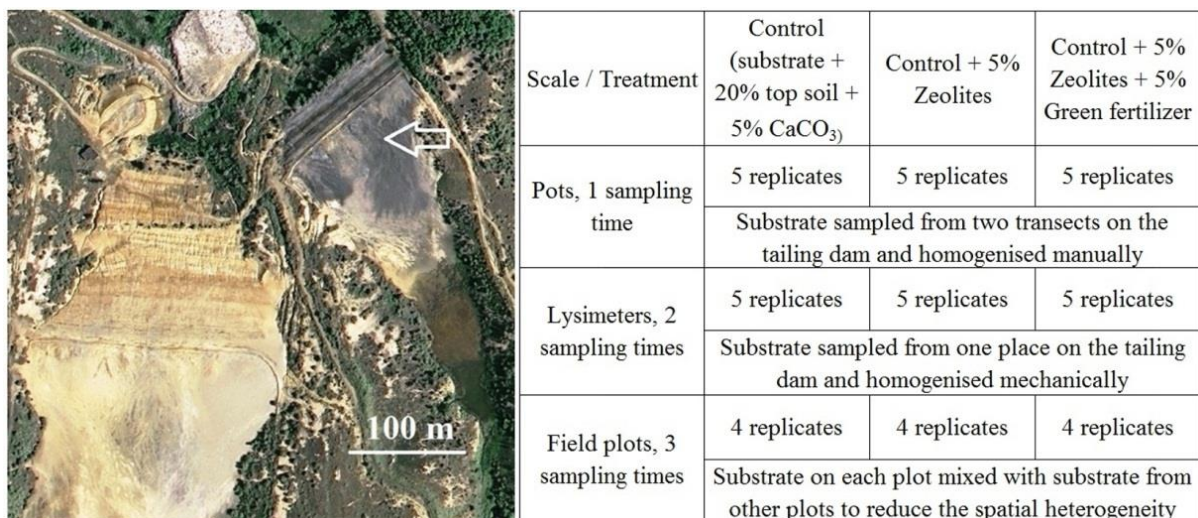


Figure 29 Left: Orthophoto imagery of the tailing dams in the Zlatna area, Romania. The small tailing dam was selected for experiments; the white arrow indicates the location of the field experiment. Right: the structure of the bivariate experimental approach.

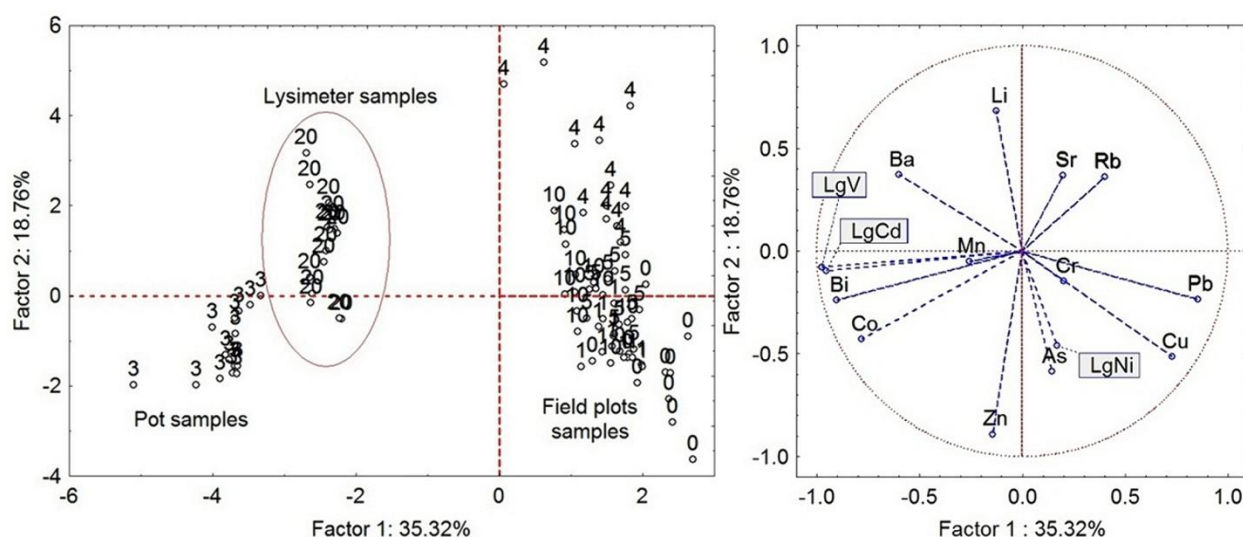


Figure 30 Biplots of sample scores (left) and of variable coordinates (right) using two PCA factors from the geochemical data. Notice the clustered distribution of the samples from the three experiments. Variables increase in the directions pointed to by the lines in the right-side graphs (for instance, samples from the pot experiments - sampled after 3 months, are shown in the left graph, have the largest concentrations of Cd, V, Bi, and Co in the substrate); the origins of the biplots correspond to the average values of the variables; the overlap or small angle between the lines of two variables or a variable and a factor indicates a strong positive correlation, while orthogonality indicates lack of correlation; the length of a variable line is proportional to the contribution of the variable to the extracted factors. (Constantinescu et al. 2019).

A preliminary inspection showed many correlations between the concentrations of elements in the plants and the physiological variables. Consequently, we decided to reduce the dimensionality of the data by PCA (figure 31). Many elements aboveground and belowground were co-correlated, allowing the extraction of three factors covering approximately 70% of the total variability in the data in total. Biplots of the sample scores for PCA factors show the strong clustering of the data by sampling times and experimental treatments (figure 31).

Table 15 summarizes the significant coefficients of correlation between physiological variables, PCA factors scores, and time since sawing. Time had an important effect on variables such as protein concentrations, pigments, lipids peroxidation, and the activity of the oxidative stress enzymes. The phosphorus status in the plants also controlled these variables (table 16). We checked the independence of these correlations by producing forward stepwise multiple regressions (results in table 16).

Table 15 Significant ($p < 0.05$) coefficients of correlation between biochemical variables, PCA factors (F1 to F3), phosphorus (P), and sampling time. NS = not statistically significant. (Constantinescu et al. 2019).

Variable	Belowground					Aboveground				
	F1	F2	F3	P	Time	F1	F2	F3	P	Time
Proteins	0.52	NS	NS	0.56	NS	NS	0.59	NS	0.33	-0.39
Chlorophyll b						0.24	NS	-0.46	0.32	-0.33
Lg Chlorophyll a		Not available					0.40	NS	-0.66	0.30
Lg Carotenes						-0.35	0.79	NS	0.08	-0.65
SOD (LgSOD)	-0.32		NS	-0.36	NS	-0.84	NS	0.60	-0.28	0.50
LgPOD	NS	0.48	NS	-0.43	-0.46	NS	-0.32	0.39	-0.35	0.52
LP	NS	0.38	NS	0.28	-0.54	NS	0.34	NS	0.16	-0.51

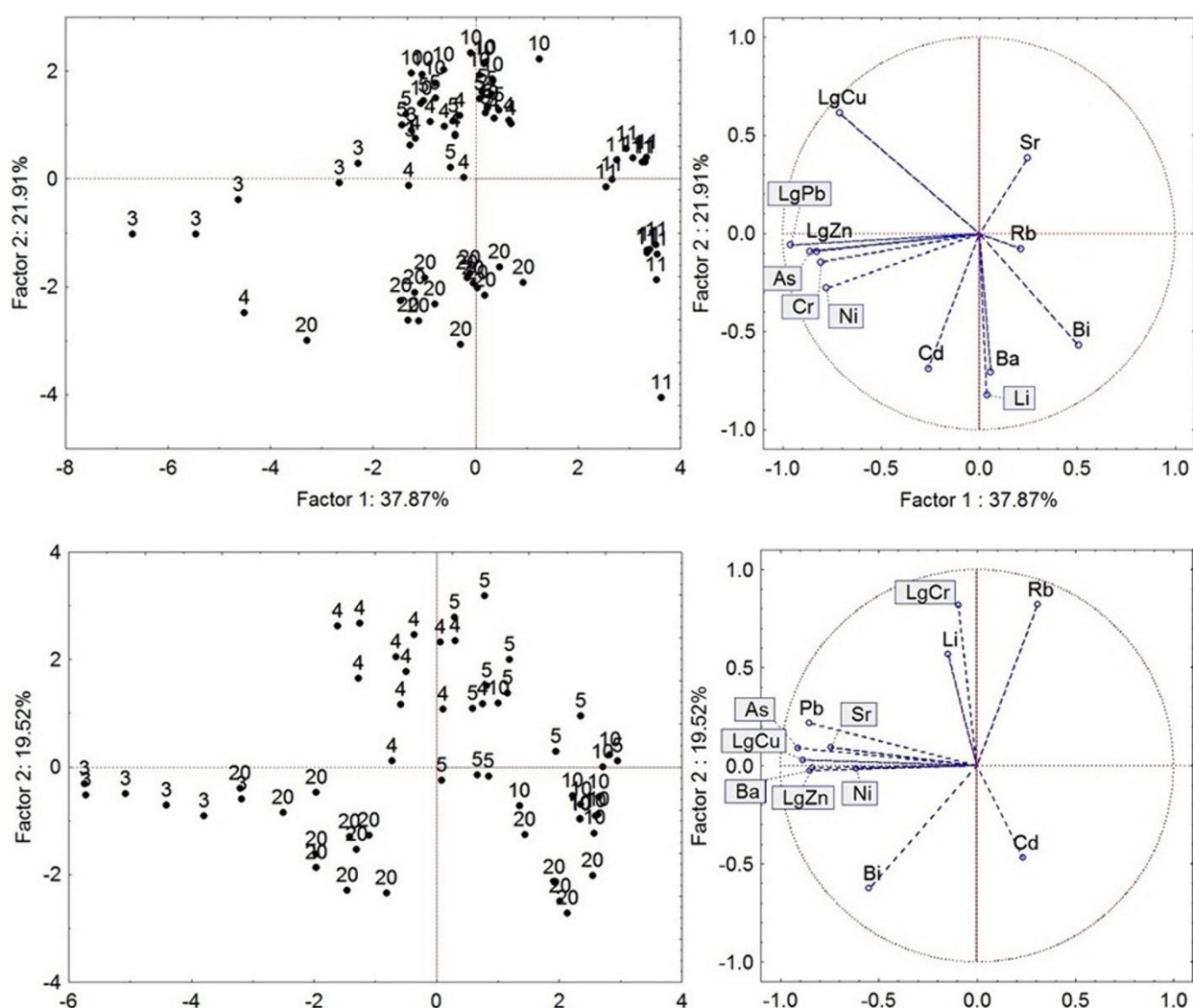


Figure 31 Biplots of sample scores and variable coordinates using two PCA factors from the root concentrations in (lower graphs) and the aboveground parts (upper graphs). Each point is a sample; the number near the point indicates the sampling time. Notice the clustered distribution of sampling times and experimental treatments. Variables increase in the direction pointed to by the lines in the right graphs; the origins of the biplots correspond to the average values of the variables; an overlap or small angle between the lines of two variables or a variable and a factor indicates a strong positive correlation; orthogonality indicates a lack of correlation; the length of a variable line is proportional to the contribution of the variable to the extracted factors. (Constantinescu et al. 2019).

Table 16 Multiple regressions for biochemical variables in function of PCA factors, P , and sampling time (significant coefficients for the standardized variables, and R^2). (Constantinescu et al. 2019).

		Toxic elements		Time	Phosphorus	R^2
	Variable	PCA F1	PCA F2			
Roots	Proteins	0.529	0.219	-	0.502	0.56
	SOD	-0.414	-	-	-0.305	0.23
	Lg POD	-	-	-0.568	-0.341	0.48
	LP	-	-	-0.810	0.367	0.38
Aboveground	LgChlorophyll a	-	-0.435	-0.857	0.240	0.63
	LgCarotens	-0.399	0.531	-0.409	-	0.75
	LgSOD	-0.760	-	0.276	-	0.78
	LgPOD	-	-	0.539	-0.307	0.39

C2.3. The control of N and P on the accumulation of toxic elements and oxidative stress in plants

I end the chapter about experiments with a field study coupled with a pot experiment (Iordache et al. 2022). It was for the first time that we directly took N and P as independent variables of heavy metals accumulation and oxidative stress both in the field and in a pot experiment.

We hypothesized that soil macronutrients control heavy metals' accumulation and toxic effects on grassland plants. In the first phase, we sampled soil and plants (26 species) from 156 locations in 12 plots distributed over contamination and altitude gradient in the 8 km² small catchment in Zlatna, Romania (pictured in figure 19). In these samples, we analyzed the concentrations of elements and the values of other potential soil control variables. The regression analysis kept total nitrogen, phosphorus, and organic carbon in the soil as predictors of heavy metal accumulation in plants at the catchment scale. In the second phase, we made a bivariate experiment looking at the effects of N and P on *Agrostis capillaris* grown in soil sampled from a highly contaminated spot. We supplemented the data set with oxidative stress variables, demonstrating that mobile forms of N and P control the accumulation and stress in plants at the pot scale. Finally, we attempted to validate the catchment and pot scale results by an extra set of 31 *Agrostis capillaris* and soil samples distributed over the same gradients as in the first phase and sampled three years later. The statistical models predicting the accumulation of Pb at the catchment scale were confirmed. The oxidative stress of *Agrostis capillaris* in the field was controlled by N and P but differently than at the pot scale. Figure 32 shows the methodological approach and details about the field results. Figure 33 shows details about the experimental results and figure 34 a comparison between field and experimental results.

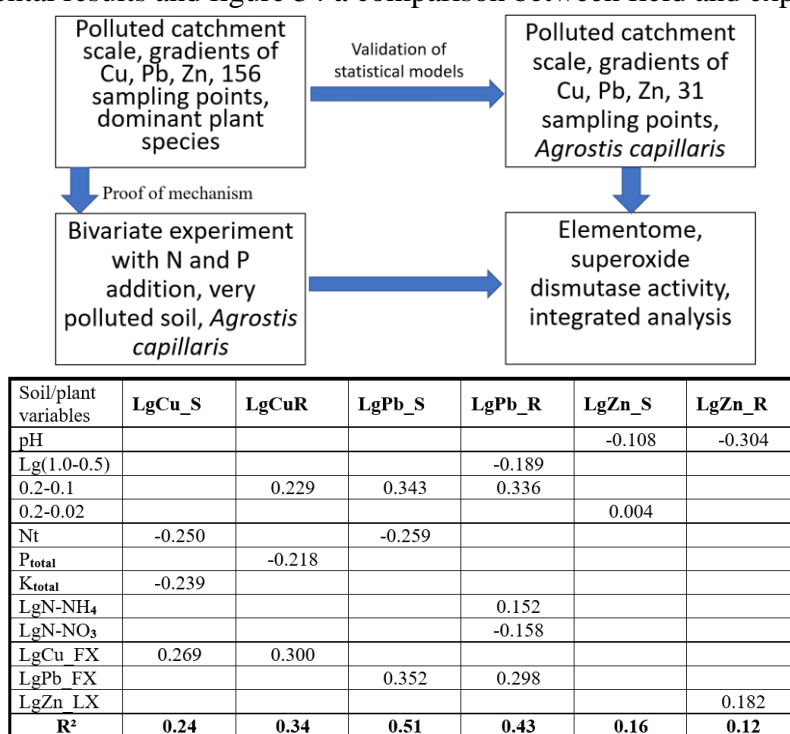


Figure 32 Up Coupled field and experimental investigations to detect the effects of N and P on bioaccumulation and oxidative stress in *Agrostis capillaris*. **Down** Standardized coefficients of the multiple regressions predicting the concentrations of Cu, Pb, and Zn in shoots (S) and roots (R) of *A. capillaris* sampled from the contaminated catchment (n=157-166) in the function of soil variables (pH, granulometric fractions, total and extractable concentrations of N, P, and K, total concentrations of heavy metals). **Legend:** FX = concentration measured in the field by F-XRF at the soil surface, LX = concentration measured in the lab by F-XRF on homogenized 0-20 cm soil (Iordache et al. 2022b).

Cu AF				Pb AF				Zn AF			
	StdCoef.	p-level	R ²		StdCoef.	p-level	R ²		StdCoef.	p-level	R ²
Intercept		0.000	0.409	Intercept		0.000	0.358	Intercept		0.000	0.202
Lg N-NO ₃ ⁻	0.416	0.000		Lg EC	0.365	0.002		pH	-0.436	0.000	
pH	0.279	0.005		pH	-0.304	0.010		Lg P Sol	-0.213	0.047	
Lg N-NO ₂ ⁻	0.243	0.011		LgN-NO ₃ ⁻	0.292	0.011					

Lg Cu TF				Lg Pb TF				Zn TF			
	StdCoef.	p-level	R ²		StdCoef.	p-level	R ²		StdCoef.	p-level	R ²
Intercept		0.003	0.386	Intercept	0.000	0.019	0.229	Intercept		0.000	0.161
Lg P soil	0.511	0.000		Lg P soil	0.458	0.000		Lg P soil	0.415	0.000	
Lg N-NO ₃ ⁻	-0.235	0.020		Soil moist.	-0.258	0.019					

Figure 33 The multiple regressions predicting the accumulation factors (root/soil, AF) and transfer factors (aboveground/root, TF) for Cu, Pb, and Zn in the function of soil variables in the experiment. The soil contamination was the same in all bivariate N and P experimental variants. (Iordache et al. 2022)

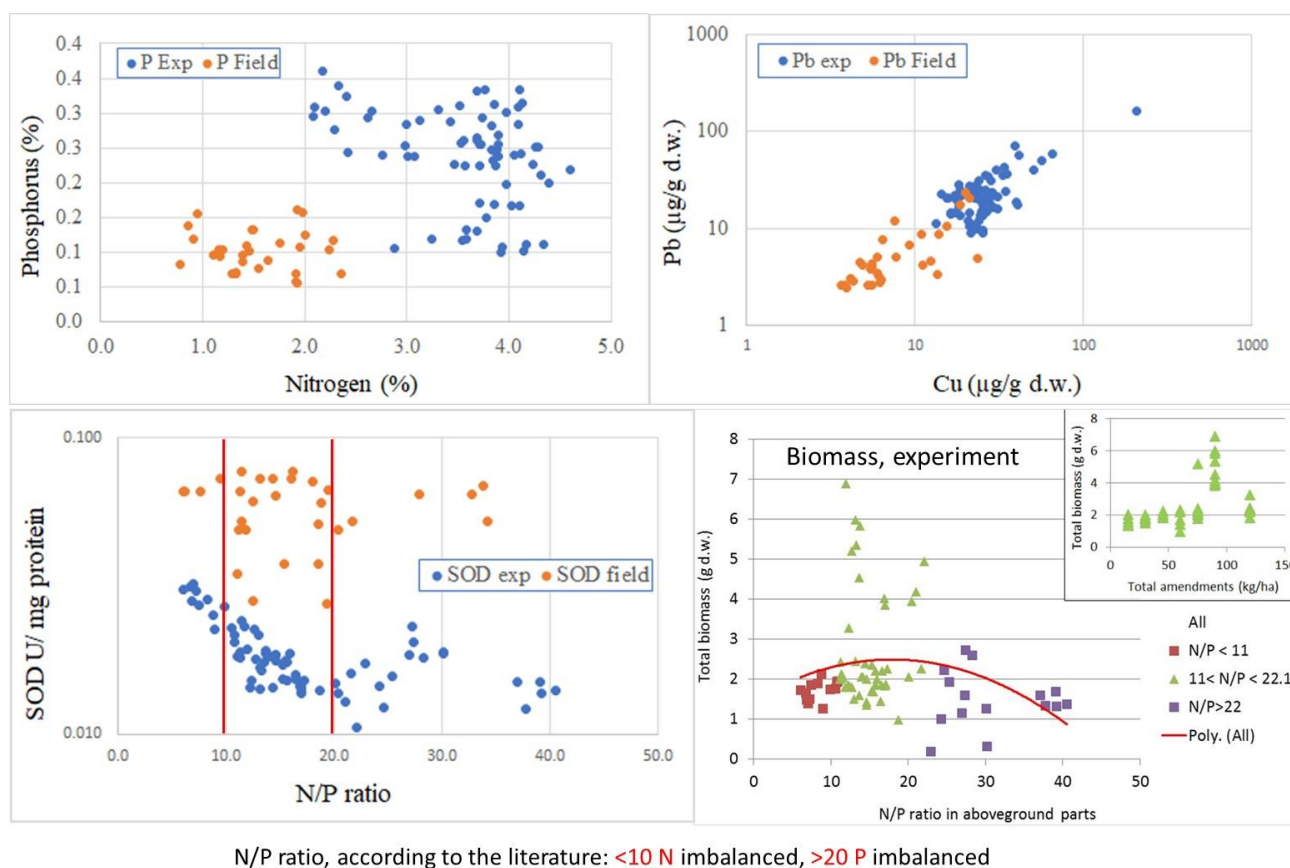


Figure 34 A comparison of several plant variables in the field and the experiment. The field and the experiment differed by the age of sampling (three months in the experiment, different moments of the life cycle in the field from June to September), by the heavy metals in soil (from a minimum to a maximum of pollution in the field, only maximum pollution in the experiment), by the N and P in soil (suboptimal in the field, from suboptimal to excessive in the experiment), by temperature and watering (suboptimal in the field, optimal in the experiment) and covered in both cases the N:P ratio in plants from N imbalanced to P imbalanced.

C3. Linking plant traits and variables relevant to hydrological models

In 2016 (Neagoe et al. 2016) we proposed a strategy (figure 35) attempting to link variables of vegetation at their measurement scale (above-ground and belowground biomass and its mechanical properties) with variables of the soil surface at model discretization unit scale (detailed morphometry and spectral properties). The structure of the strategy is 1) to build models predicting the relevant plant variables from experimental and field studies in the function of soil variables and other relevant driving factors (e.g. types of human impact), 2) to build models relating surface roughness, and soil cohesiveness in the function of LiDAR and remote sensing measurements, and 3) to build coupling models relating the plant scale models with hydrological and erosion models (including up-scaling or down-scaling methodological models). Our approach is complementary to that formulated in general biodiversity and ecosystem services terms and allows the formulation of detailed research hypotheses/research projects dealing with coupled ecological, soil, and hydrological processes.

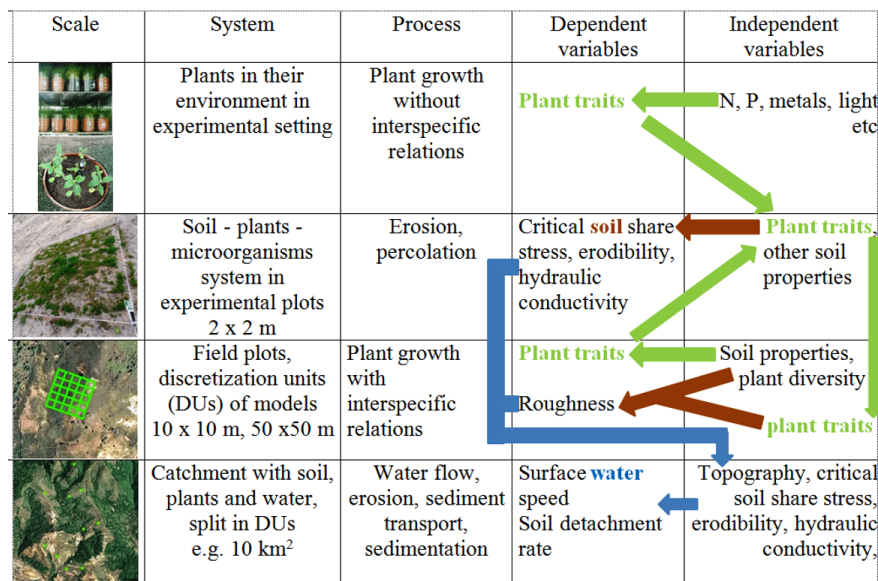


Figure 35 The causal chain from small-scale independent variables (N, P, metals, other physiological variables) to water flow and erosion using plant traits as intermediary variables (from Neagoe et al. 2016).

Figure 36 shows our new research strategy to link the local effects on grasslands (either from impacting projects or from bioremediation projects) with catchment scale consequences on water and sediment flows. The approach operationalizes the theoretical framework developed by Iordache et al. (2012) for a specific set of coupled processes.

Since then, we advanced in the subproblem of relating the morphometric aboveground traits of plants with the porosity of the plant cover at the scale needed for hydrological models such as the one presented in chapter D2. Iordache et al. (2022) communicated the first results (figure 37), and Iordache and Neagoe (2023) published a TRL2 LIDAR-based technology for the assessment of aboveground vegetation functional Traits and the roughness and porosity of plant cover (figure 38).

Results⁴ (article in preparation) include the LIDAR characterization and metrics computation for an experiment at a 2x2 m scale proving that preliminary explored metrics of the points cloud are

⁴ from the 2023 report of the exploratory research project METTELFLUX, www.mettelflux.com, experiment by Aurora. Neagoe, Virgil Iordache and coworkers, LIDAR and processing by Ersilia David (Oniga) and coworkers).

significantly different between experimental variants and correlated with the plant cover by cm scale layers measured by plant ecologists). Once the basic metric of volume has proved very sensitive to small differences between aboveground vegetation traits one can expect the more elaborate metric describing vegetation porosity by layers relevant to water flow would be also sensitive and relevant as an input to erosion models with spatially distributed vegetation influence.

Modeling at each scale suppose:

- Selection of dominant processes
- Selection of relevant variables.

New variables at soil-plant systems and catchment scale beside those influenced by plants traits.

In function of the empirical situation plant effects can be quantified or will be screened out by other dominant processes and variables.

Ecological and hydro-ecological research hypothesis.

Surface water speed, soil detachment rate	Critical soil share stress, erodibility, hydraulic conductivity	Topography, rainfall	Other relevant variables
Critical soil share stress, erodibility, hydraulic conductivity	Plant traits	Other soil properties	Other relevant variables
Plant traits	Species, N, P, microorganisms	Metals	Other relevant variables
Dependent variables	Independent variable		

In red variables modified in bioremediation projects

Figure 36 The new strategy for coupling processes with different scales, from plants to small catchments. The major difference compared to usual approaches is the use of plant traits/plant functional diversity as an independent variable to predict changes in soil and surface properties, instead of structural variables of plant community. This approach would allow the design of local management measures in the function of consequences at large distances downslope and downstream. (the picture is from Neagoe et al. 2016, and the explanation is from a research project).

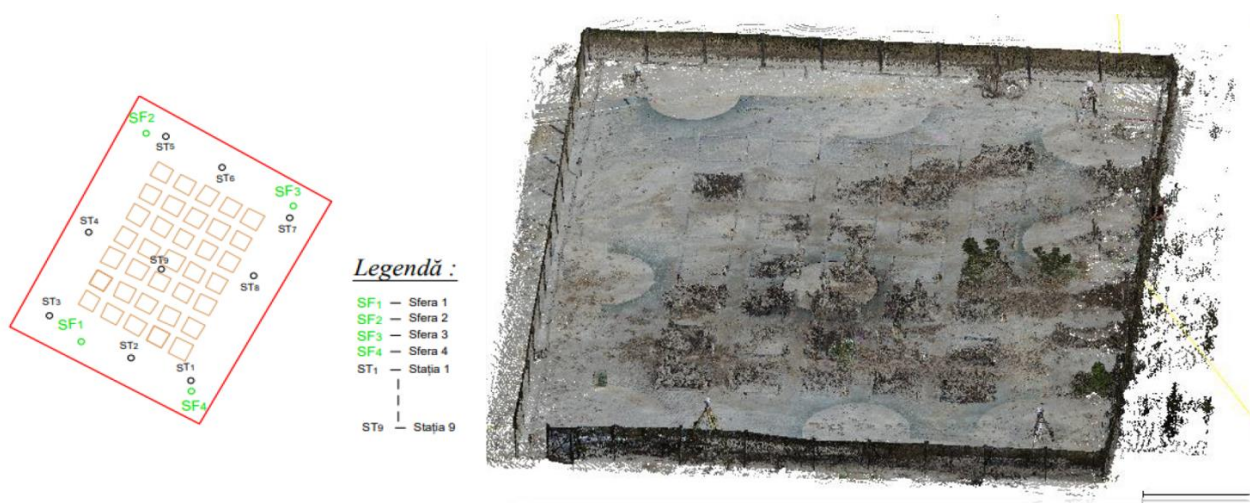


Figure 37 Vegetation LIDAR raw data (right) for a bivariate field experiment, with details of the measurement method. The data processing and interpretation led to results allowing the development of the technology schematized in figure 31 (from Iordache et al. 2022c).

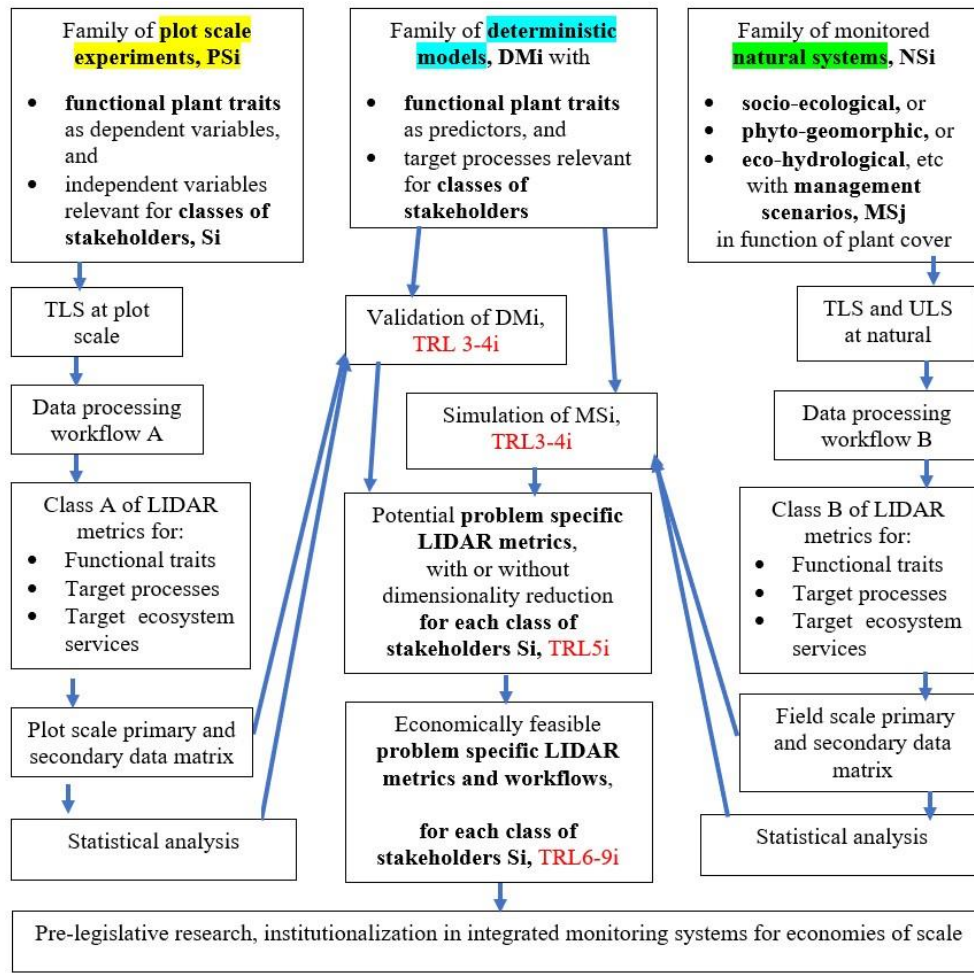


Figure 38 Graphical abstract of the TRL2 stage of the technology (Iordache and Neagoe 2023) We conceptualized it as a custom-oriented integrated tool-box of procedures/workflows and software modules for extraction of LIDAR metrics describing functional plant cover traits, deterministic models of processes describing the role of plants in the production of target ecosystem services, and coupled experimental scale–field scale investigations for validations and simulations. The development of the technology toward higher TRLs is on the one hand reactive to market needs, and on the other hand proactive for the institutional evolution of integrated monitoring.

D. Mathematical modeling

To get an image of the problems we wanted to solve let us have a look at several details of a cellular automata model predicting the transport of metals by erosion from mining catchments (figure 39 from Iordache et al. 2011b). One can notice that 1) the vegetation is included only to control the deposition of the eroded sediment, 2) the initial density and height variables do not have spatial structure and are the same all over the river basin, without accounting for the differences in the type of habitat and internal heterogeneities inside each habitat, and 3) the density varies between 0 and 1 without the possibility to empirically check the value. Such a model can be used to qualitatively simulate that vegetation has influence, but cannot be used to test hypotheses using field and experimental research, and even less to assist the management of coupled soil-water-vegetation processes in contaminated areas.

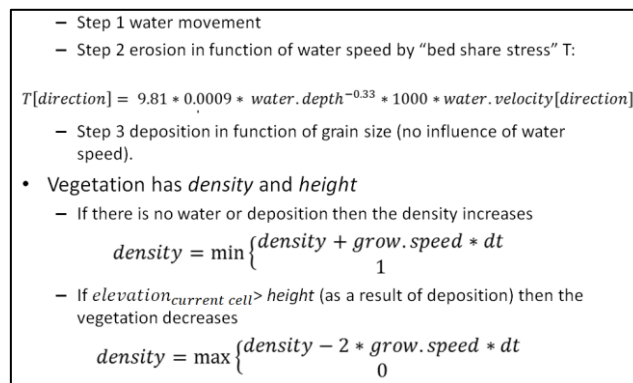


Figure 39 Slide describing how the role of plants is accounted for in the open-access cellular automata erosion model CAESAR-TRACER (Iordache et al. 2011b).

The first idea was to improve the cellular automata approach by changing its details. Although this could not realistically solve the vegetation-erosion coupling, it led to important results about how to port data from the plant scale to the discretization units of the erosion model scale (the problem underlined in figure 14 in this thesis), which were published in Ion et al. (2014, chapter D1) and complemented with another method for interpolating data (Ion et al. 2020). For the role of plants, a deterministic model of the processes was built including the spatially distributed vegetation traits as “porosity” (Ion et al. 2015 for the one-dimensional form). Later, our mathematician colleagues developed the 2D form of the model (e.g. Ion et al. 2022), while we moved to the problem of empirically measuring the vegetation porosity over large catchments to feed the mathematical model (using LIDAR as presented in chapter C3).

D1. A data porting tool for coupling models with different discretization needs

Predicting the long-distance effects of local environmental changes requires a coupling between local and regional models of ecological and abiotic processes (Ion et al. 2014). Examples include the integration of local vegetation processes with regional transport models for heavy metals (examples have been provided in table 5 in this thesis) or the local resources development with the movement of animal species.

Direct coupling of the models is technically possible but allows less flexibility for further model development. Alternatively, more common and flexible geographical objects are used as an interface among models of processes occurring at different space-time scales. One specific problem with this integration strategy is that the kind and properties of the geographical objects used as input to or output from local and regional models are usually different.

The differences arise due to methodological constraints related to the measurements of the space variables and to the modeling techniques. Table 17 summarizes the types of geographical objects which can occur. It can be seen from the inspection of this table that raster data and vector data are not basic terms in geographical ontology. We used this framework to be able to later introduce the real georeferenced ecological measurements of plant traits (chapter C3). In this context, there is a need to build spatial interpolation algorithms for porting rectangular raster information to other networks with cells of a different size or geometry, i.e. a method of Data Porting (DP). These algorithms should be developed in such a way to preserve as much possible the original measured space variables. We tackled the particular situation of variables treated by a field-type approach, observable at a scale much smaller than the derived geographical objects and the empirical precision of geographical location, having the size of the derived and not empirically constrained polygons.

The data porting tool was applied on data from our model sites, namely Ampoi's Valley with large cells (100 m cell size) and Paul's Valley (already presented in figure 19), a subdomain in Ampoi's basin with much smaller cells (10 m cell size). Figure 40 presents pictures of the same portion of Paul's Valley terrain constructed on different rasters.

Table 17 *Types of geographical objects occurring directly and indirectly in the modeling of the coupled environmental process. The field-type approach allows a rigorous description of the error and empirical verification, while the discrete-type approach does not allow a good treatment of errors, and usually involves a filtering of empirical data. (Ion et al. 2014).*

Approach	Measurement, observation	Primary („real”) geographic objects		Derived („methodological”) geographic objects (resulted from data modeling and plane discretization)
Field type (properties with relation of spatial location)	Variables z observable at a scale much smaller than the derived geographical objects and the empirical precision of geographical location	Tuples of space variables spațial <x,y, z ₁ , ..., z _n >	Interpolated field (the infinite set of tuples)	Substrates with attributes (polygons, contour lines, regularly distributed points as centers of a plane discretization). The polygons are characterized by a variation function of the variables inside them. The size of the polygons is not empirically constrained.
	Variables z observable at a scale larger than the potentially derivable geographical objects and the empirical precision of geographical location	Tuples with x and y in the center of the observation polygon or line transect		Substrate with attributes. It makes no natural sense to have the size of the discretization units smaller than the observation scale of the spatial variables.
Discrete type (substrate located in space with properties)	The observation scale does not influence the approach. Usually makes use of old geographical maps or methodological objects resulting from field approach.	Points, polygons, lines filling and empty geographical space.		Field obtained by planar enforcement (points with a certain value inside the discrete object, by class, and a constant value in the empty space)

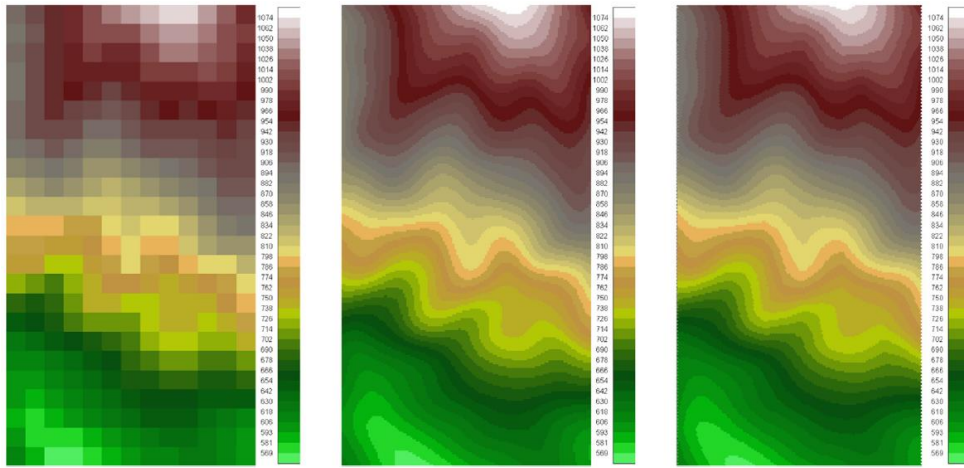


Figure 40 Relief from Romanian Paul's Valley. All the figures represent the same zone from Romanian Paul's Valley and are obtained as follows: the left one from a 13 x 24 regular raster data with square cells of 100 m size, the middle one from a 130 x 240 regular raster data with square cells of 10 m size. The figure on the right is obtained on a hexagonal raster (of 5.7735 m cell size) applying the data porting tool to the same data input as for the first figure. (Ion et al. 2014).

We also explored the consequences of data porting on the process of water flow reporting the cellular automata model in this article. It is important to note that from an ecological point of view, cellular automata with hexagonal cells are much more realistic than those with square cells, which are much more frequent only because of the technical simplicity of the data systems. For this reason, we adopted the solution with hexagonal cells. In the computation of the *water velocity of the cell i* we used a *Manning-type empirical law* without direct relation to the vegetation properties. *The basic assumption on the water flux across the cells is that the water of any cell flows out to the neighboring cells toward which the water velocity of that cell points to, and the water enters a cell only from the neighboring cells whose water velocities point to that cell.* A comparative portrait between the method on rectangular raster and our method for water flow among cells is illustrated in figure 41.

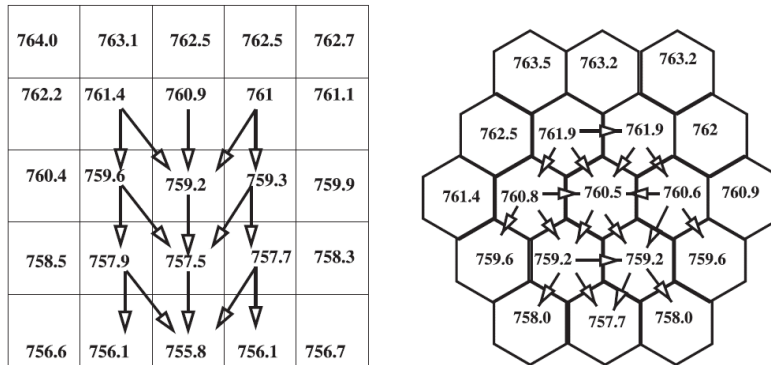


Figure 41 Water flow among cells in rectangular (left side) and hexagonal (right side) rasters using Tarboton and our rules, respectively. Data written inside cells represent altitudes and they come from a small region (the same on the left and on the right) of the Romanian Paul Valley. The values of the rectangular raster slightly differ from those of the hexagonal one because they represent two different models of the same terrain surface. (Ion et al. 2014).

Figure 42 is a snapshot of a water flow on Ampoi's Valley modeled using the method described in this section. Figure 43 contains three images of the same zone cut out from Paul's Valley. The first one is a photo where one can observe the ravines of this region, while the other two are images constructed from GIS data and include the water accumulation zones found in two different ways.

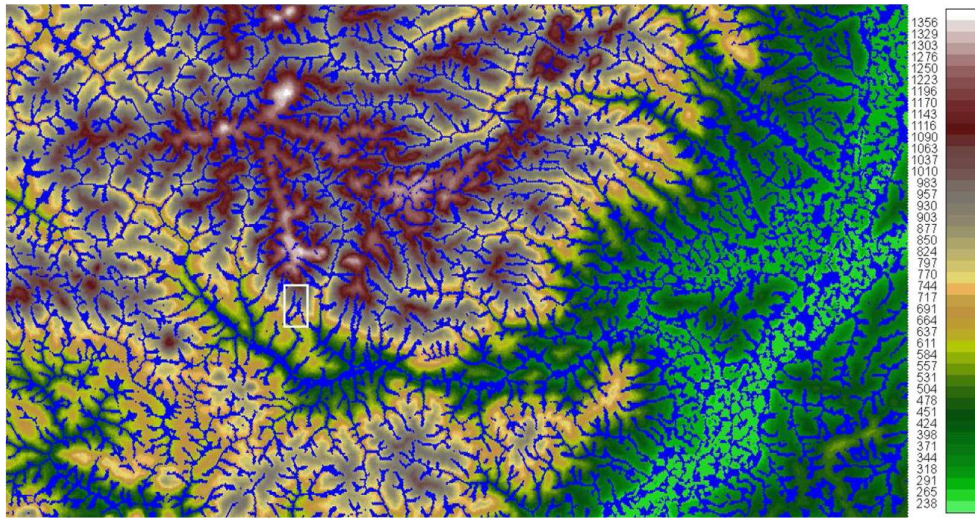


Figure 42 Water accumulation zones in Ampoi's hydrographic basin. Starting from the real elevation GIS data (542 columns by 310 rows of cells with 100 m side length) of Ampoi's landscape, we captured the areas of concentrated water flow using a hexagonal cellular automaton. The hexagonal raster (with cell side of 57.735 m) was obtained by porting the GIS data following our method. Starting with a uniform shallow water level on the entire landscape, we processed the water flow across the cells using the cellular automata law. The blue area in the figure represents the hexagonal cells where the water layer exceeds the initial level. The white border rectangle inside this figure marks the area from Paul's Valley we referred to in figure 43 (Ion et al. 2024).

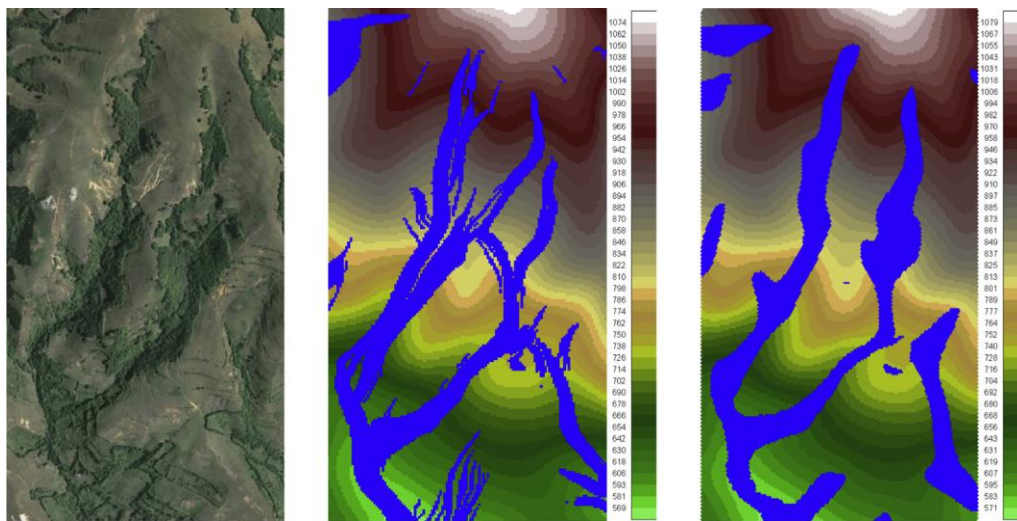


Figure 43 Potential water accumulation zones in Paul's Valley. The left figure is an aerial photo of this region. The relief from the image in the middle is given by the same 130 x 240 GIS raster data with square cells of 10 m size used for the middle picture from figure 40. The relief from the right picture is generated from the hexagonal raster (of 5.7735 m cell size) obtained by applying our data porting tool to the same raster used for the middle image. The blue transparent areas represent the potential water accumulation zones determined by an iterative process. The picture in the middle is obtained using Tarboton's rules for water change among cells (the cellular automata with squares in figure 40). For the picture on the right side, we used our water routing method. One clearly observes that the accumulation zones indicated by this method overlap almost perfectly with the ravines and are less spread out than the ones identified in the middle image. (Ion et al. 2024).

The water routing method presented in our article has a physical base and it is a simplified version of a discrete form of shallow water equations. One of the advantages of this approach is that the higher isotropy between the cells of a hexagonal raster produces a more appropriate model of the transport phenomena. Another potential advantage of using this approach is that it can be easily

incorporated into more elaborate water flow models providing a first step for a very quick investigation of the terrain topography and the potential water accumulation.

Besides the use for the research program presented in this thesis, this 2D model is useful for studies on problems with water distribution: determination of dry or flooded regions, landscape water flow, vegetated bed rivers, and dam break problems.

Further research directions included (Ion et al. 2014):

1. To develop the software in order to be compatible with variables that have restrictions on the size and the form of their discretization units as a result of the observation scale and method (as resulted from table 17).
2. To develop a multiresolution analysis by using cubic spline wavelets in order to examine the GIS data (considering also data de-noising and compression).

The results of the second research direction were published by Ion et al. (2020) where we introduced a cubic spline wavelets method intended to interpolate a big set of R^2 -randomly distributed data. The approximation using spline wavelets has many advantages, especially when one needs to evaluate the model function many times. Also, the model function is not stochastic, as in statistically-based interpolation methods, which provides a base for the empirical validation point by point of the predictions. This is highly relevant when using interpolation for the functional traits of plants measurable over large scales (chapter C3).

D2. Accounting for the role of plants on the water flowing over hill-slopes

As already mentioned, our technical problem was to include measurable traits of plants inside the model for water flow and soil erosion. In turn, the chemical changes due to the export of elements (N, P, and heavy metals by runoff or leaching – chapter C2.1) would influence the plants' development (chapters C2.2 and C2.3) and change the plant traits next growing seasons and generations.

The presence of plants on a hill creates a resistance force to the water flow and influences the process of water accumulation on the soil surface (Ion et al. 2015). The large diversity of growing plants on a hill makes the elaboration of a unitary model for the water flow over the soil covered by plants very difficult. We assumed that the plants form a dense net of rigid vertical tubes and that the water fills the “voided” space up to a level not higher than these plant tubes (see figure 44 for some graphical details).

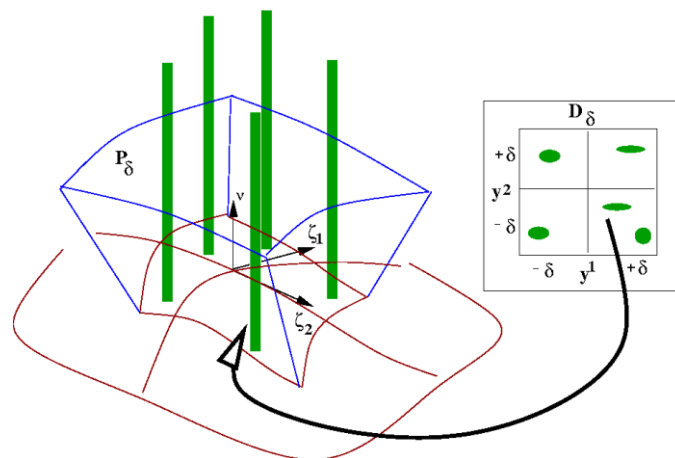


Figure 44 The representative element of the volume P_δ used for averaging. The bottom surface $z(y^1, y^2)$ of P_δ has a representative width δ along two orthogonal directions on this surface. ξ_1, ξ_2 are the tangent vectors at $z(y^1, y^2)$ and v is the unit normal to this surface. The water depth h associated to P_δ is the averaged value of the physical water depth h inside P_δ (Ion et al. 2015).

One assumes that the terrain exhibits topographic variation but with small curvature and that the terrain surface is locally almost plane. One also supposes that the viscosity of the fluid and the fluctuation of the velocity field have a small effect as compared to the bed friction and plant resistance. Starting from the general principles for mass and momentum balance laws and invoking the above assumptions, one obtains the following basic model for water flow on vegetated hills:

$$\begin{aligned} \partial_t(h\beta\theta) + \partial_a(h\beta\theta v^a) &= \beta(m_r - \theta m_i), \\ \partial_t(h\theta\beta v^c) + \partial_a(\theta\beta h v^c v^a) + h\theta\beta\gamma_{ab}^c v^a v^b + h\theta\beta\partial_c w &= -\beta K(h, \theta)|v|v^c, \quad c = 1, 2, \end{aligned}$$

where θ is the porosity of the vegetation cover; w is, roughly speaking, the altitude of the water surface; m_r , m_i are the water supply rate (from rain) and the water loss rate (by infiltration), respectively.

These equations were obtained by averaging the macroscopic variables over a representative element of volume P_δ placed on the land surface $z(y^1, y^2)$ of the flow and illustrated in figure 44.

The model described above is mathematically too complicated for many practical applications, but it is a good basic model to generate simplified models of certain realistic problems. Such models can be obtained by considering stronger assumptions on the soil surface topography and the structure of the plant cover. The porous analogy for the fluid-plant physical system was used especially for the case of submerged vegetation where the flow is assumed to be plan parallel.

We introduced a simplified variant of the full model which allows small variations in soil topography and plant porosity and presented some numerical results obtained with our scheme (figure 45).

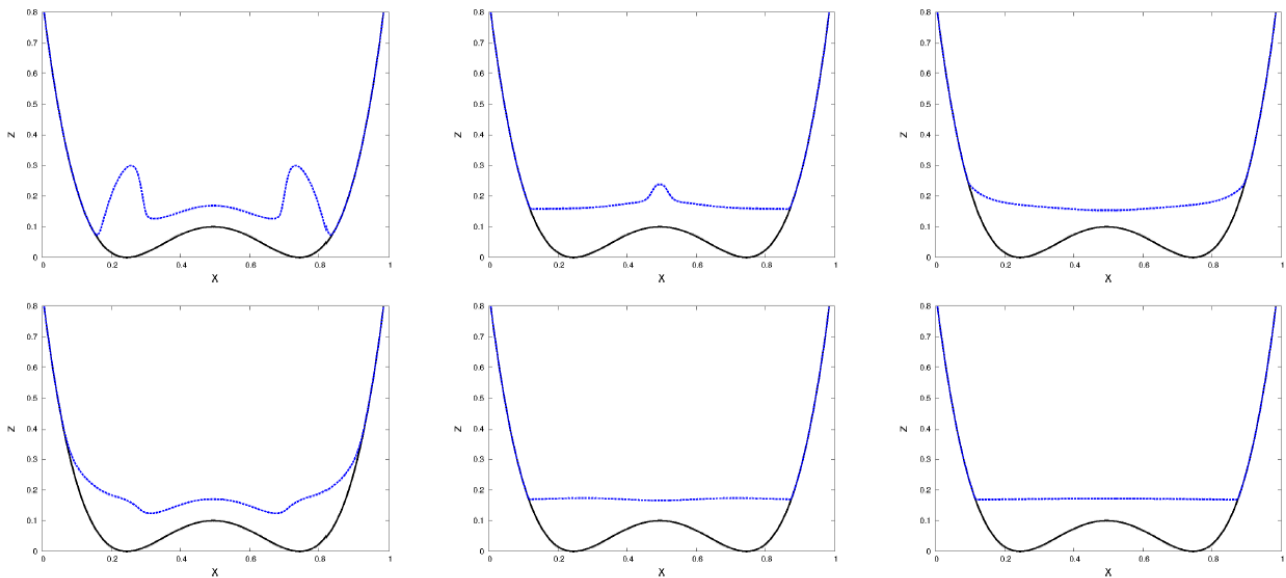


Figure 45 The dashed and continuous lines represent the water and soil surfaces, respectively. The first row of pictures gives the dynamic of the free water surface on bare soil, i.e. absence of vegetation, at times $t = 0.1, 2$, and 3 . The second row gives the dynamic of the free water surface on a soil covered with vegetation at the same moments as before. One can observe the attenuation effect of the flow due to the vegetation. (Ion et al. 2015).

The modeling equations mainly address a hydrographic basin that exhibits variation concerning the soil surface orientation, slope, and plant cover density. It is quite general and allows one to solve

many practical problems. To use it, one needs tools for terrain data acquisition concerning physical parameters of the terrain and of the vegetation and some high computational infrastructure.

Figure 46 illustrates how the model works with a 2D example of the influence of porosity on the water velocity in our model catchment (Ion et al. 2022, without me as co-author, but extending our 1D model). Later, our mathematician colleagues added the erosion process to the 2D form of the shallow water equations from Ion et al. (2015) using the Hairsin-Rose model for soil erosion and considering the presence of the plants on the soil surface.

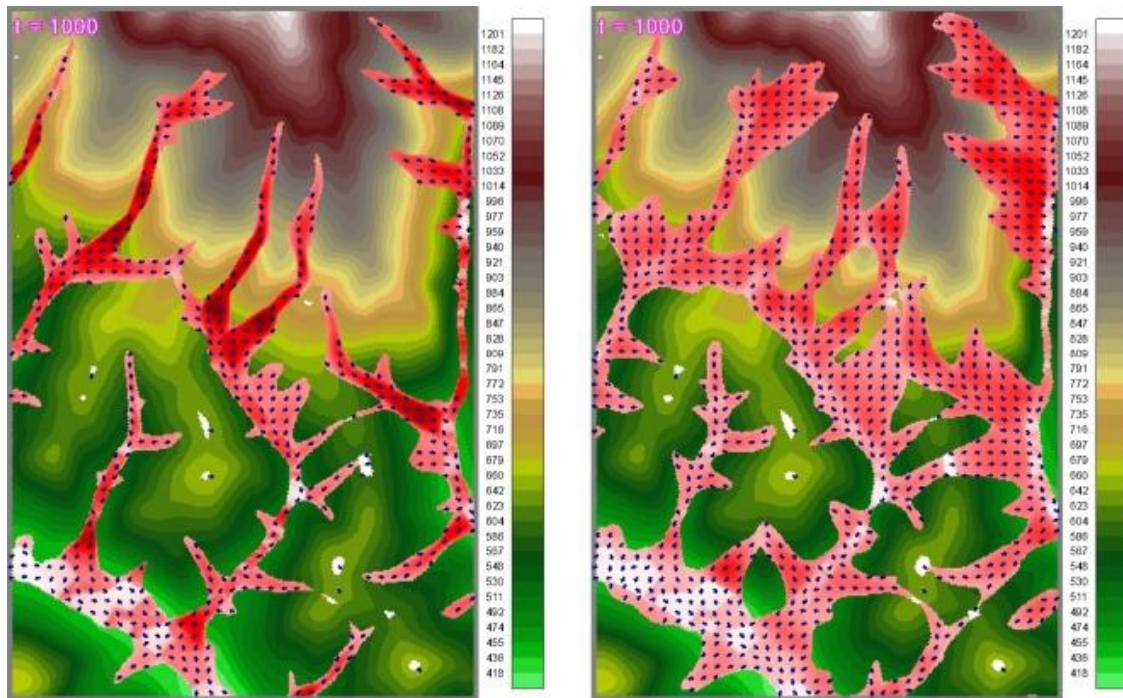


Figure 46 Snapshots of water velocity distribution in Paul's Valley hydrographic basin for two different uniform vegetation densities: $\theta = 0.993$ (lower density) and $\theta = 0.974$ (higher density) on the left and right picture, respectively. As expected, the velocities are smaller when vegetation is denser. (Ion et al. 2022).

A main strength of the current model is that it addresses the dynamic process of the plant-soil-water interaction. It can simulate the root plant effect on the soil particle cohesivity and the effect of the plant stems on the water dynamics. Experimental data are required to calibrate the model parameter. The data can be collected by point source measurements and then extrapolated on the entire surface of the basin by some porting data schemes (Ion et al. 2014, chapter D1), or from satellite, aerial photographs, or LIDAR techniques. The model is part of an information system including also other models developed in the past project (optimization of the CAESAR erosion model – figure 39 - concerning the vegetation module, and a cellular automata new erosion model on a hexagonal grid).

At the end of this chapter, I would like to underline again two key aspects:

- **The local vs. global impact of variables** in ecological/environmental models. In ecological and environmental models, the mathematical fields of variables are only at the level of data models, they don't have a physical reality in the physical space. When we model an interpolation as a continuous function by spline wavelets the global impact of local changes is only a methodology to be checked by later empirical measurements of the values in the terrain at locations different than the initial set of data. In the models of processes, the local changes of variables may lead to an effect that propagates at a large scale or their impact can be screened out at large scales. Which scenario will be real is a matter of empirical research

and mathematical simulation, but in no way local effects will have direct global effects, as in the case of the fields used in the theories of physics. This leads to the fact the processes/clusters of processes can be relatively decoupled in their functioning, up to a certain time scale. This was the point of using simplified structural models of the kind presented in figures 6, 7, and 49 to focus on a key target process and several coupled ones.

- The space-time variability of variables. The importance of spatially distributed ecological variables in models is crucial because of the reality of the heterogeneity in space. Sometimes the heterogeneity does not have a large-scale impact on the modelled processes, but sometimes, when thresholds are surpassed, the impact occurs (for instance when local stressful conditions of plant development lead to the initiation of strong sheet erosion, which eventually generates positive feedback towards larger scale erosion processes). As an extra example, we show below the distribution of Cu in a floodplain downstream of a tailing dam (figure 47 from Iordache et al. 2022). The spatial heterogeneity of Cu was controlled by the upstream-downstream position of the plot (50x50 m grid+ centres of the plots) and the distance from the river, and controlled in turn the distribution of plant species together with other soil variables, such as nutrients. The variability in time will be a focus of future research (see part II).

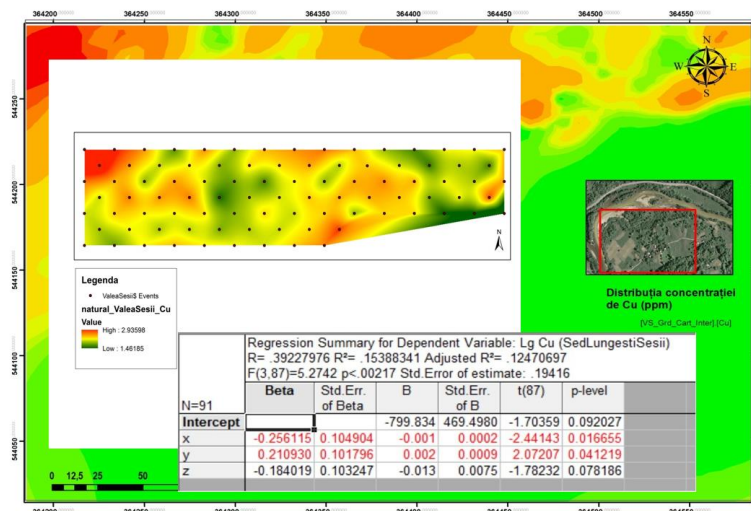


Figure 47 An example of the spatial heterogeneity of Cu in the soil of a floodplain sector located downstream of a contaminating tailing dam (Iordache et al. 2022).

I will use the results of this chapter in the research directions presented in part II of this thesis.

E. Environmental management and institutional development

In this chapter I will present four contributions, two of them in the “ecological hierarchy” approach (Iordache and Bodescu 2005, Iordache et al. 2005) and two in the “processes at many scales” approach (Iordache 2020, Iordache and Neagoe 2023). As we have seen in chapter A2 they could translate into one another, the first one using the processes of the service-providing units of the species located in the management are of interest, and the second one by modularizing the results at the needed/imposed site/regional scales already specified in the regulations or corresponding to the responsibilities of the organizations involved in the management of natural resources and services.

E1. Integrated monitoring of emergent ecosystem services

In Iordache and Bodescu (2005) *we used four specific methodological aspects/principles*:

1. *a multiple inclusion principle*; this allowed to surpass the nested hierarchies by overlapping in space ecological systems at a given hierarchical level, for instance, including in both of them parts that contributed to the emergent properties in each of the larger scale ecological systems. For instance, in figure 48 we present how small riparian forests are included in landscapes of large scale.

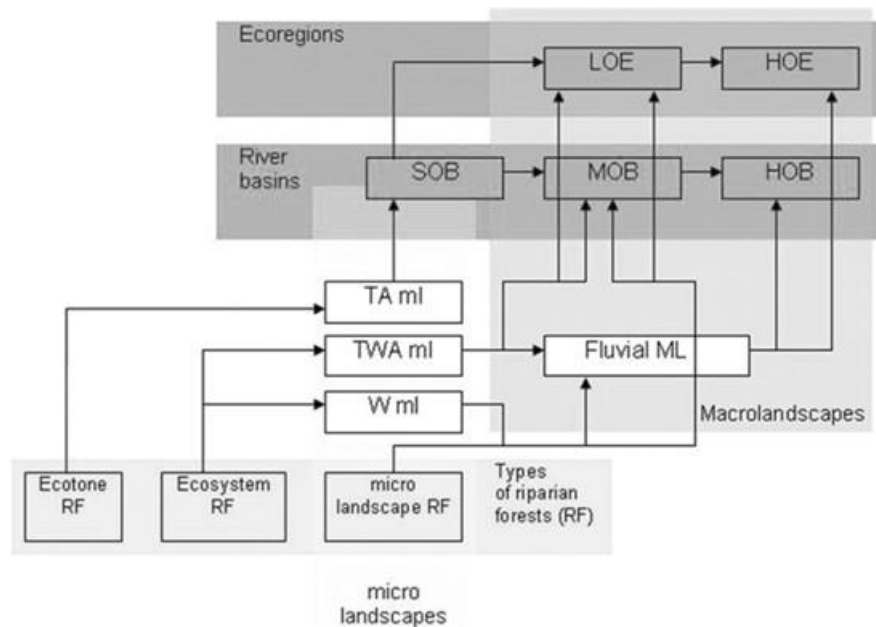


Figure 48 *Inclusion (black arrows) of riparian forests in their integrating systems. The included systems are structural elements of the higher systems in which they are included. It results that at low-order ecoregion or medium-order river basin level, all types of riparian forest should be taken into consideration for the design of the management. At an even higher level, practically the full river corridor should be considered. Legend: ml = micro-landscape, ML = macro-landscape, TA = terrestrial-aquatic, TWA = terrestrial-wetland-aquatic, W = wetland, SOB = small order river basin, MOB = medium order river basin, HOB = high order river basin, LOE = low order ecoregion, HOE = high order ecoregion; a river corridor consists of the TA micro-landscapes, the TWA micro-landscapes, and the fluvial macro-landscapes of a river basin. (Iordache and Bodescu 2005).*

2. *a differentiation between natural ecological systems and natural capital*; this allowed us to differentiate from an evolutionary point of view between ecosystems before the speciation of humans and after the development of human institutions. Natural capital in this approach has a relational property resulting from the interaction with humans that does not exist in natural ecological systems. In our times this is only an analytical distinction that allows us to detail the content of the above-mentioned relational property in terms of ecosystem services delivered/managed by specific institutions according to their hierarchical level of production.

3. *a coupling of the monitoring of natural capital with management through natural resources and services;*
4. *a distinction between systemism and holism.* This was needed to decouple the approach from spiritual holistic approaches such as deep ecology, as well as from the collectivistic use of ecological knowledge in political ideologies.

Coupling the above-mentioned principles with the existing knowledge about a fluvial system (the lower Danube River system – LDRS) as described in the introduction has led us to:

- a refinement of the structural model of the socio-environment;
- a tentative list of the indicators to be included in an integrated monitoring system of the LDRS
- a decentralization principle for structuring the specific information system for LDRS.

Table 18 presents the list of indicators of the natural ecological systems by hierarchical level and table 19 the socio-ecological indicators by institutions needed at each hierarchical level in this approach.

Table 18. *Indicators characterizing the natural ecological systems of LDRS (TDM = trophodynamic module) (Iordache and Bodescu 2018).*

Type of system	Resources and services provided to SESs	Indicators to be assessed
Regional landscape	Maintenance of local landscapes diversity	Number of local landscapes of each type and their morphological characteristics
	Maintenance of species diversity associated to TDMs emergent at regional level	Number of populations of migratory species (fish, birds)
	Renewable resources	Sustainable harvest levels of migratory species
	Regional microclimate improvement and groundwater recharge	Water retention and evapotranspiration
	Water quality improvement	Retention of sediment and pollutants
	Transportation pathway	Morphological characteristics of channels
Local landscape	Maintenance of ecosystems diversity	Number of ecosystems of each type and their morphological characteristics
	Maintenance of species diversity associated to TDMs emergent at local landscape level	Number of populations of species with high mobility at local landscape level (fish, reptiles, amphibians, mammals, birds)
	Contribution to regional micro-climate improvement	Parameters for determining the local water budget
	Contribution to water quality improvement	Sediment retention, pollutants retention, pollutants export by land use, nitrogen export by denitrification
	Renewable resources	Sustainable harvest levels of species with high mobility at local landscape level
Ecosystem	Maintenance of species diversity	Number of TDMs and of low mobility/ sessile populations (macroinvertebrates, plants)
	Renewable resources	Sustainable harvest levels of vegetation (wood, reed, medicinal plants), macro-invertebrates and fish

Table 19 Indicators characterizing the SESs (all hierarchical levels) (A); Indicators characterizing the relation of SESs with natural ecological systems (B); Indicators characterizing the managerial institutions emerged as a result of the interaction of SESs with natural ecological systems (all hierarchical levels) (C).

A	
Emergent properties	Indicators to be assessed
Economic wealth	Size of the economy as measured by gross product, level of infrastructure
Social welfare	Employment rate
Viability	Rate of change of the labor force over time, index of diversity in employment, current sustainable employment relative to population, level of social cohesion
Independence	Percentage of locally based economic activity
Individual wealth	Per capita income relative to the average income in the integrating economy, food supply per capita relative to minimum nutritional needs, probability of sufficient food being available over next 10 years
Equity	Ratio of historical to current coefficients of income and/or food distribution, social stratification, involvement of women in local institutions
Public functional modules	Identified socio-economic objectives, regulatory and enforcement approaches, interaction with upper levels of government
B	
Emergent properties	Indicators to be assessed
Ownership status of NC (local level)	Surfaces and morphometry of owned parts of natural capital, for each type of ownership
Functional modules at the interface with the natural capital (all levels)	Number of functional modules, and number and dimension of organizations thereof, including managerial institutions (for the details in the case of managerial institutions, see Table 3C)
Contribution of NC to economic wealth (all levels)	Natural capital rents, cumulated for all used resources and services (originating in LDRS and in the full ecological footprint of SES)
Sustainability (all levels)	Ecological footprint of SES relative to productive surface of owned NC
C	
Emergent properties	Indicators to be assessed
Effectiveness	Level of success of stated management and regulatory policies
Viability	At all levels: level of financial and organizational viability, extent of capacity building effort At local level: extent of incorporation of local socio-cultural factors (community decision making, traditional ecological knowledge and management methods)

In this approach, one can identify the following principles for the design of integrated, systemic monitoring (Iordache and Bodescu 2005):

- 1. Decentralization of the monitoring; at each socio-economic level the set of indicators needed for the specific portfolio of societal objectives should be monitored; this set of indicators should be extended subject to constraints imposed by the monitoring needs for reaching the societal objectives at higher hierarchical socio-economic levels; The development of a competitive market of laboratories could be promoted, which would serve monitoring at all levels. Databases could be under the direct control of the public institutions (local, regional, and national) re- responsible for their creation and maintenance.*
- 2. Public availability of the data concerning natural ecological systems and socio-economic systems; the private organizations that have financed directly and indirectly the monitoring could have free access to the databases at the local, regional, and national levels;*
- 3. Openness of the monitoring institutions to civil society control; the monitoring is part of management.*

E2. Designing floodplain restoration

We have seen in the previous chapter that a realistic approach to the relationships between the natural and social processes and the hierarchy of ecological systems led to complexities that would imply changes in the institutional framework for the management of ecosystem services triggering cooperation between the different institutions. This in turn proved to be not realistic from a socio-political point of view, as demonstrated by the future dynamics of the sustainable development policies, the major mechanisms being the path-dependency of the socio-ecological systems and more specifically the resistance to institutional change. The resistance to institutional change reflects the social equilibrium between the real present interests of the users of the natural capital, which cannot be overturned by normative approaches. We explored such a situation in a case study focused on the optimization of ecosystem services delivery by the multifunctional restoration of a large island in the Danube floodplain (Iordache et al. 2005).

At the time of our analysis (and also in the present, as no restoration occurred in the area) *the main users are farmers. After restoration ecotourism could become a further important user group as in the Danube Delta. Table 20 lists the potential effects of restoration on current users' interest. The following remarks interpret some of the points made in this table:*

- *Most local users gain by restoration, including fishers, but their potential for lobbying is low, compared with governmental users.*
- *Foresters reflect interests located both at the governmental and the local level. They have a high lobby potential and may be interested in restoration. However, their incentives are attenuated by the long time needed for transforming agricultural systems into riparian forests.*
- *Farmers (with high lobby potential) are against restoration, as their benefits will strongly decrease after restoration. As long as most of the embanked areas are state property, the economic inefficiency of farming can be masked by governmental subsidies.*
- *Conditions for tourism in restored areas of LDRS would be strongly improved after restoration, but there are no current users at the local level to lobby for this. Some lobby for tourism at this moment could come only from the governmental agencies responsible for the development of this economic sector.*
- *Water quality services will be strongly improved after restoration; however, the setting of restoration for nutrient retention was under pressure both because of the reduction of the nutrient input in the Danube catchment compared to past times and because of a lack of understanding about the time scales of elements retention in floodplains and rigorous estimations of the budgets of elements across scales (which depends on monitoring of the type presented in chapter E2).*

In Table 21 we indicated eight main objectives for further development of the riparian communities. The following comments elucidate the possibilities:

- *The portfolio of objectives should include at least the following ones (1 to 4 in table 21): sustainable production of natural resources and services, economic efficiency and viability, distribution equity, and employment. Objectives 1 and 2 would make fishers, foresters, and water authorities to be interested in restoration, both at the local and governmental levels.*
- *The inclusion of the objectives of distribution equity and employment would strongly enhance the interest of local people in restoration, and would also be of relevance for the governmental social policies.*
- *the increase in fish export is limited, besides others, by the fact that there is not, on foreign markets, a high demand for the currently offered dominant species. Restoration of LDRS might change the situation in this respect by the fact that many economically valuable fish species depend on the improved lateral connectivity of large floodplains. Also, the stock dimension will increase, thus contributing to objective 5 (export promotion and generation of foreign exchange).*

Table 20 Elements for analyzing the influence of the potential development of LDRS by restoration on the current users' interests for such a development. Legend: ""+, ++" = increase in the production of resource/service, NA = not applicable, MWEP = Ministry of Water and Environmental Protection, L = local (within LDRS), NL = not-local, Gov = governmental, * excepting for Danube Delta and Small Island of Braila.

Resource/service	Direction of change after restoration	Time of benefits manifestation after change	Current user/manager	Level of final current dominant beneficiary
Resources				
1. Fish	++	medium	fishers	L
2. Wood and game species	+	long	foresters	NL (Gov)
3. Medicinal plants, honey	++	medium	villagers	L
4. Systematic agricultural crops	--	NA	farmers	NL (Gov)
5. Traditional agricultural crops	+	medium	villagers	L
Services				
6. Maintenance of species diversity and ecological systems diversity	++	long	MWEP	NL
7. Absorption of secondary products	0	NA	industry	L
8. Water quality improvement	++	short/medium	MWEP	NL
9. Flood mitigation	++	short	MWEP	L
10. Regional microclimate improvement and groundwater recharge	++	medium	MWEP	NL
11. Conditions for tourism	++	long	none*	L
12. Transportation pathway	0	NA	transporters	L
13. Remarks	Directly related to the intensity of the user interest for restoration	Manifestation after long time decreases the intensity of the interest	If there is no current user, there is no current interest	Final beneficiaries at G level are more influential than those at L level

- *The area is currently dominated by the agricultural sector. Fishery post-harvest sector development as a result of increasing stocks might contribute to objective 8 (industrial diversification). Various fish products might be produced for export in Western Europe, following the model already in place in the Danube Delta.*
- *Objective 7 (maintaining a regional balance of development) might be appropriate for the LDRS district socio-economic systems, which are suffering from economic and social problems, as well as objective 6 (decreasing urban-rural drift) for the local socio-economic systems, taking into consideration their current depopulation trend/*

There is a potential conflict of interest between farmers and other sectors about the integrated development of LDRS. Such intersectoral conflicts are recognized at the governmental level in terms of conflicts between the strategies for the development of different sectors: extraction, agriculture, forestry, transport, energy, or tourism. In this context, the restoration solution balancing the interest of the farmers and other users could be a multifunctional farming system with more or less developed riparian forests separating the wetlands (shallow lakes) from the agricultural fields, which also

would include forest belts. A refined hydrological management would be needed to maintain both the functionality of the lakes and of the agricultural fields

Table 21 Elements for choosing the portfolio of objectives that maximize the potential interest for the development of LDRS by large-scale reconstruction. Legend: G = at the governmental level, L = at the local level, Gov = governmental, LA = local administration, MWEF = Ministry of Water and Environmental Protection (Iordache et al. 2005).

Societal objective of the LDRS management	Potentially for		Potentially against	
	G	L	G	L
Basic objectives				
• Sustainable production of high level of natural resources and services	fisher foresters	fishers foresters	farmers	farmers
• Economic efficiency, economic viability	MWEF			
Optional objectives				
• Distribution equity	Gov	LA		
• Employment	Gov	LA		
• Export promotion and generation of foreign exchange	Gov			
• Decreasing urban-rural drift	Gov			
• Maintaining a regional balance of development	Gov			
• Industry diversification	Gov			

E3 Designing remediation of mining areas by accelerating succession at multiple scales

I have shown in the theoretical and methodological chapters of this thesis how we developed from the hierarchical approach used in chapters E1 and E2 to an approach based on processes at multiple scales and a complementarity between them. Our geographical focus on environmental management shifted also from the large rivers to the upstream catchments where the industrial sources of pollution with heavy metals occur and this problem is of larger public institutional interest. In Iordache (2020) I developed a multi-scale process approach for the remediation of such areas touching coupling in the text the theoretical, methodological, and application aspects. The starting question was to what extent the manipulation with microorganisms could accelerate the ecological succession in novel and remediated ecosystems (mining dumps, tailing dams, contaminated soils on the hills and in the floodplains). This question reflected our research interests and the results presented in chapter C2 of this thesis.

Thinking restoration or remediation in relation with ecological succession has a large theoretical and methodological heterogeneity because it cross-cuts disciplinary fields with different strategies to reduce the dimensionality of the natural complexity. First of all, succession and community assembly are different and complementary theoretical frameworks relevant to this problem. Community assembly studies investigate the rules and mechanisms relating local diversity patterns and the regional species pool, which are characterized by key concepts like species co-occurrence, functional traits, and dispersion, and usually lack a temporal dimension. Succession studies have key concepts like disturbance, ecosystem development, legacy effects, and threshold effects, and place the processes controlling the community structure in a temporal context. Common concepts relating these two research traditions could be species pool, priority effects, dispersal filters, abiotic filters, and biotic filters.

In an integrated model, one would expect community assembly theory to contribute more to the first phases of community dynamic, controlled mainly by dispersal and abiotic variables, and succession theories more in the later phases, with a larger influence of intraspecific and interspecific biotic interactions.

In this context, the objective of this contribution was to screen the literature about the succession of soil microorganisms and groups directly related in the trophic network with soil microorganisms (figure 49), about the coupling processes between these groups, and to extract relevant information about how and in what context manipulating the soil microorganism might be useful for the acceleration of succession as a management objective.

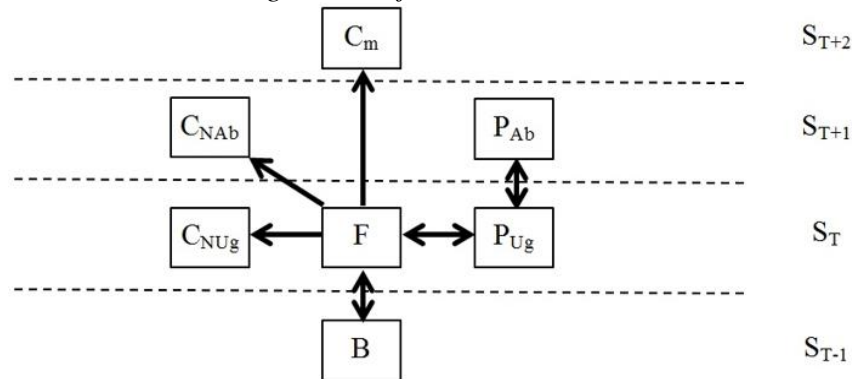


Figure 49 Structural model accounting for the role of fungi in the local network of interactions between organisms involved in the successional processes at the community and ecosystem scale. Each square represents a group of statistical populations of different species (trophic dynamic module) including one or more service-providing units (smaller groups of populations differentiated in function of their ecological role). **Legend:** F = fungi, B = bacteria, P_{Ug} = underground parts of plants, P_{Ab} = aboveground parts of plants, C = consumers, C_{NUg} = fungivorous underground invertebrates, C_{NAb} = fungivorous aboveground invertebrates, C_m = fungivorous small mammals, S_T = target scale (characteristic to fungi), S_{T-1}, +1, +2 = scales smaller and larger than the target scale. (Iordache 2020).

The structural model from figure 48 is limited to processes at the site scale. Coupling between site scale processes can be done by biotic or abiotic processes of larger scale (chapter B2 of this thesis). Manipulation of microorganisms can be just an operational measure in a portfolio of coupled scale-specific management activities serving various restoration objectives. After analyzing the available knowledge, I arrived at the following potential steps for devising a restoration/remediation / new ecosystem construction plan including the use of fungi for accelerating the ecological succession:

- Investigate the site and the surroundings at several scales (figure 50). The scales selected for the proposed approach depend on the realistic discontinuity analysis of the species distribution classified by functional groups, and not on classifications of the landscape units serving other management objectives.
- Estimate the relative importance and dispersal and habitat suitability for species recolonization. Describe the relevant succession processes by community and the coupled integrated processes. Describe the spatial structure of soil variables in the sites to be restored. Use modeling tools to simulate the potential trajectories of coupled successional processes. Information about the potential solutions for fungi manipulations can be obtained from the study of chronosequences relevant to the management situation (with primary or secondary succession) in the same landscape.
- Evaluate if the site can be a control point in the landscape or its potential functional relation with landscape/catchment control points.
- Evaluate to what extent objectives at the site scale can be formulated in terms of states and phases with transitions in between.
- Evaluate to what extent small-scale hot-spot and keystone vegetation structures can be included in the site.
- Adopt a multifunctional and multiscale approach in formulating the potential objectives in the design phase: which ecosystem services are to be restored, and which species to be recovered with their habitat and microhabitat needs.

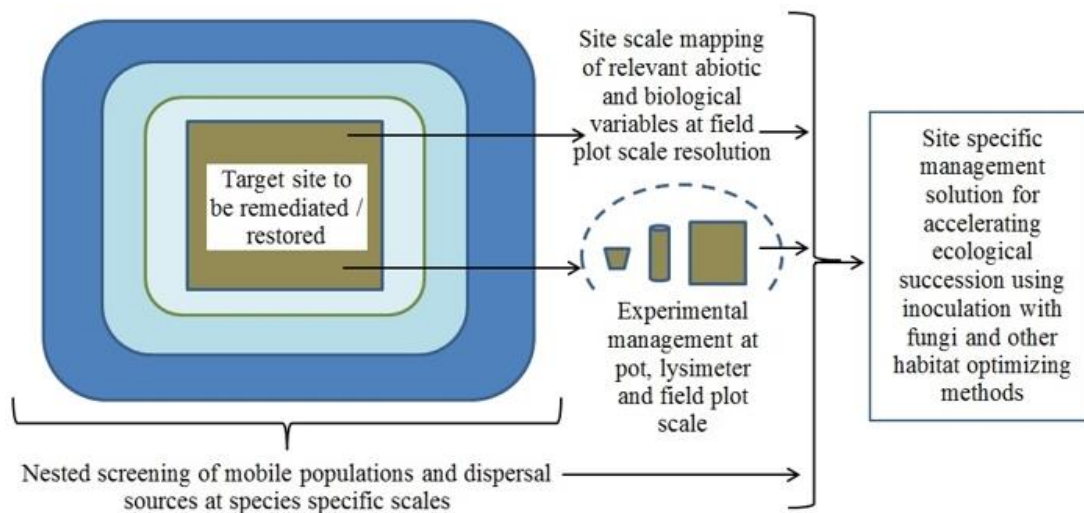


Figure 50 Multiscale field and experimental approach for designing a portfolio of operational measures including soil microbial manipulation for the restoration of a site. It is complementary with the use of non-native species when the construction of a new ecosystem is needed. (Iordache 2020).

- Adopt flexible endpoints of restoration in the function of the abiotic and biotic characteristics, concerning states, phases, and uncertainties. Associate specific activities in time with specific phases and states. Devise a plan to navigate the trajectory of the site towards this conceptual landscape
- Perform multiscale experiments to detect the effects of microbial inoculation on the relevant ecophysiological and ecosystem processes involved in succession.
- Facilitate dispersion or inoculation in a spatially structured approach, geomorphologically sensitive (valley, ridge, slope), and sensitive to discretization units (service providing unit) scale of fungi. In appropriate dispersing conditions planting a diverse community of trees in reclaimed soils could yield a diverse community of belowground fungi with no need for inoculation. Late microbes can be inoculated from the beginning in the construction of new ecosystems. Mycorrhizal fungi are key for coupling succession processes, they expand the niche of the plants and have effects in a cascade towards microhabitats for invertebrates and later mammals.
- Provide environmental conditions in a spatially structured approach to facilitate species or to filter some of them out. Design the trophic niche with nutritional terms based on stoichiometric ecological knowledge. Construct microhabitat heterogeneity for invertebrates with allochthonous particulate organic matter (relevant also for controlling the mobility of heavy metals in mining areas). Reclaimed soil from mine lands used for improving conditions suffers many disturbances related to the distribution of soil microflora community, mycorrhizal fungi, and enzymatic activities in soil. The reuse of such soil may benefit from inoculation with microorganisms (bacteria and fungi).
- Create spatially structured vegetation cover for microhabitat diversity. Inoculate spatially structured: around plots of vegetation facilitating by priority effects in artificial ecosystems, at potential keystone structures to facilitate vertebrates. Research areas in this field are the cheap production of inoculum and the in-situ management methods for effective restoration.
- Construct keystone structures with specific fungi communities supporting them for small mammals and other vertebrates. Include management by disturbances in later phases to control the system towards desired states. Spatially extensive disturbances may homogenize pre-existing differences within patches and reduce variability, while smaller disturbances may enhance within-patch variability by creating heterogeneity.
- Ensure connectivity (matrix permeability) with the surrounding landscape elements to enhance the viability of the metapopulations of mobile organisms.

E4. Catalyzing the development of ecosystems of innovation for environmental services

In chapter D1 we took a normative approach, in line with the sustainable development policies, in chapter D2 we touched on the real limitations toward such ideals of integrated management, in chapter D3 we provided a roadmap and methodological tools to stimulate the potential integrated management of biodiversity and mining problems in contaminated areas, and in this chapter, we arrived at catalyzing the inter-disciplinary cooperation by complex bottom-up and top-down mechanisms. To do this, I used the results described in chapters A3 and B4, namely a general concept of resilience, its application to ecosystem services management from ecological population and community levels to socio-ecological systems, and a method of knowledge mapping.

The CiteSpace analysis by the Web of Science domain has the results presented in table 22. The most important ones are Environmental sciences, Ecology, Plant sciences, Soil science, Water resources, Geosciences multidisciplinary, and Agronomy. The total number of domains was huge. The set merging all other sets covered 87 domains with at least ten articles, the extended set of the selected reviews had 44 domains, and the extended set of the 121 primary articles belonged to 26 domains. No scientific discipline can cover all basic and applied aspects of the complex cause-effect chain, from stressors to ecosystem processes by SPUs, and the long-term feedback presented in chapter B4 of this thesis.

Table 22 *The percent of articles belonging to the most important Web of Science domains in three CiteSpace data sets: four merged sets, the extended set of articles citing the 60 selected reviews, and the extended set of articles citing the 121 selected primary articles (Iordache and Neagoe 2023).*

Web of Science domain	Percent from primary articles		
	In four merged data sets	Citing core reviews	Citing core primary articles
Agronomy	2.90	4.98	4.80
Biodiversity conservation	2.76	2.79	2.48
Ecology	9.15	14.93	10.50
Engineering environmental	3.32	1.48	2.16
Environmental sciences	23.20	14.68	19.47
Forestry	1.96	4.44	3.15
Geosciences, multidisciplinary	2.97	3.52	8.10
Green & sustainable science & technology	1.77	0.79	1.06
Microbiology	2.60	1.18	1.02
Multidisciplinary sciences	2.61	3.51	1.46
Plant sciences	6.74	15.49	8.93
Soil science	6.60	9.45	12.39
Water resources	4.04	3.48	7.87

The textual analysis of the fundamental science reviews (table 23) revealed that they belong to three scientific domains: physiology, ecology (most of them), and hydrology. The highest complexity of the reviewed topics (regarding knowledge bodies covered) occurs in ecology. In applied science reviews (table 23) the diversity of disciplines was more significant, from agronomy to ecology, environmental engineering, geological engineering, geomorphology, and water management.

The disciplines identified in table 23 use many resilience concepts for their scientific objects and processes, as shown in figure 51. Ecology developed the well-known dichotomy between engineering and ecological resilience. Geomorphology uses its notions of engineering resilience (not necessarily naming it this way) and imports holistic resilience from ecology for socio-ecological situations (particularly catchments). The classic physical concept of resilience is used in agronomy - when it comes to soil mechanical properties, and also in ecophysiology and ecological engineering - when

the mechanical traits of plants are of interest. Organizations directly involved in managing natural resources and ES use simpler forms of resilience relevant to their time scale of action. Economic sectors and governments also refer to holistic ecological resilience and other complex concepts for long-term sustainability purposes.

Table 23 Information about review articles. Level of the cause-effect chain from 1 to 5 as in figure 1, O = organism, P = population, C = community, E = ecosystem. Econ = economic objectives, Bdv = objectives related to biodiversity, Soc = objectives related to regulating ES, Soc Econ Bdv = priority objectives related to regulating ES, second priority economic objectives, third priority objectives related to biodiversity. (Iordache and Neagoe 2023).

Type of review	Scientific field	Number of reviews	Level of the cause-effect chain	Stressors	Hierarchical level	Prioritization of objectives
Fundamental research	Ecology	3	1&2	Hg, elemental imbalances, light, water, cold, drought	O, P, C, E, Global	Not applicable
		2	1&2&3&4	All types	O, P, C, E, Global	
		1	1&2&3&4&5	Water and nutrients (low) availability	O, P, C, E	
		5	1&2&4	Climate and land-use change, elemental imbalances	O, P, C, E	
		1	1&2&5	Drought, lack of nutrients, C-N-P imbalances, grazing	O, P, C	
		1	1&4	All types	C, E	
		1	1&5	Multiple, including nutrient co-limitation	E	
		15	2	Mechanical, water, warming, eutrophication, global changes, imbalance of N and P, HMs, pesticides	O, P, C, E	
		1	2&3	General (not specified)	O, C	
		1	2&3&4	Not discussed	E, Landscapes	
		1	2&3&4&5	Not discussed	O, P, C, E	
		3	2&3&5	Not discussed	From genome to the biosphere	
		2	2&4	Not discussed	O, C, E	
		1	2&5	Not discussed	O, E	
	Hydrology	1	4	Not discussed	E, water bodies	
	Physiology	2	2	HMs	O	
		3	1&2	Many abiotic and biotic, including HMs	O	
Applied research	Agronomy	2	1&2&5	Many, including nutrients imbalance	O, P, C, E	Econ, Bdv
		1	2	Not discussed	O, P, E	Bdv, Econ
	Ecology	1	4	Not discussed	O, E	Bdv, Econ
		1	5	Not discussed	E	Bdv, Econ
		2	1&2&4	Climatic and HMs	O, P, E	Soc, Econ
		2	1&2&5	Climate change, nutritional and	O, P, C, E	Bdv, Econ

Type of review	Scientific field	Number of reviews	Level of the cause-effect chain	Stressors	Hierarchical level	Prioritization of objectives
				contaminant stressors		
		1	1&3&4	Many	E	Soc, Bdv, Econ
		1	1&4&5	Many	E	Soc, Bdv
		2	1&5	Chemicals, N and P imbalance	O, P, C, E	Bdv, Soc, Econ
	Environmental Engineering	1	2&4&5	Not discussed	O, C, E	Soc, Econ, Bdv
	Geological Engineering	1	1&2&4&5	Climate change	O, C, E	Soc, Econ, Bdv
	Geomorphology	1	2&3&4	Not discussed	O, E	Soc, Econ, Bdv
	Water management	1	5	Nonpoint pollution with nutrients	E	Econ, Bdv

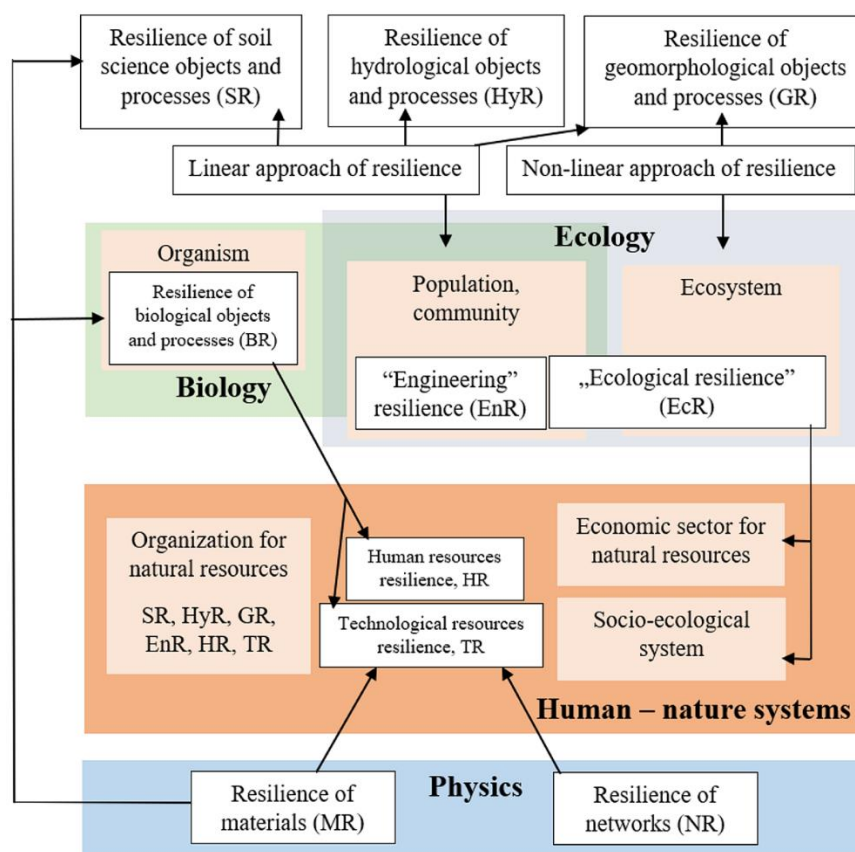


Figure 51 Concepts of resilience relevant for managing socio-natural processes, particularly ES, at several scales (from organizations to the economic sector and the whole socio-ecological system). The operationalization of the hierarchical concept for resilience introduced in chapter B4 can use various technical concepts presented in this figure, depending on the fundamental and applied research networks' objectives, structure, and organizational composition (Iordache and Neagoe 2023).

To organize a long-term research network of contaminated areas, one needs institutional frameworks catalyzing the cooperation and communication between disciplines with different traditions and vocabularies. Facing the need for such integration, scientists can follow proactive, reactive, and

inactive pathways. The proactive way means to invest in the environment to make it more appropriate for integration; the reactive is to respond in the short term to opportunities and threats existing in the environment, and the inactive means to perform disciplinary science as usual without interest in the integration. Knowledge production is compatible with all attitudes, but its speed of change to a more integrated form will depend on reactive and proactive attitudes. One can classify the driving factors for interdisciplinary cooperation as top-down and bottom-up. From amongst top-down approaches, we discussed in this contribution the innovation ecosystems and environmental securitization. Out of bottom-up factors, we mentioned the ontologies for coupling the vocabularies of different scientific fields.

One can develop a gradient linking the locally integrated ontologies (for specific stressors – SPUs and ES in well-defined action arenas) with larger-scale ontologies (figure 52) at intermediary levels. Such an approach unifies the normative and descriptive dimensions of sustainability science. Normatively oriented ontologies can support large-scale policies, while ontologies needed for integrating interdisciplinary knowledge can support the implementation of policies by producing operational tools for managing ES and resilience.

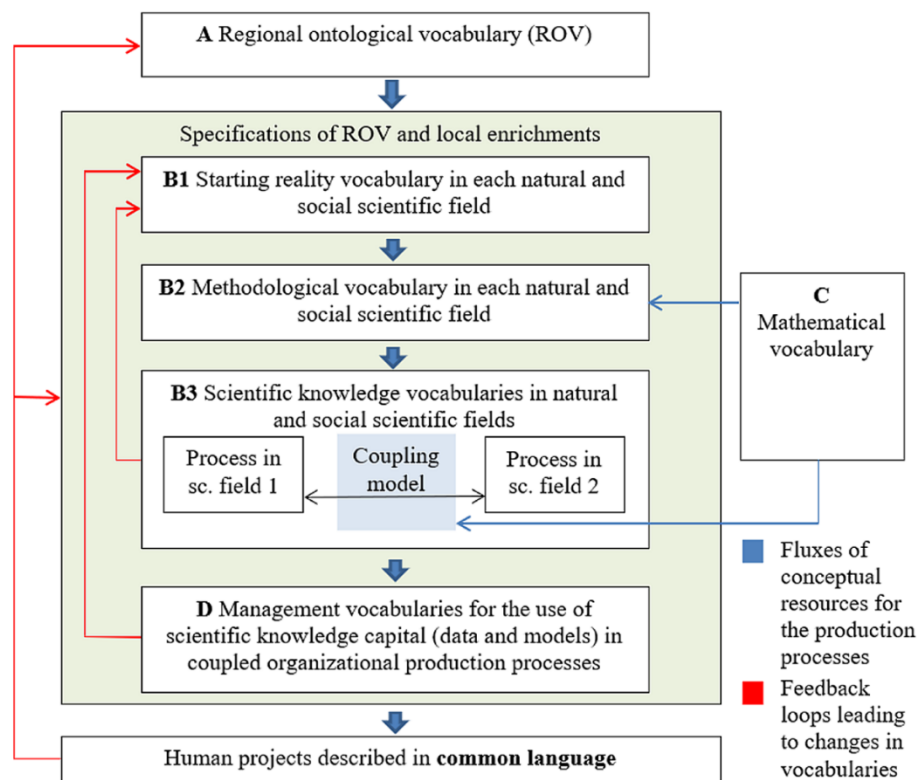


Figure 52 Types of technical vocabularies and coupling models needed for the integrated management in socio-ecological systems at the action arena scale by coupling sectoral objectives involved in the production of ES (Iordache et al. 2018).

Another important topic approached in this contribution was **how the complexity of the cause-effect chain is reflected in the research hypotheses and objectives**. The causal chains in basic research articles vary from very short ones (stressors acting on organisms) to complete causal chains, including feedback effects (table 24a). The investigated causal chains are longer in ecology than in ecohydrology. Several articles deal simultaneously with the effect of stressors on traits and the upscaling of traits to the SPU scale (1_2_3 causation, as in figure 16, chapter A3 of this thesis). Other articles simultaneously cover upscaling and impacts on ecosystem processes (2_3_4 causation as in figure 16). This suggests that breaking up complex problems into testable hypotheses is possible, although not at a scale enabling targeted reviews. In the applied science articles (table 24b), one can

notice again several scientific fields involved, pointing out the need for inter-disciplinary cooperation at the tactical level, too. Most articles approach short causal chains (table 24a and 24b), and the number of hypotheses or objectives by article tends to be small. This points out the need for portfolios of complementary research projects to couple the ES and resilience problems.

Table 24a Cause-effect chain length in fundamental science articles ($n = 82$) (Iordache and Neagoe 2023).

Scientific field	Cause-effect chain / Types of variables	No of articles	Scientific field	Cause-effect chain / Types of variables	No of articles
Agronomy	1_2	1	Ecology	1_2_4	10
	1_3_4	1		1_2_4_5	2
Ecohydrology	1_2_4	1		1_4	1
	2_3_4	1		1_4_1	2
	2_4	1		2	6
	2_4_1	1		2_3	5
Ecology	1_2	23		2_3_4	6
	1_2_3	10		2_3_4_5	1
	1_2_3_4	2		2_4	3
	1_2_3_4_1	2		2_4_2	1
			Geomorphology	2_4	2

Table 24b Cause-effect chain length in applied science articles ($n = 39$). Econ = economic objectives (resources with market value), Soc = social objectives (regulating ES, without market value), Bdv = objectives related to biodiversity (intrinsic species and habitats value) (Iordache and Neagoe 2023).

Scientific field	Objectives	Cause-effect chain / Types of variables	No of articles	Scientific field	Objectives	Cause-effect chain / Types of variables	No of articles
Agronomy	Econ	1_2	3	Ecology	Bdv	1_2_4_5	1
	Soc or Eco&Soc	2_4	7		Econ	1_2_5	2
Ecohydrology	Soc	2_3_4	4		Soc	2_3_4	2
	Soc	2_4	3		Soc or Bdv	2_4	4
	Soc	4	1		Bdv	2_4_5	1
Ecology	Bdv or Econ	1_2	1	Geochemistry	Econ	1_2	1
	Bdv or Soc	1_2_3	1	Geological Engineering	Soc	4	1
		1_2_3_4_5	1		Soc	2_4	2
				Water management			
	Soc	1_2_3_5	1		Soc	2_3_4_5	1

For reasons of space, I will not touch here on the issues of *downscaling the stressors and upscaling the effects of functional traits and the long-term feedback of traits on stress factors*, nor on the specific

hypotheses to test the framework, partly presented in C3 of this thesis and partly included in the complementary thesis of my co-author (Dr. Neagoe).

The scheme presented in figure 16 and operationalized in this contribution is convergent with ecological autocatalysis, which was already used in the area of traits–functioning relationships. Describing the feedback loops from figure 16 for each stressor - SPU–ES coupling would provide empirical support for the negative and positive feedback loops occurring in the ecosystem functioning across scales. This solution does not homogenize the measurement units to the same substance or energy currency (as in systems ecology). It keeps them as raw measurements and uses piecemeal integration in a population of models of lower complexity. The methodology itself described in this chapter is built in an autocatalytic way (figure 53).

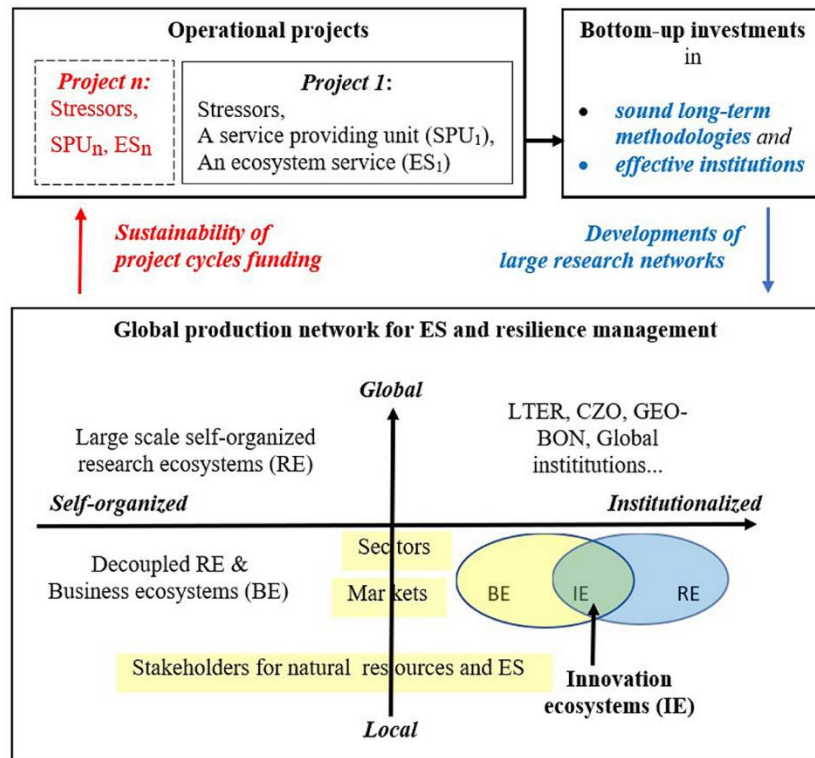


Figure 53 The autocatalytic nature of the proposed conceptual methodological framework. The transfer of fundamental knowledge to business ecosystems for the management of biogeochemical services in networks of contaminated areas allows strategic investments in effective institutions for cooperation, tactical investments in coherent inter-disciplinary methodologies, and finally, the long-term funding of projects dealing with operational complex problems in ecosystems of innovation and other entities for long-term research. (Iordache and Neagoe et al. 2023).

The future usefulness of the proposed conceptual methodological model depends on factors specific to HMs research and more general characteristics relevant to any socio-ecological research but applied in areas contaminated with HMs. A procedure for operationalization includes the following steps, by analogy with standard modeling activity:

- **Calibration.** In this phase, the specific details for the hierarchical heuristic resilience concept are set in the function of the SPUs of interest, the potential processes involved in the production of a target ecosystem service, and the structure of the system at the socio-ecological scale (types of relevant organizations, scientific kind of knowledge capital used in their decisions, and in particular the types of resilience concepts needed to manage the processes involved in the production of the target ES, as described in figure 50).
- **Sensitivity analysis.** The role of this phase is to screen out the small-scale processes with no quantifiable effect at the large scale of biogeochemical processes. This would depend on the

relative size of the SPUs compared to the discretization units of biogeochemical processes but also on the heterogeneity of the rates of SPU processes in time and space. This phase cannot be performed without a deep understanding of the existing mathematical models to simulate the coupled biological–abiotic processes. The availability of such models is a strong constraint for the development of the approach. For instance, microbial processes might not be directly relevant to the control of runoff chemistry and erosion. They can be screened out for these processes. Still, they can be suitable for predicting percolation in the vadose zone by clogging mechanisms and having a role in reactive transport. They can be retained as SPUs for such biogeochemical services. It all depends on the system's structure after the calibration phase.

- *Validation.* In this phase, the feasible ecosystems of innovation are devised, and the coherent portfolios of fundamental and applied research are organized in the frame of long-term programs. While the calibration and sensitivity analysis of the conceptual methodological model is site-specific, the validation would gain very much from an international organization of programs, economies of cost, and data sharing, all the advantages typical to long-term research and monitoring networks. As in any modeling, the complexity of research and innovation transfer networks should be optimal, neither holistic nor sectorial, but with inter-sectorial cooperation that can be managed and funded sustainably.

The validation phase, and in particular the knowledge transfer to end-users, is constrained by the availability of technologies not directly related to HMs research, as shown in figure 36 (chapter D3 of this thesis) for the upscaling of aboveground plant traits controlling the export of elements by runoff, the erosion. One can expect similar difficulties to occur for any SPU-ES couple, needing interdisciplinary cooperation to surpass them.

The results of the validation phase can feed policies for integrated monitoring and management of contaminated sites. Due to the diversity of institutional settings worldwide, it is not likely that the knowledge transfer mechanism would be the same everywhere. A scheme with levels of complexity, as depicted in table 6 of this thesis, from black box to grey box to white box approach, can be helpful in any social and political context. In the absence of international networks, the context of the tired scheme would vary from one socio-ecological system to another depending on the availability of data and models and on social and political variables. International cooperation in HMs research would increase the pace of models and database development, as was the case for biodiversity conservation objectives.

The difficulty of producing an overarching ES directive in the EU suggests that for HMs effect on biogeochemical services, an approach cross-cutting existing regulation might be more feasible. One can capitalize on already existing regulations applicable in contaminated sites, choose a particular ecosystem service relevant to key stakeholders (identified in the calibration phase of the conceptual methodological model), and work for realistic methodologies to account for the effects of HMs on the selected SPU, the relevant biogeochemical processes, and finally the production of the ecosystem service. In this way, the environmental regulations would not be changed at the level of laws, which would be a process too complex to be controlled by scientists, but at the level of law enforcement by methodologies and operational plans depending more on scientific knowledge.

To conclude:

- complex problems such as the resilience of ecosystem services must be disentangled and organized such as to make them tractable on the scale of research projects and long-term programs. By analogy with computing systems, we structured the integrative literature review using as conceptual classification of constructs a nested collection of at keys (attributes) and values (variables belonging to the set corresponding to each attribute). The most general key is the approach for the knowledge and management of ecosystem services, with three values: black box, grey box, and white box. Each secondary key has two values, ontological-epistemic

issues, and methodological issues. Mapping the literature bodies allows a qualitative description of the values of tertiary keys. An alternative conceptual-methodological framework introduced innovative values of the white box approach issues. On the ontological-epistemic side, one proposed a cross-scale model of producing biogeochemical services under HM stress and a concept of resilience as a systemic property mirroring the organization of the cross-scale model. On the methodological side, one assessed the possibility of a hierarchical organization from projects to research programs to innovation ecosystems and long-term research networks.

- At the research program and research network scale, one suggests operationalizing the conceptual, methodological model in contaminated socio-ecological systems by a calibration, a sensitivity analysis, and a validation phase. In the validation phase, innovation ecosystems are devised, and the coherent portfolios of fundamental and applied research are organized in the frame of long-term programs. We suggested a pragmatic approach, with optimal complexity of the networks and agendas, capitalizing on existing legislation frameworks and innovating at the level of the methodologies for their enforcement.
- At the metatheoretical level of complexity, one can test the hypothesis that there are epistemic niches for solving different problems with different local ontologies by different strategies of dimensionality reduction. This could explain the separation of knowledge clusters and scientific schools of thought, point out their complementarity, and decrease unconstructive competition. Such results could feed the development of hierarchical ontologies needed for the efficient functioning of complex interdisciplinary networks. Once the meta-theoretical details are clarified the best methodological strategy could be to use a population of different ontological-epistemic frameworks in the same research program and long-term research network instead of specializing them in a single paradigm (as was the case with long-term ecological networks).
- The complex cross-scale processes which are modellable as in figure 16 cannot be understood under the umbrella of an epistemically homogenous theoretical frame and need coupling between many scientific fields. Organizing the programs and networks in an interdisciplinary and transdisciplinary way decreases transaction costs and increases the chances for financial sustainability and effective biogeochemical services management. A calibration–sensitivity analysis–validation scheme as proposed at the end of the discussions could optimize the costs of developing and maintaining such institutional structures. The optimization would be towards a polycentric organization of the innovation ecosystems/research networks, with research and management agendas distributed across levels of problem complexity from SPUs processes to coupled SPUs and abiotic processes to socio-natural processes. Such a structure can easily adapt to the changing natural and socio-economic reality by eliminating or adding modules (local centers with relatively homogenous ontological-epistemic assumptions) to deal with the mutations occurring in the complex problems to be solved in areas contaminated with HMs and their integrating landscapes, and at the same time maintaining the social capital developed by past cooperations.
- The contributions' novelty comes from the structured complementarity of the complex deterministic approach of HMs' impact on biogeochemical services with other procedures, from the innovative conceptualization of the resilience of biogeochemical services to HMs stress, and from the potential of catalyzing long-term research networks and innovation ecosystems for contaminated areas.

F Teaching

I used the input from the theoretical and methodological research to organize for undergraduate students a mapping of the main theories and concepts in ecology (basic, applied, and knowledge transfer issues). Table 25 presents a simplified classification of the main epistemic strategies in use to simplify the very large complexity of large-scale productive processes spanning across the natural and social realms. On the other hand, to solve a certain problem, one does not need all of them at the same time, but rather a toolbox of instruments to select the needed ones in every situation.

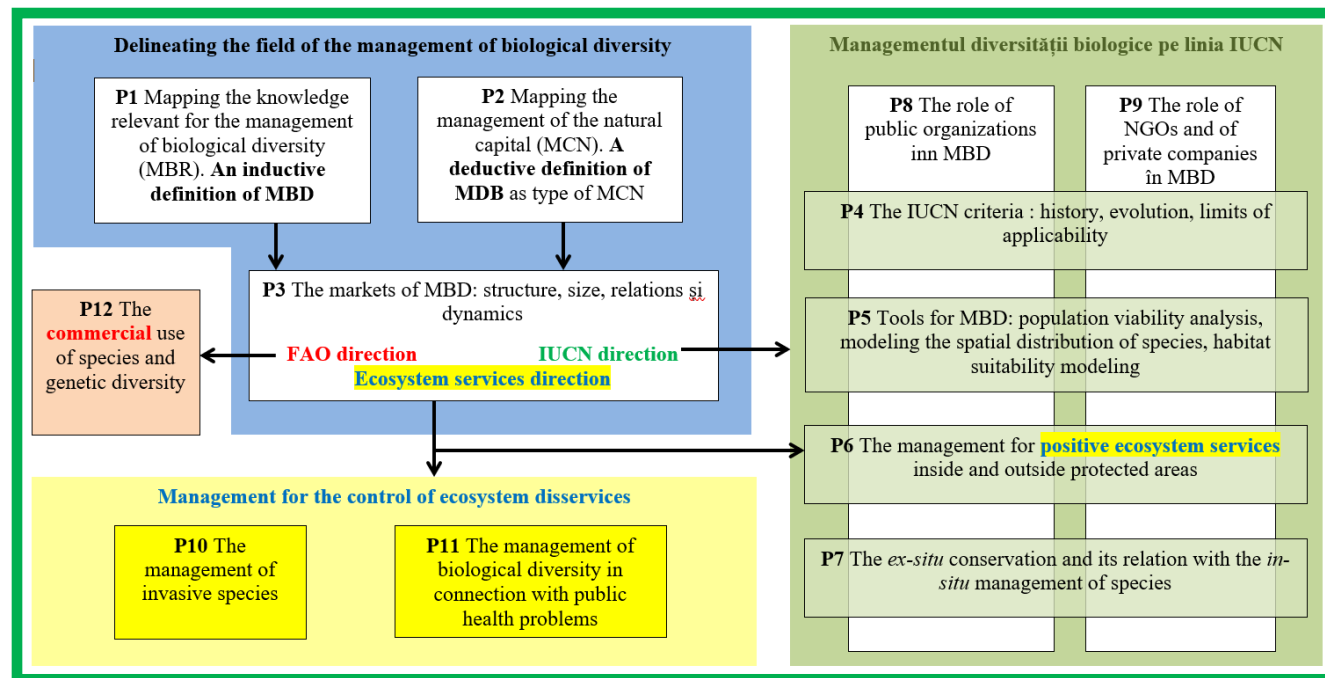
In figure 54 on the next page, one can see the relationships between the graphical abstracts of four disciplines developed in this approach and their main topics. The general ecology is conceived in such a way as to be useful for people from biochemists to classic biologists to ecologists and to point out the complementarity of their roles in solving complex problems. The idea was to catalyze problem-oriented cooperation between future professionals of different specializations. The complementarity was clear from the very beginning by the fact that three ecological strategies have a biological tradition and two of them belong to earth system science (table 25). It is the same idea that was used already in the E4 chapter to point out the complementarity of different sciences and specializations when dealing with the resilience of complex productive processes and the development of ecosystems of innovation.

Table 25 A simplified classification (for teaching purposes) of the epistemic strategies reducing the complexity of productive processes in the complementary natural and social domains. The gradient of blue color suggests a continuum from individualistic (Gleasonian) positions to holistic (Clementsian) ones. The strategies E1, E2 and E3 traditionally belong to the domain of biology, while the E4 and ES5 strategies belong to earth system science.

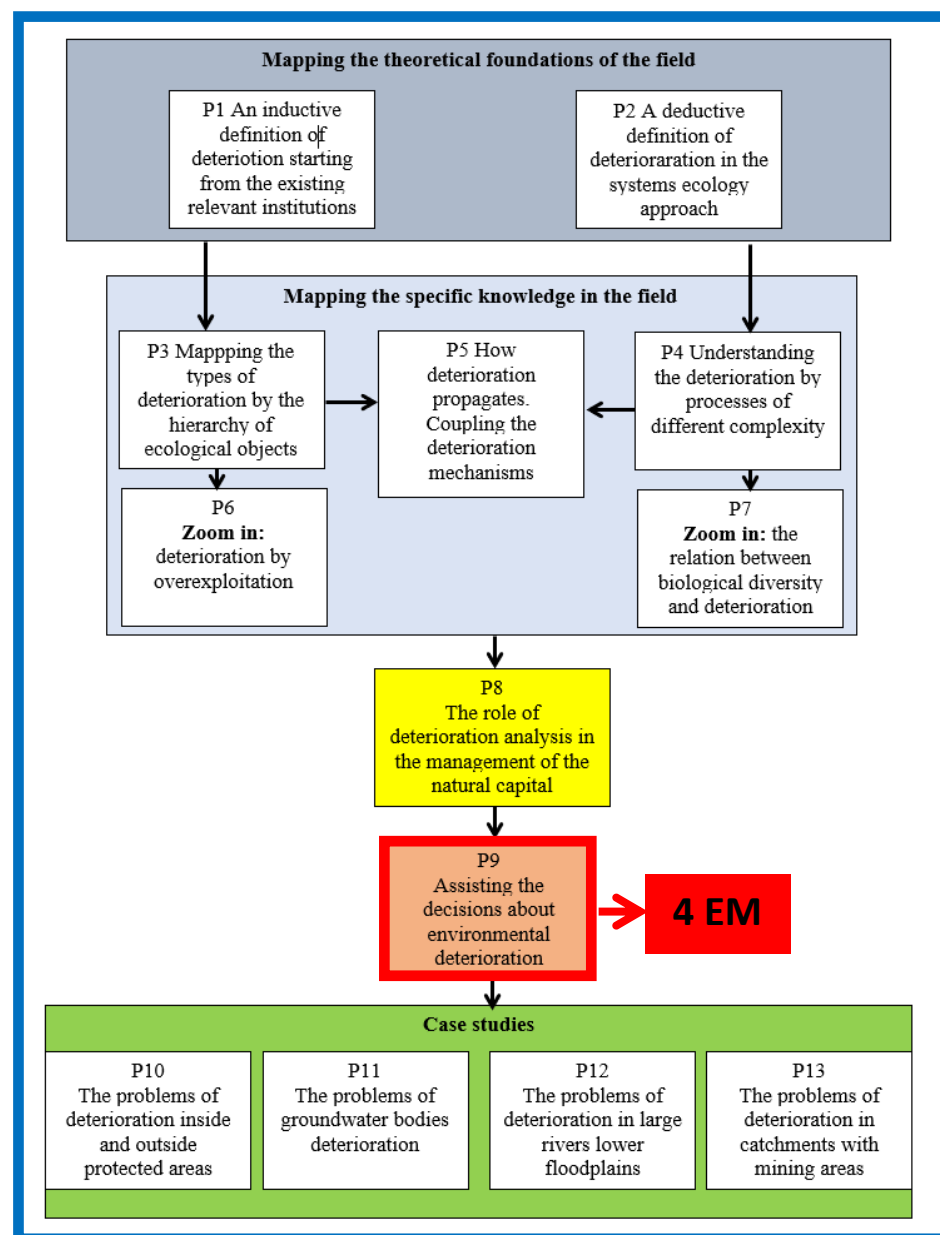
Field	Ecological objects and processes					
Epistemic strategy	E1 Eco-physiological	E2 Population ecology	E3a Community ecology	E3b Systems of coevolved populations (biocenoses)	E4 Ecosystem ecology	ES5 Systems ecology Theories about adaptive cycles
	S1 Management theory, organisational studies	S2 Ecology of populations of organizations	S3a Ecology of communities of organizations. Action arenas	S3b Theories about the evolution of culture/institutions	S4 Industrial ecology, other physicalist approaches	Theories about general social and economic structures
Field	Social, economic and cultural objects and processes					

Another teaching contribution capitalizing on the results from research (besides the usual BSc, and MSc theses, as well as contributions to PhD theses) was peer learning about knowledge mapping using the software CiteSpace complemented with methods of conceptual analysis (for instance Iordache 2024). I did this for teachers and researchers in the fields of biology, geography, and geology.

3 Management of biological diversity



2 Environmental deterioration



4 Ecological monitoring (EM)

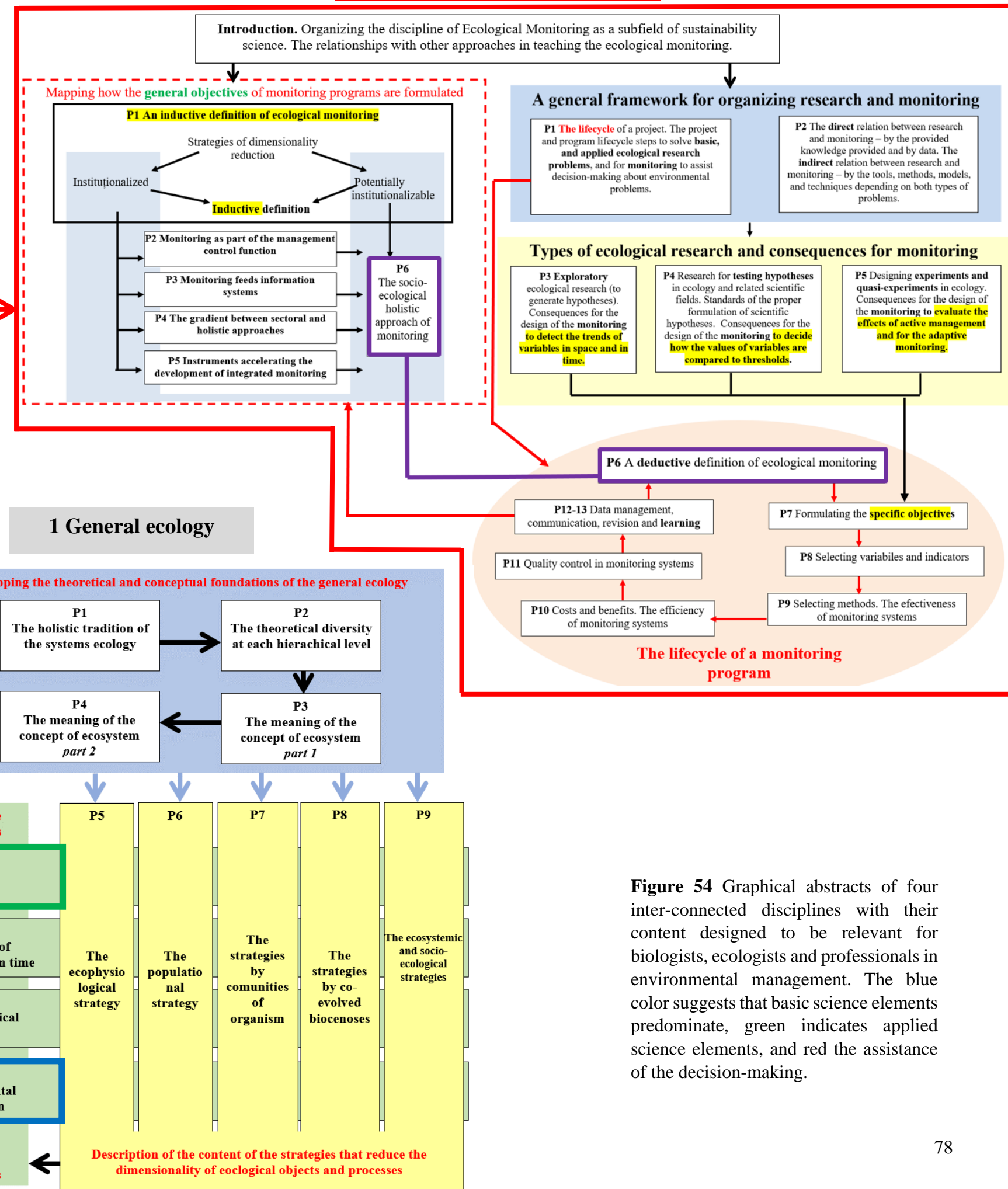


Figure 54 Graphical abstracts of four inter-connected disciplines with their content designed to be relevant for biologists, ecologists and professionals in environmental management. The blue color suggests that basic science elements predominate, green indicates applied science elements, and red the assistance of the decision-making.

Part II – Future perspective in research and academic fields

“The goal of the eco-evo-devo approach is to uncover the rules that underlie the interactions between an organism’s environment, genes, and development, and to incorporate these rules into evolutionary theory”. “The thermodynamic view of evolution deals with the laws and principles that control energy transformations as species and ecosystems increase in power output.” “In the eco-evo-devo (ecological evolutionary developmental biology) approach to evolution, species are organized by taxonomic similarity (who is related to whom within trophic levels). In the thermodynamic approach, species are organized functionally (who eats whom as energy flows through trophic levels). [...] To understand evolution and to apply the understanding to conservation of species, the scientist has to understand how species are related to each other functionally as well as taxonomically within an ecosystem.”

Carl F. Jordan (2022), systems ecologist

I started this part with a citation from a recent book by Emeritus Professor Jordan, Odum School of Ecology, University of Georgia, to point out the convergence of his results with our results obtained in the ecology school at the University of Bucharest. Systems ecology does not replace, is complementary with, and co-evolved with other research strategies. Formulating a career development plan on this background is constrained by 1) the research gaps and uncertainties in the bodies of knowledge, and 2) the institutional settings, both of them with their independent dynamic. To the extent possible the structure of a strategic plan should be **modular**, and **polycentric**, allowing for its adaptive management in function of 1) the evolving global research agenda, 2) the organizational internal policies, and 3) the national and international research policies. My **strategic goal is to contribute to the development of scientific knowledge and the formation of human resources in interdisciplinary and transdisciplinary life sciences and socio-ecological academic programs**. The quantifiable **objectives** are:

1. To develop theoretical foundations for the integrated modeling of biological and socio-ecological processes;
2. To produce scientific knowledge about the role of plant-soil systems in the production of ecosystem services associated with hydrological and biogeochemical processes;
3. To develop new insights in the field of eco-hydrology at the slope, floodplain, and catchment scale;
4. To design improvements in the institutional frameworks for the integrated management of natural resources and services.

The success of such an agenda depends on the art the long-term research, which is to couple operational projects in programs in a creative mode. The operational research lines of this program are organized in the same as the previously presented contributions: by theoretical, methodological, empirical, mathematical modeling, environmental management, and institutional development directions.

In the **theoretical** direction, I am interested in two operational topics:

- Comparative ontology of environmental sciences. It will start from results published by Iordache et al. (2012) and will follow the approach presented in figure 52.
- The problem of time in biology and earth systems science. Upscaling the processes from the SPU scale to the site/ecosystem scale needs to be done not only in space but also in time. Until now we have worked only on the upscaling in space. *Limitations come from how time is conceptualized in such hybrid processes, ranging from developmental ones at the organism scale to landscape*

ones. The inspection of the recent trends in the development of general theories in biogeochemistry (Bianchi 2021, Bianchi et al. 2021) shows a holistic interest in understanding highly complex processes, often linking ecology and biogeochemistry with hydrology under the pressure of climate change. This holism differs from the Odum style biogeochemistry because of the multiple scales and types of processes engaged. There is no agreement on how such processes can be leveraged to formulate generalizable knowledge beyond the profile of systems. Existing inquiries from the philosophy of science (Huneman and Bouton 2017, Baedke and Manus 2018) have already shown that the concept of time is not homogenous within and between scientific disciplines. Time can be used as an ordinal or quantitative variable, discrete or continuous, parameter or variable in modeling, or as the stage or timing of developmental events. Some aspects of the conceptualization of time in other disciplines, for instance, the importance of the order of events, are not so much considered in biogeochemistry. A potential solution can be a combination of theoretical (at the interface between general theory formulation and philosophy of science) and experimental research of aspects of time not so often accounted for in biogeochemistry (the length of life of organisms and the order of factors driving their development and role in biogeochemical processes). The effect of the order of stress factors acting on SPUs and regulating ES has not been conceptualized or investigated so far. Recent and essential contributions to this area are the article by Jackson et al. (2021) about the temporal dynamic of multiple stressors and the book about time in ecology by Post (2019). (Iordache and Neagoe 2023). Several other ideas about time in biology have been communicated in Iordache (2021).

The methodological topic is coupled for the time being with the institutional development in a Fulbright project implemented at the host institutions CUNY Advanced Science Research Center, Brooklyn College, Cary Institute of Ecosystem Studies with host scientist Peter M. Groffman, Ph.D., Professor of Earth and Environmental Sciences. The Fulbright project (FP) with the title “Knowledge transfer for the development of a Critical Zone Observatory in a Romanian urbanized catchment” is included below

Background of the FP:

The research in experimental catchment shifted from comparing inputs and outputs and quantifying pools and fluxes to a more mechanistic understanding of ecosystem processes within watersheds (Campbell et al., 2021). The mechanisms of resilience to disturbance and specifically to climate stress are a research priority of long-term research and monitoring sites (Campbell et al., 2022; Contosta et al., 2023) and are related to the priority of up-scaling and down-scaling processes between experimental plots to full catchments (Halpern et al., 2023) and from hot spot and moments to larger time scales (Inamdar et al., 2022).

The University of Bucharest is involved in the strategic objective of developing a Critical Zone Observatory in a highly polluted catchment, with the mining and smelting industry in its structure (news is available here). Iordache and Neagoe developed a cross-scale conceptual and methodological framework for the resilience of biogeochemical services to heavy metals stress in contaminated catchments (Iordache and Neagoe, 2023) and later applied a national research project (under evaluation) for a stoichiometric approach to elements retention in buffer zones under climate stress (Appendix 1 of this detailed statement). The mentioned project would transfer knowledge for the development of the strategic CZO (Objective 3 in the exploratory project REBIOS-ST).

Research agendas or frameworks are lacking that connect research questions to available data for specific combinations of existing networks in ecology and environmental science (Jones et al., 2021). We do not have yet reliable methods for predicting nutrient retention capacity at the watershed or regional scales, the processes and the space and time scales being extremely context-dependent (Severe et al., 2023). This heterogeneity is even larger in urban and industrial watersheds (Welty et

al., 2022). Innovative conceptual frameworks and methodologies (Gan et al., 2023) are needed to surpass such difficulties.

Goal and objectives of the FP

In this context, the goal of the Fulbright research activity is to transfer conceptual, methodological, and institutional experience from the U.S. LTER network to the future long-term CZO to be developed in Romania. The goal of the Fulbright visit is complementary to existing national efforts and is decisive for appropriate institutional development of the local long-term and monitoring institutions, taking into consideration the extensive experience of the U.S. host.

*The specific **objectives** are:*

- 1. To formulate hypotheses in a stoichiometric approach for elements retention in transversal and longitudinal buffer zones testable across sites and scales in US-Romania coupled research projects implemented in LTER/CZO sites.*
- 2. To identify the up-to-date methodologies for implementing ecological stoichiometry projects in LTER/CZO networks.*
- 3. To produce a road map and an operational plan for the effective and efficient development and implementation of a CZO in an urban and industrial Romanian basin.*

Methodology and deliverables of the FP

The first objective will be approached by standard knowledge mapping and analytical review methods in cooperation with scientists from the host institution. Time allocated: one person month.

The second objective will be supported by visits at the research sites, involvement in running field activities at riparian U.S. sites, labs, and data processing as decided by the host, reviews of methodological documents, other activities resulting from brainstorming and workshops at the host institution. Time allocated: two person months.

The third objective will capitalize on the extensive institutional experience in LTER design and the experience of the host and on the results from first and second objectives of the Fulbright visit. The strategic and operational documents will be developed according to the standards of good practice of U.S. LTER sites for the specific questions to be addressed in the future by the Romanian CZO and adapted to its socio-ecological structure.

Impact of the FP

The short-term scientific impact is related to the submission of a review and perspective article as the common product of objectives 1 and 2. The long-term impact consists of catalyzing the institutional development of a CZO by the results of objective 3 and the future cooperation between U.S. and Romanian institutions for testing hypotheses in US-Romania coupled projects.

The Fulbright methodological project with institutional implications is complemented by a **national exploratory project** dealing with the resilience of biogeochemical services to climate change stress which has an empirical and an institutional development dimension. I present several elements of this project still under evaluation in bellow. The background, objectives, and hypotheses of the project “The REsilience of BIOgeochemical Services to climate change stress in a Critical Zone Observatory: problems related to Space-Time upscaling REBIOS-ST” (the project has a reference list of 121 articles which is not included here and has been communicated in Iordache 2023b):

*The issue approached in this project is **how the effects of climate stress on the ecosystem scale retention of elements in biological and abiotic compartments of the river basins propagate at larger scales in space and time and change the overall buffering of elements in the river system.** This kind*

of cross-scale approach (figure 54) is feasible only when long-term research and monitoring institutions are organized. For this reason, the project has an objective dedicated to institutional development. The high dimensionality problem of the resilience of biogeochemical services to climate change stress in river systems is usually simplified to be compatible with standard research and monitoring programs. One classic approach is to focus on single elements or classes of elements (e.g., nutrients like N and P or toxic elements like many heavy metals - HM). Another one is to tackle separate processes (e.g., hydrological or biological) at the same space-time scale. Another often-worked possibility is to describe the climate changes only as a change in the flooding patterns, disregarding the separate effects of temperature and precipitations at the ecosystem scale. The research priorities extracted from the literature are combined in the issue structure presented in figure 54.

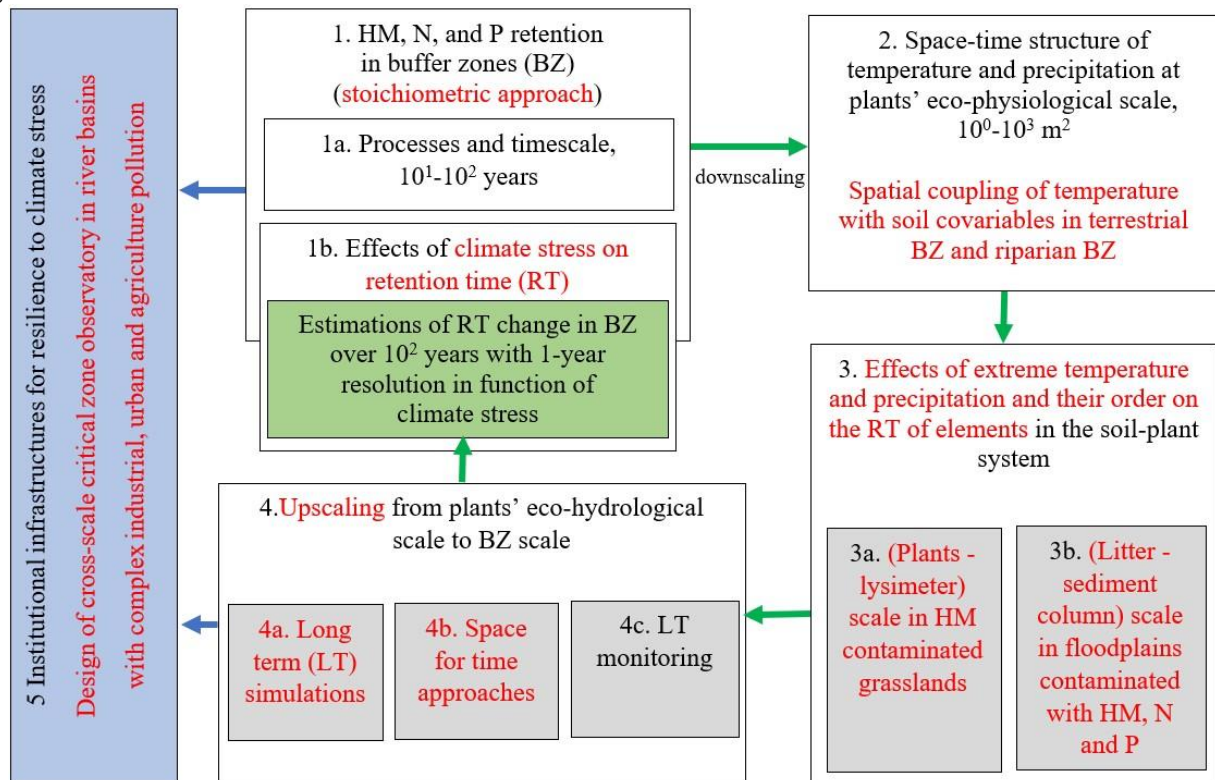


Figure 55. Scientific (white and green boxes), methodological (grey boxes), and institutional (blue box) fields relevant to the project's goal. In red are critical problems corresponding to the elements of difficulty. Green arrows show fluxes of knowledge and data about processes underlying the production of biogeochemical services related to HM, N, and P retention in contaminated river basins. Blue arrows show the data and knowledge transfer for institutional design (Iordache 2023b).

The limitations of current approaches in relation to the state-of-the-art in the field. To identify the limitations of current approaches, we made a combination of systematic review, mapping knowledge fields with the software Citespace, inspection of the clusters, and selection of key articles.

Difficulty element 1. There is no information about climate security issues of buffer zones or the integrated retention of N, P, and HM (figure 55). When we focused on the literature about the retention of heavy metals in floodplains/river systems, the result was rich. Still, its analysis with Citespace showed that many of the clusters of the network of citing articles are not directly relevant (figure 56). After inspection, only clusters 8 (HM in floodplains) and 10 (HM) proved to be important for our purpose. Most of the other literature deals with HM as independent variables and ecological risk assessment. There are studies about the effect of climate change on HM retention, but they are limited to the effects of changes in flooding patterns and intensity. The literature about HM in soils is huge, but the information is rather scarce regarding HM retention time in soils of contaminated

landscapes (85 articles). The combined effects of rainfall and temperature on HM retention in soils were not investigated. The retention time in the soil is perceived as a biogeochemical service only in peculiar management contexts around mining and industrial point sources.

Difficulty element 2. Although it will not be approached in the project, we also looked for the downscaling of temperature and other stressors at a small scale in grasslands (one of our model ecosystems) and floodplains (figure 53). The literature is not well developed, and the problems' complexity requires a project in itself.

The objectives of the projects are:

- **Objective 1** To test hypotheses about the effects of the stress due to extreme temperatures and precipitation events during the growing season of plants and their order in time on processes involved in the storage and remobilization of elements in grasslands contaminated with heavy metals
- **Objective 2** To test hypotheses on the effects of the stress due to extreme temperatures and precipitation events during the growing season of plants and their order in time on processes involved in the storage and remobilization of elements in floodplain islands of different contamination, age, and position from upstream to downstream
- **Objective 3** To produce catalyzers for a CZO research and monitoring ecosystem dedicated to the problem of the resilience of biogeochemical services in contaminated river systems.

I formulated explicit hypotheses for testing in objectives 1 and 2 (not presented here). As for the objective 3, in November 2022⁵, a network of seven Romanian institutions with experts from plant science, ecology, hydrogeology, geophysics, environmental sciences, microbiology, hydraulics, geodesy, and industrial ecology agreed to get involved in the development of a critical zone observatory dealing with coupled geological, hydrological, biological, and technological processes in the highly polluted areas. This project is intended to complement the Fulbright one and provide input to the chain of projects leading the development of this CZO.

Another operational line to follow in the research program is the **technological development of environmental services** of the kind presented in figure 38. We have such a project aiming at moving to TRL4 our TRL2 results. I will give several details below about the project with the title “TRL3 LIDAR-based technology for the assessment of aboveground VEgetation functional Traits and of the Roughness And Porosity of plant cover – LIVETRAP” (still under evaluation):

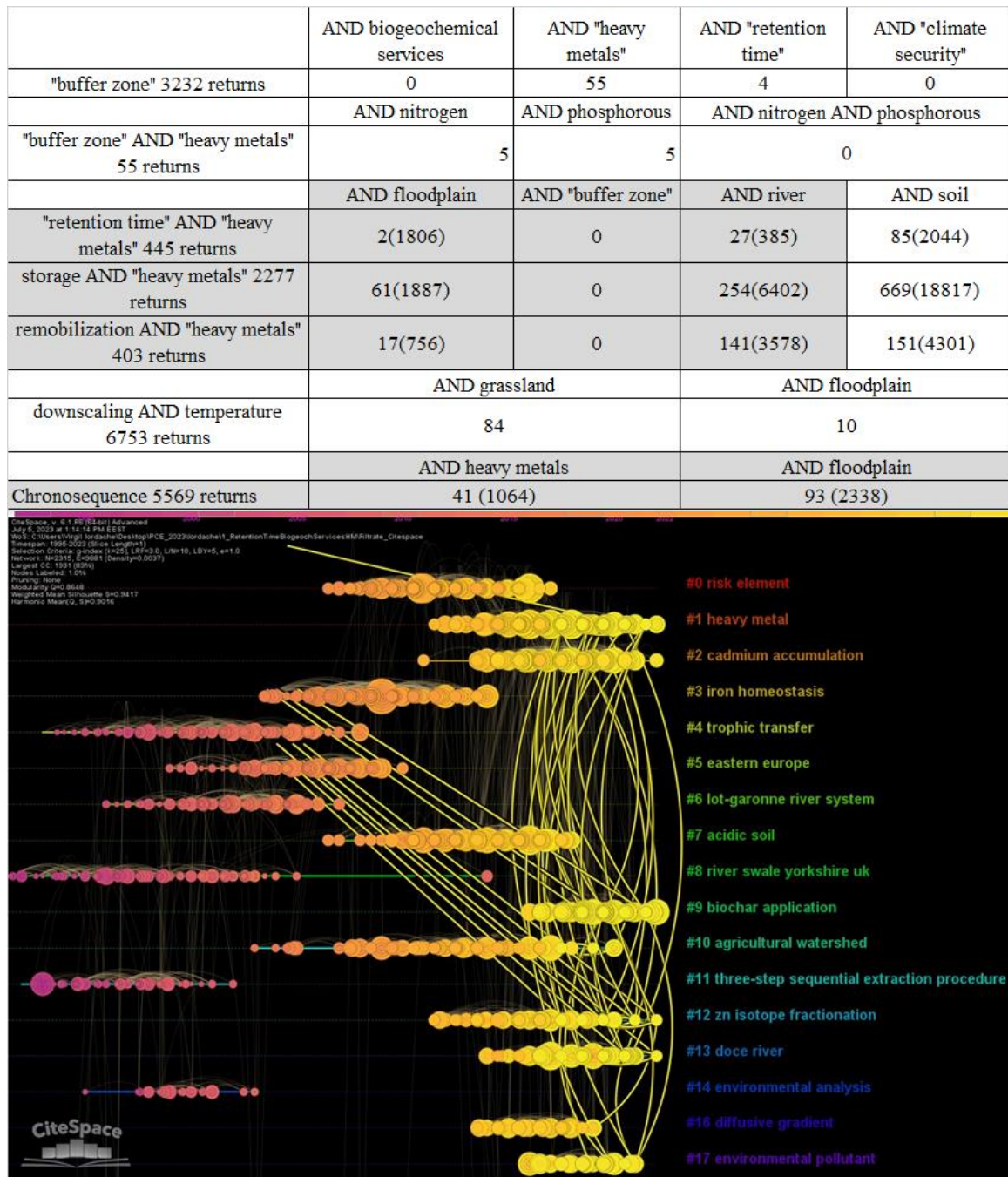
The goal of the project is to produce a TRL3 LIDAR-based technology for the assessment of aboveground vegetation functional traits and the roughness and porosity of plant cover. The technology is applicable for the quantification of hydrological and erosion control ecosystem services in the restoration ecology industry, river basin management, environmental impact assessment, and other types of services in the field of environmental and natural resources management.

The objectives of this project are:

- Objective 1** To experimentally validate at plot scale a deterministic hydrological model using a set of LIDAR metrics describing the roughness and porosity of plant cover
- Objective 2** To simulate plant management scenarios at catchment and land cover units scale with a deterministic hydrological model using a set of LIDAR metrics describing the roughness and porosity of plant cover
- Objective 3** To design the TRL3 environmental service with scientific feasibility fully demonstrated

⁵ <https://unibuc.ro/cercetatori-si-profesori-ai-universitatii-din-bucuresti-printre-initiatorii-unui-observator-al-zonelor-critice-in-apuseni-valea-centrala-a-muresului/>

The graphical abstract of the LIVETRAP project can be seen in figure 57.



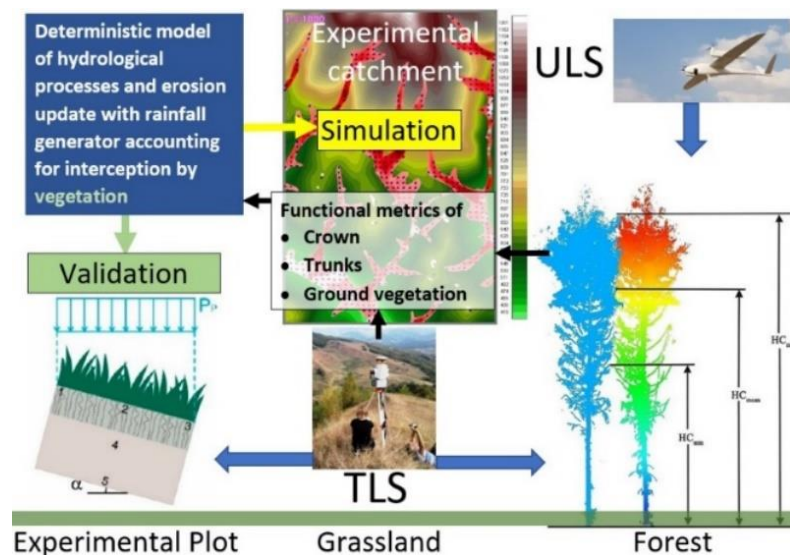


Figure 57 Graphical abstract of the project LIVE-TRAP. In the graphical abstract, the forest image is from Wang et al. (2021), and the image of the plot experiment is from Mendes et al. (2021).

Another line of the research program is to catalyze **the development of an ecosystem of innovation associated with the CZO** (project in development). Specific objectives within this ecosystem of innovation would be to produce several TRL2 technologies and an overarching TRL6 one dealing with the cumulative impact assessment. In a coming presentation at the European conference of the Society for Ecological Restoration (Iordache et al. 2024, August 2024) with the title “Grounding the landscape scale restoration for biogeochemical services on cumulative impact assessment: a process-based approach” *we will present this project that triggers the mutual reinforcement between the restoration industry and other environmental business sectors using the institutional framework of cumulative impact assessment (CIA), as part of the procedures for environmental impact assessment (EIA) and for strategic environmental assessment (SEA). The problem is the impact of many types of projects on decarbonization, retention of nutrients, and of heavy metals provided by head and intermediate catchments with mining and smelting industries. Including ecosystem services (ES) in CIA is currently limited to mapping ES production and scenarios of ES change by spatially distributed impacts. We add to this screening stage of CIA a process-based stage coupling the service-providing units of plants and biogeochemical processes by aboveground and belowground functional traits. The first step of the second CIA stage is a spatial multifactorial diagnosis of the trees' stress under atmospheric and soil pollution at 100x100 m² resolution, with potential consequences on elements budgets in the soil-plant-atmosphere system via functional traits. Another step consists of a LIDAR and geophysical methods-based upscaling of the aboveground and root traits data from tree scale to catchment and floodplains level. This will be coupled with the data from the integrated forest and water monitoring in a Critical Zone Observatory, and simulations of the production of the biogeochemical services using mathematical models for predicting the migration of pollutants taking into account vegetation traits on hillside areas and floodplain areas. The last step is the prioritization of forest management actions, restoration of contaminated ecosystems, remediation of tailings and mining dumps, and forested treatment wetlands for acid mine drainage. The technological development of the CIA process and instrumental technologies needed is hosted by an innovation ecosystem supported by ontologies, pre-legislative research, and procedures for pilot integration of pollution monitoring and management in headwater catchments and floodplain sectors.* (Iordache et al. 2024). The production flow chart of the TRL6 CIA method is presented in figure 58.

In the professional community, I intend to catalyze together with my colleagues from the field the link between scientific knowledge from the research ecosystems and the know-how from the business ecosystems capitalizing on the current role of the President-elect of the large-scale ecosystem

restoration section of the Society for Ecological Restoration (Iordache and Gaglioti 2024). It seems that this connection is critical for changing the trajectory of the production of ecosystem services from the current decline to recovery at national and global scales.

On the teaching side, my goal is to continue to catalyze the interdisciplinary cooperation between biologists, ecologists, and persons from other fields relevant to integrated environmental management, both at the undergraduate level and in an interdisciplinary doctoral school. An operational objective for undergraduate students will be to produce a textbook using the existing lecture notes with the structure presented in figure 53 at an international academic press.

I served a full mandate in the National Council for Ethics in Scientific Research, Technological Development, and Innovation, including academic contributions to the development of the scientific field of research ethics (Iordache 2023). This line may continue depending on the needs of the public institutions. Another direction that may continue is the involvement in the management of research institutes, using the experience gained as a member of the board of the National Research and Development Institute for Industrial Ecology – ECOIND.

All these experiences are useful for coordinating the development of the future CZO, the associated ecosystem of innovation, and portfolios of projects, which are my main scientific priorities in the future.

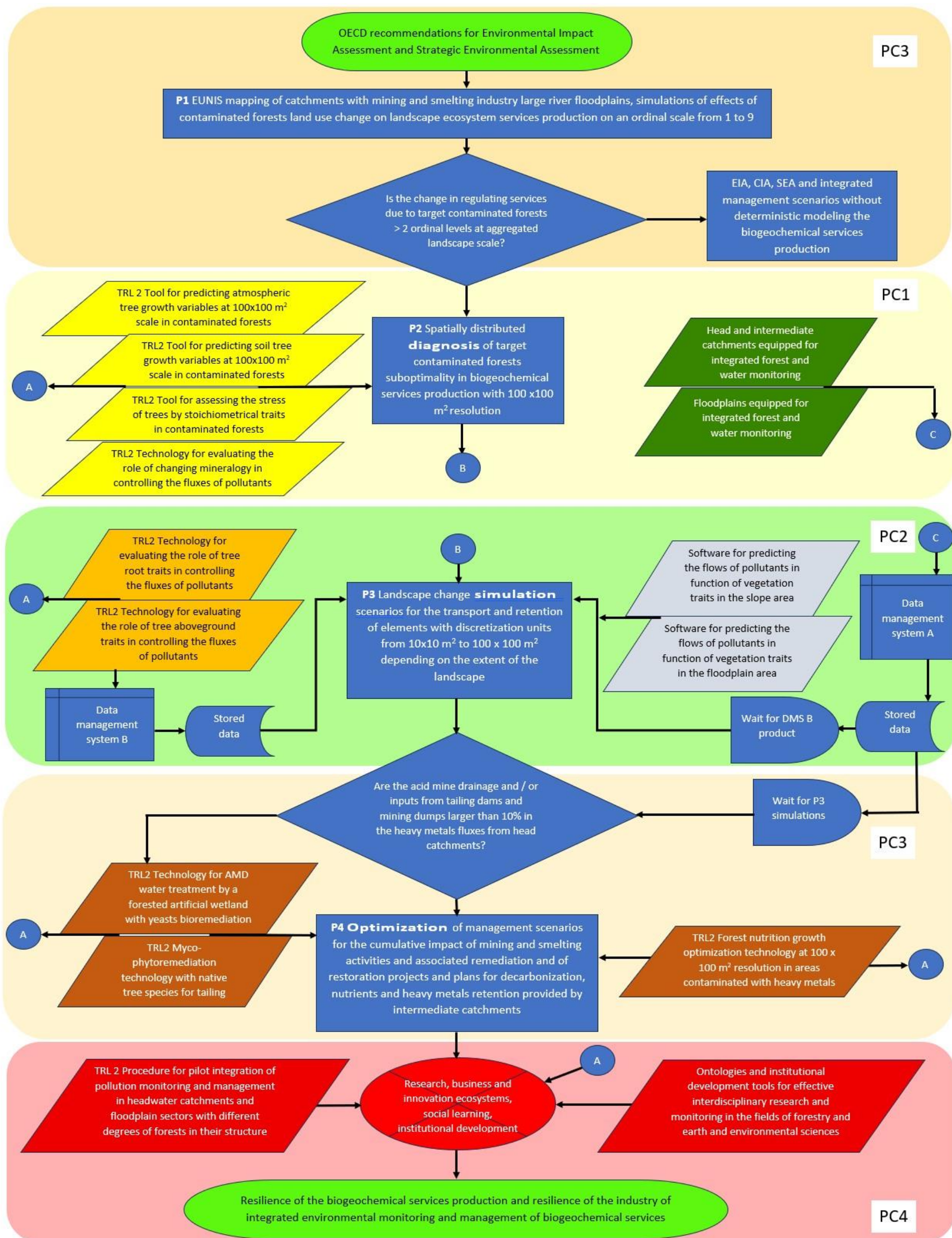


Figure 58 Production flow chart of the **TRL6 cumulative impact assessment (CIA)** method (environmental service) of forestry and water management activities optimizing the biogeochemical services (decarbonization, nutrients, and heavy metals retention) in head and intermediate catchments with mining and smelting activities. PC1, PC2, and PC3 are the three vertical inter-disciplinary subprojects, is a cross-cutting trans-disciplinary sub-project. Besides the TRL6 environmental service, we will produce **nine TRL2 instrumental technologies and procedures** needed for the development of the CIA method which can have much larger and diverse specific markets. All services and technologies will benefit from the institutional development of a functional innovation ecosystem at the interface between the research and business ecosystems developed in PC4. A **critical zone observatory** for interdisciplinary monitoring and research in industrially polluted head and intermediate catchments will be developed in direct association with the innovation ecosystem.

Conclusions

The research program developed on the following lines: theoretical, methodological, disciplinary and interdisciplinary, mathematical modeling, knowledge transfer for decision making, and the development of institutional frameworks for complex environmental problems

The main theoretical contributions are a reconstruction of the Darwinian law of growth with reproduction, a reconstruction of the potential socio-ecological complexity from the elementary productive processes (including deriving structural models of communities connected to target groups of organisms; our case studies have been ectomycorrhizal and arbuscular mycorrhizal fungi), a conceptualization of the relationship between multi-scale productive processes at organismal, population and community scale and the standard nested hierarchy of ecological systems, and a general concept of resilience.

The methodological contributions are an integrated technique for knowledge mapping and conceptual analysis, a framework for integrated modeling of metals biogeochemistry based on the standard nested hierarchy of ecological systems, a highly complex methodology for upscaling ecological processes from a relatively smaller community scale to larger target scale, a simpler complementary framework for integrated modeling based on coupled biological and abiotic processes occurring at different scales, and a methodological framework to study the resilience of biogeochemical services to heavy metals stress.

The empirical contributions published by now are in two directions, one related to scale-dependent patterns of the distribution of organisms in contaminated areas, and one consisting of experimental investigations of biogeochemical processes in soil-plant systems. In the first direction, we found that the decrease of richness in contaminated sites compared to reference sites seemed to be larger as the scale of the organism was smaller, in each site, and a positive correlation between the coefficient of variation of mites' species richness (log-transformed) and the coefficient of variation of the scores extracted by PCA from in situ measurements of geochemical variables on the tailing surface in each station with a plot of 2 m². In the second direction, we investigated the leaching of elements from soil-plant systems, and the control of toxic elements, and P on plant oxidative stress. The main findings were that the inoculation with mycorrhizal fungi and/or plant growth-promoting bacteria changes the export of elements by water and plants and their relative importance, decreases the export of metals by plants although increases the biomass, depending also on the plant species, and decreases the concentrations of elements in leachate. The order of hydrological events with different water chemistry leading to leaching also controlled the total budgets of leached elements and their stoichiometric ratios. A portfolio of coupled experiments at pot, lysimeter, and plot scales revealed that P and toxic elements co-control oxidative stress, the control of the toxic elements and P on the oxidative stress depends on the age of the plants and the scale of the experiment, the nitrogen, phosphorus, and organic carbon in the soil were predictors of toxic elements accumulation in plants at the catchment scale, and the oxidative stress of *Agrostis capillaris* in the field was controlled by N and P but differently than at the pot scale. While these contributions focused on the effects of heavy metals and nutrients in the soil as independent variables, a complementary approach in the field was to look for the effect of morphometric plant traits on the properties of the vegetation cover controlling the water flow on a hillslope at the scale of the discretization units of the models (50x50 m). In this way, one could have information on the feedback effects of soil pollution on the transport of pollutants themselves, via the ecotoxicological effect on vegetation. We produced and published a TRL2 custom-oriented integrated tool-box of procedures/workflows and software modules for extraction of LIDAR metrics describing functional plant cover traits, deterministic models of processes describing the role of plants in the production of target ecosystem services, and coupled experimental scale-field scale investigations for validations and simulations.

The mathematical modeling started from the problem of including spatially explicit the role of vegetation in erosion models (and associated transport of heavy metals). This led to two complementary problems, one of porting data between scales (different discretization of the model), and one of the deterministic hydrological model with plant variables controlling the flow. Both of them were part of the larger research problem of predicting the long-distance effect of local pollution via ecotoxicological effects on plants and the transport of elements by water. We produced a data porting tool and demonstrated it on a model catchment using cellular automata of water flow without vegetation components. Then we produced a 1D model accounting for the role of plants on the water flowing over hill-slopes, using vegetation porosity as a plant variable, which could be measured in the field by LIDAR. The model was later extended by our mathematician colleagues to a 2D form with erosion processes.

The environmental management contributions are in a classic nested hierarchy approach (approaches for the integrated monitoring of emergent ecosystem services and restoration of a large alluvial island), and in a multi-scale process approach (triggering an accelerated succession in contaminated areas by inoculation with microorganisms -kind of an eco-remediation technique coupling site scale and landscape scale measures, and a complex approach for catalyzing the development of ecosystems of innovation for environmental services – using bottom-up and top-down measures). In this last contribution, we also make use of a large family of concepts of resilience relevant to managing socio-natural processes, particularly ecosystem services, at several scales (from organizations to the economic sector and the whole socio-ecological system, which is highly innovative as an integrated interdisciplinary tool.

I used the conceptual and methodological results in a simplified form also to organize the teaching, especially by classifying the epistemic strategies reducing the complexity of productive processes in the complementary natural and social domains and pointing out the complementarity and cultural/scientific co-evolution of ecophysiology, population ecology, various types of community ecology, ecosystem ecology and holistic approaches such as systems ecology and sustainability science. This led to a coherent and interconnected structure of four teaching disciplines in biological (general ecology) and environmental sciences (environmental deterioration, ecological monitoring, and management of biological diversity). At stake was to stimulate interdisciplinarity for solving complex missions instead of competition between experts specializing in various fields and sub-fields.

The future research lines of the research program are also on theoretical, methodological, empirical, mathematical modeling, environmental management, and institutional development directions. I am interested in the comparative ontology of biological and environmental sciences and the problem of how different is conceptualized time in different fields and sub-fields of research. The methodological direction is coupled with the institutional development of a Critical Zone Observatory for catchments with important industrial activity in their structure (including mining). Here I have an already funded Fulbright project for knowledge transfer from experienced institutions and researchers in the field of long-term ecological sites and a large-scale project draft (but with a consolidated network of organizations) for an innovation ecosystem oriented towards the development of a cumulative-impact assessment method in catchments with multiple types of impacts. In this framework, we will implement exploratory projects (for instance one dedicated to the resilience of biogeochemical services to climate change stress, using a stoichiometric approach of elements retention in transversal and longitudinal buffer zones) and projects for technology development (for instance developing to TRL3 the already mentioned LIDAR-based technology). In the scientific societies, I intend to focus on a better link between scientific knowledge from the research ecosystems and the know-how from the business ecosystems, which is critical for the improvement of environmental management in general, and of ecosystem services production in contaminated catchments in particular.

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