Scientific modelling can be accessible, interoperable and user friendly: An example for pasture and livestock modelling

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Abstract

This article describes the adaptation of a non-spatial model of pastureland dynamics, including vegetation life cycle, livestock management and nitrogen cycle, for use in a spatially explicit and modular modelling platform (k.LAB) dedicated to make data and models more interoperable. The aim is to deliver an existing, locally successful monolithic model, into a more modular, transparent and accessible approach to potential end users, regional managers, farmers and other stakeholders. This allows better usability and adaptability of the model beyond its originally intended geographical scope (the Cantabrian Region in the North of Spain). The original model, named Puerto, is developed in the R language and includes 1,491 lines of code divided into 13 script files and linked to 19 input tables. The spatiotemporal rewrite is structured around a set of 10 namespaces called PaL (Pasture and Livestock), which includes 198 interoperable but independent models. The end user chooses the spatial and temporal context of the analysis through an intuitive web-based user interface called k.Explorer. Each model can be called individually or in conjunction with the others, by querying any PaL-related concepts in a search bar. A scientific workflow is built as a response, which is run to produce result datasets and a report with information on the data sources and modelling processes used, delivering results with full transparency. We argue that this work demonstrates key steps needed to create more Findable, Accessible, Interoperable and Reusable (FAIR) models. This is particularly essential in environments as complex as agricultural systems, where multidisciplinary knowledge needs to be integrated across diverse spatial and temporal scales in order to understand complex and changing problems.

Introduction

Extensive farming, when paired with the conservation of natural vegetation, has historically been capable of sustaining food production in agricultural areas while maintaining ecosystems in good condition (European Environment Agency, 2004; Hendrickson et al., 2008; Lemaire et al., 2014). Since the 1950s, the increase of labour costs and beginning of widespread mechanisation and fertilizer application in the developed countries (Hayami & Ruttan, 1971; Billen, Lassaletta & Garnier, 2014) led to important changes such as the intensification of land use and the expansion of farming scale. This paradigm shift benefited from the European Union's Common Agricultural Policy (CAP) subsidies scheme. These policies simultaneously contributed to disincentivizing low-input land uses, causing land abandonment and afforestation in extensive agricultural areas, while also decreased agricultural commodity prices due to overproduction of intensive farming (Strijker, 2005; Pe'er et al., 2014).

Today, multiple human activities, such as urban development and tourism, are adding further pressures to ecosystems in addition to the increased productivity of intensive agriculture. These activities are moving pasture from mountain areas (Daugstad, Mier & Peña-Chocarro, 2014) to more accessible locations closer to urban centres (Fernández-Giménez & Fillat Estaque, 2012). Agricultural intensification in concentrated areas is threatening ecological sustainability and the provision of ecosystem services (van Zanten et al., 2014; Balbi et al., 2015). Such pressures are leading to ecosystem degradation by reducing biodiversity and threatening species linked to low-intensive agricultural production (Pimentel et al., 1992; Donald, Green & Heath, 2001; Henle et al., 2008), and by depleting plant resources, increasing contamination by leachate and soil erosion (Pimentel et al., 1995; Kumar et al., 2005; Tan, Lal & Wiebe, 2005; Rosegrant, Ringler & Zhu, 2009; Cordell, Drangert & White, 2009).

At the same time, farmland abandonment in rural areas can cause: (i) loss of woodland clearings, (ii) increased fuel loads and fire hazards and (iii) negative impacts on biological diversity (MacDonald et al., 2000; Casasús et al., 2007). The improvement of farmers' socio-economic conditions, extensive farming evolution and the balance with the environment require more efficient use of pastoral vegetation, including proper livestock management (grazing rotations by species and across time and space (Gibon, 2005)) and the controlled use of fire to preserve pasture availability (López, 2002; López-Sáez et al., 2016). The lack of quantitative tools for the analysis of such processes has been a major limitation for smarter and more sustainable management of mountain pastureland (Bernués et al., 2011).

Agricultural production systems have benefited from technological advances primarily developed for other industries such as mechanization, synthetic fertilizers, genetic engineering and automation. The information age brings new technology that can transform agriculture to low-input, high-efficiency and sustainable systems (Zhang, Wang & Wang, 2002; Balbi et al., 2015), such as cloud computing, remote sensing and artificial intelligence (Putfarken et al., 2008; Janssen et al., 2017; Kamilaris, Kartakoullis & Prenafeta-Boldú, 2017). The agricultural industry is now capable of gathering more comprehensive data on production variability across both space and time (Angelov, Iglesias & Corrales, 2018). Data and models can play an important role in sustainable agriculture, optimizing resources, providing key spatial-temporal information and

identifying the most appropriate and effective practices for better management (Vries, Teng & Metselaar, 1993).

One main issues preventing the full use of these new technologies in agricultural modelling arises from the multidimensional nature of needed data and models that are produced by different scientific domains from climatology to ecology and social sciences (Farina, 2000). Although an agricultural system can be designed for a specific purpose, such as crop production or animal breeding, understanding it requires knowledge from diverse fields (e.g., agricultural production, natural resources and human factors) (Argent, 2004; Jones et al., 2017). These components cannot be studied in isolation (Hieronymi, 2013), since they interact with each other and with their environment (Wallach et al., 2019).

The Puerto model (Busqué, 2014) was created in response to some of the above-mentioned agricultural systems challenges. The Puerto model was developed at the Centre for Agricultural Research and Training of Cantabria (CIFA) as part of its research on the structure, growth and utilization of pastures in the Cantabrian rangeland (Marcos, Lodos & Rodríguez-Arango, 2003). Puerto is an empirical dynamic model based on established biophysical relationships and constants between vegetation's life cycle (including growth, senescence death and litterfall), livestock grazing process (livestock ingestion, digestion, excretion and weight change) and the nitrogen cycle (nitrogen uptake, soil cycling and leaching). It evaluates existing nitrogen and grazing imbalances (under- or overgrazing) and their relationship with animal productivity. Puerto's four main goals are to: (i) provide a tool to support pastoral management; (ii) quantify and assess grazing system and nitrogen cycle imbalances; (iii) enable managers to develop strategies to resolve imbalances; and (iv) visualize the effects of management actions through scenarios. This model has proven to be a valuable tool for modelling pastureland in Cantabria and was used in several regional projects (Busqué, Fernández & Fernández, 2006; Bedia, Cabañas & Busqué, 2009) at different temporal and spatial scales. Although its reliability and usefulness have been validated and improved over the years, this model is essentially inaccessible to a non-initiated programming audience, and Cantabrian land managers must rely on technical consultancies to use it. Further, Puerto has always been used in isolation, never contributing to more comprehensive computational modelling workflows. We argue that these limitations arise from three choices made in Puerto's modelling philosophy, which are typical to modern environmental modelling:

1. the model's interface is not user friendly, it is coded in R and is only usable by advanced R users, with each run requiring the modification of source files to point to input data;
2. it is monolithic and cumbersome (1,491 lines of code divided into 13 script files and linked to 19 input tables), which makes understanding of its computational workflow difficult;
3. it lacks transparency in the definition of multiple parameters, which lack semantics and appear as acronyms defined as fixed values in the code.

These limitations are common practice in most current scientific modelling exercises, which are not developed as Findable, Accessible, Interoperable and Reusable (FAIR) scientific artifacts (Parker et al., 2002; Wilkinson et al., 2016).At the same time, the importance of accessibility, interoperability and reusability of models and resources is increasingly recognized by modelling communities. While novel approaches are available to facilitate that (van Ittersum et al., 2008; Verburg, Eickhout & van Meijl, 2008; Ewert et al., 2009; Peckham, Hutton & Norris, 2013), none has yet reached the necessary levels of practicality, generality and community acceptance to make a dent into a still widespread model and data curation malpractice.

The aim of this article is to demonstrate the implementation of Puerto into a semantic-first modelling approach, which aims to better achieve the FAIR criteria. This redesign makes the models, from now on referred to as the Pasture and Livestock (PaL) namespace(s), and their results more accessible to end users such as farmers and policy-makers. PaL is written in k.IM, a semantic modelling language designed for the k.LAB modelling platform. K.LAB is powered by artificial intelligence, and in particular by machine reasoning, for the interoperability of data and models (Villa, 2007; Villa et al., 2017). PaL will be part of ARIES (ARtificial Intelligence for Environment and Sustainability), the best known application of k.LAB (Villa et al., 2014; Bagstad et al., 2014). ARIES is an open-source platform for interoperable models and data backed by an international and multidisciplinary community, producing a web-based platform linking, synthesizing and providing easy access to integrated knowledge to address a wide range of sustainability problems. In this article, we describe the PaL implementation and its application to a study area in Northern Spain. In the methods section, we describe the key requirements and distinctions of the semantic modelling approach as applied to Puerto and PaL. Our results compare the outputs of Puerto and PaL when applied to a region in eastern Cantabria and illustrate key end-user features of the k.LAB modelling environment. Finally, our discussion and conclusions describe implications of this approach for environmental modelling more generally and agricultural modelling specifically.

Materials & Methods

Study area

The study area was selected to match the location where the original model has been most frequently applied. The Pas, Miera, and Ason watersheds (43°20′36″N, 3°44′28″W) are adjacent to the Cantabrian mountain range in the eastern Cantabria region, covering a terrestrial, riverine and estuarine system of 173,700 ha (Fig. 1). This study area, with its river basins draining into the Cantabrian Sea, has a temperate hyper-oceanic climate, defined mainly by mild temperatures and high humidity due to regular precipitation and fog. Although the average annual temperature is 14º C, snow is common in the mountains from late autumn to early spring.

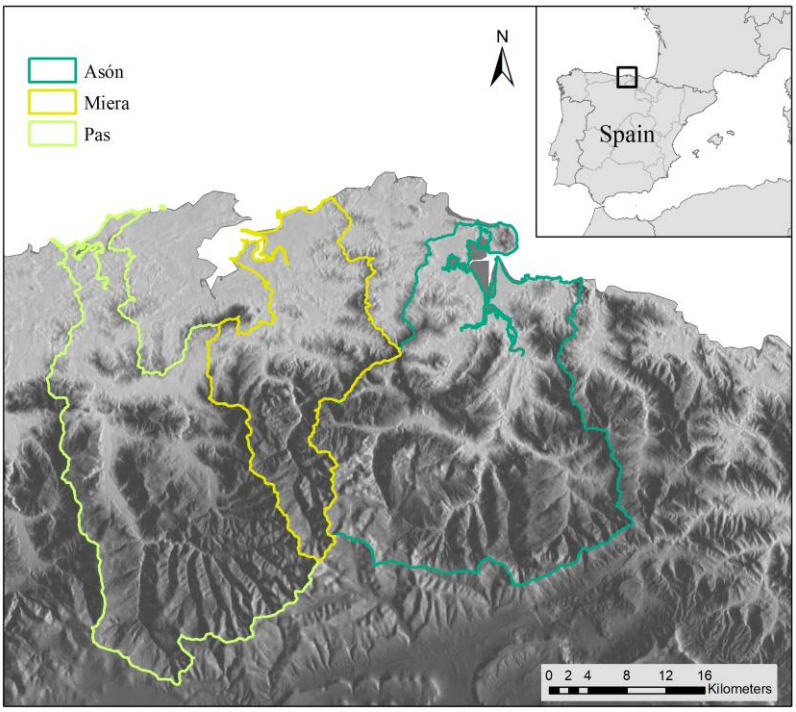


Figure 1 Location of the case study, the Pas, Miera and Ason in watersheds in northern Spain.

This unique landscape is a product of the combined use of fire and livestock grazing for over 400 years (Montserrat & Fillat, 1990). As a consequence, almost 75% of the landscape consists of managed grasslands and shrublands, relegating mature forests to headwater basins and marginal lands with low agricultural value on steeper slopes. The pastoral lands are dominated by nine pastureland types and multiple livestock types, including cattle and mares (Fig. 2).

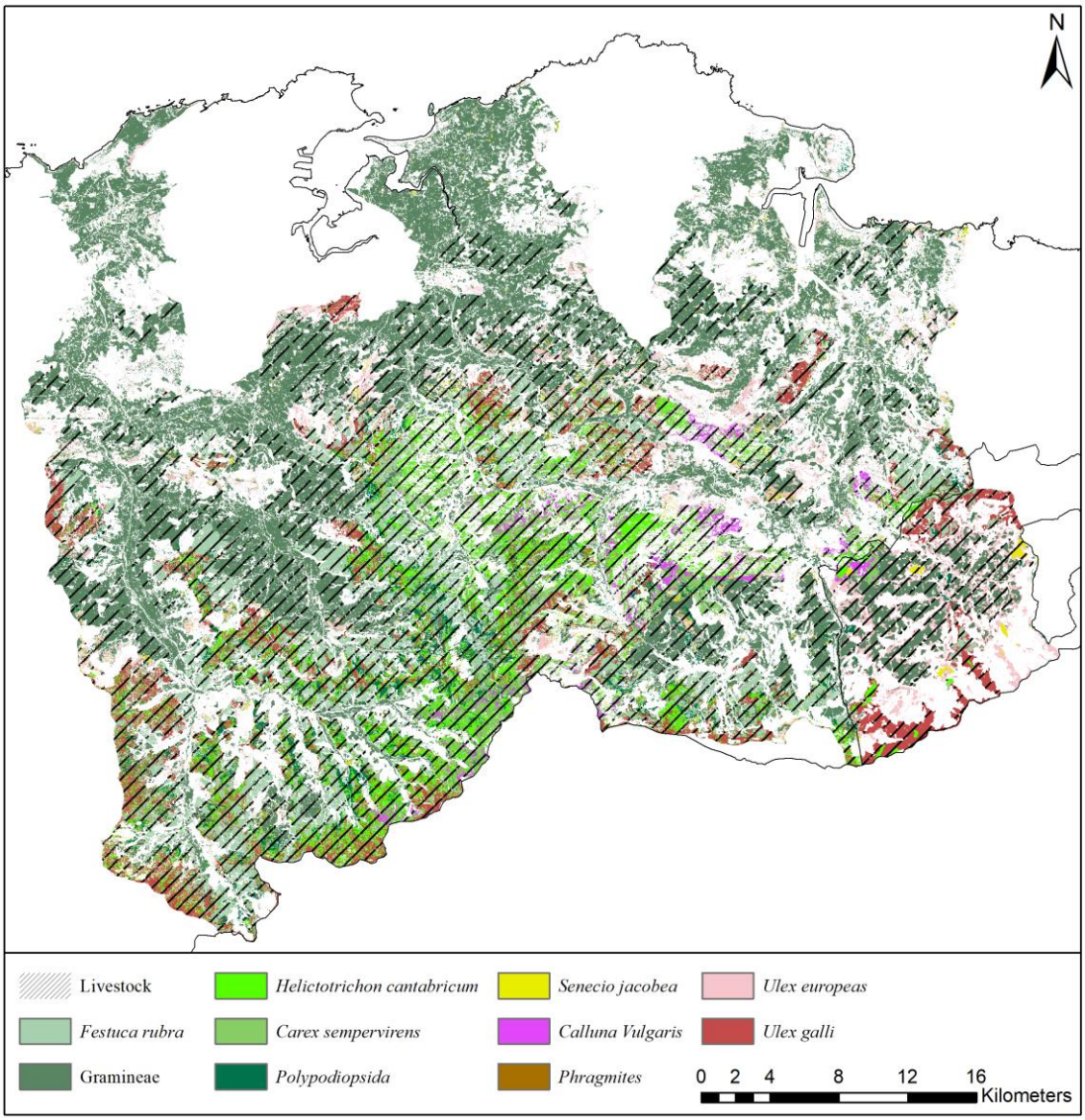


Figure 2 Distribution of livestock and pastureland types in the case study.

There are three climatic sub-regions influenced by the mountain ranges (including the "Picos de Europa" mountain range) and the ocean. The coastal zone, which is under high human pressure, has widespread grasslands and eucalyptus plantations (*Eucalyptus globulus*) on gentle slopes. The central part is the most rugged, with elevation ranging between 100-1200 m a.s.l., dominated by semi-extensive pastures grazed by livestock. Large areas are occupied by *Ulex europaeus*, *Erica tetralix*, *Pteridium aquilinum* or *Carex asturica* and productive plantations of *Pinus radiata*. The mountain ranges in the south, with steep slopes and a more complex management, have a great diversity of plant communities used by livestock.

Model description

The Puerto Model

Puerto's main code can be divided into four components. The first component consists of climate, topography and soil, which affect vegetation growth and livestock ingestion of forage. The second part captures the entire life cycle of vegetation including growth, senescence and litterfall. The third component focuses on the nitrogen cycle, including mineralization, plant reabsorption and leaching. Finally, the last component describes grazing, ingestion, weight variation, and excretion of manure and urine of livestock.

Puerto needs with a substantial set of input data and parameters to be initialized, derived from literature or field measurements, related to vegetation, soil, climate, the nitrogen cycle and, optionally, livestock management. In total, it requires 56 data inputs as tables and 27 constant parameters. After initialization, it executes dynamic transitions over a modeller-defined temporal horizon, by daily timestep for entire years, simulating the management of pastoral systems. Outputs are produced as R tables associated with each management unit of pastureland, such tables can be transformed into vector data by a technician proficient in Geographical Information System (GIS) software so that the results can be displayed spatially.

The Pasture and Livestock namespaces

The Pasture and Livestock (PaL) namespaces provide an integrated modelling framework for the Puerto model designed to better adhere to the FAIR Principles while making the model more accessible for nontechnical users. They operate under the k.LAB open-source software platform and k.IM semantic annotation and modelling language (Table 1) (Villa, 2007; Villa et al., 2017) the only programming language using semantics as the primary organizational principle. The k.LAB platform connects a network of data, models, and semantic resources distributed globally on the semantic web. The code of PaL in k.IM language is available online at the Bitbucket repository (https://bitbucket.org/integratedmodelling/im.ecology.grassland.livestock/).

Semantics are used to annotate all resources (i.e., data and model components) in PaL namespaces, using a well-established and expert-vetted vocabulary (Arp, Smith & Spear, 2015). The concepts used to build the model components and to represent data are not built specifically for a model, but come from a shared, network-accessible worldview which provides uniform definitions encompassing concepts and the relationships between them. The use of semantics to describe data and models enables an artificial intelligent algorithm to build meaningful connections between inputs and outputs by making inferences and ranking each model component for the best fit to the concepts required as input. Any resource available in k.LAB can be automatically and accurately interpreted by a receiving system (Martínez-López et al., 2019) as a response to a query. Such a modelling approach is modular by design, parsimonious and logically consistent, which makes the knowledge contained in the resources unambiguously and more transparently sharable while making the model more accessible for non-technical users. By providing a web-based query tool with intuitive spatial and temporal context selection (k.Explorer), the scientific information in models and data can be displayed in understandable and accessible fashion, without compromising on rigor and machine-readability of results.

Table 1 Comparison between R and k.IM language for the "Potential above ground biomass caused by growth" model. Colour coding in the k.IM language denotes different types of semantic meaning: brown denotes processes, green qualities, and blue attributes that can be combined to describe semantically meaningful scientific observables (Villa et al., 2017).

Concept	**Language**	**Code**
Potential above ground biomass caused by growth	R	setkey(Fhijt,com2);setkey(pl1$B3,com) T1<-pl1$B3[Fhijt][,.(IDMancha,com=i.com,com2=com,t,diay,FT,FR,FH,FTRH,xi,ph,prPerc, crecpot=FTRH*xi*ph)]
	k.IM	**model** im:Potential ecology:AboveGroundBiomass **caused by** biology:Growth **in** g/m^2 'AboveGroundBiomass caused by Potential Growth' **observing** im:Maximum ecology:Biomass **caused by** biology:Growth **in** g/m^2 **named** xf, **percentage of** ecology:Vegetation biology:Growth **caused by** *ecology:VegetationLimitingFactor* **named** ftrh, **occurrence of** ecology.incubation:PhenologyActivity **named** ph **set to** [xf*ftrh*ph];

PaL is structured into 10 k.IM code files (namespaces), which integrate multiple data and models related to climatic growth limitations, vegetation's life cycle, livestock grazing and the nitrogen cycle. PaL generates spatially explicit outputs at user-specified temporal and spatial scales. In case the user does not want to change the output characteristics, a set of default output properties is defined. These features are: spatial resolution of 50 meters, daily time step, time period between 2018 and 2050. Each model finds its input data on the network, previously annotated from international and recognized data providers from regional to global scale and from the literature; the choice of data is done by the k.LAB AI based on fit to the context and the scale chosen by the user. The user can also provide data to override any of the PaL components, be them input datasets or computational logics for each of the concepts involved in the model. Outputs include multiple open-source models, algorithms and spatial outputs of primary interest to pastureland managers. For example, selected results include the amount of above and below ground biomass of vegetation, concentration of nitrogen leaching or livestock weight gain. These outputs can be used for quantitative analysis of pastureland sustainability (or assessment of farmland requirements and tradeoffs). The set of namespaces in PaL consists of 10 thematic namespaces that describe the interactions between vegetation, animals and their environment (Fig. 3, Table 2).

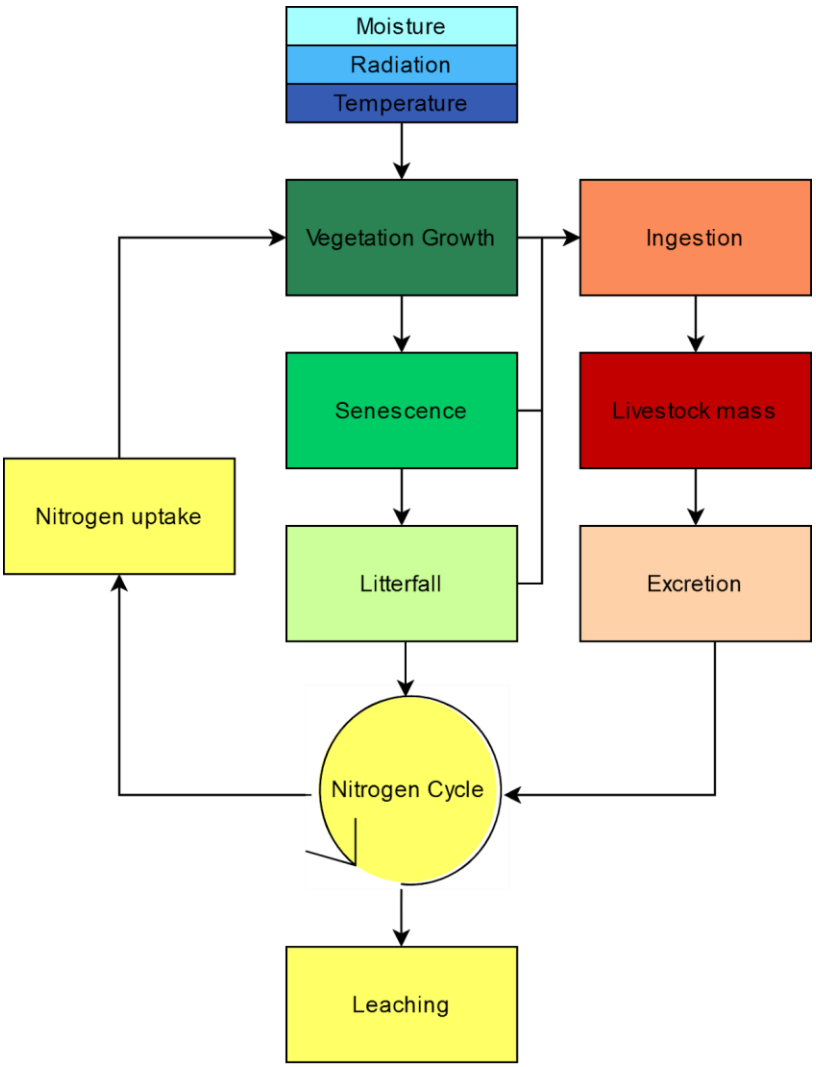


Figure 3 Workflow of PaL namespaces related to climatic growth limitations, vegetation life's cycle, livestock grazing and nitrogen cycle

Table 2 Description of PaL namespaces related to climatic growth limitations, vegetation life cycle, livestock grazing and nitrogen cycle.

Namespace	**Description**
Moisture	All processes involving the limitation of vegetation growth due to soil moisture.
Radiation	All processes involving the limitation of vegetation growth due to solar radiation.
Temperature	All processes involving the limitation of vegetation growth due to atmospheric temperature.
Ingestion	All processes related to grazing and digestion.
Livestock mass	Set of models related to livestock weight change.
Excretion	The process of livestock solid and liquid manure.

Nitrogen	Nitrogen concentration and nitrogen proportions in the N-cycle (including leaching and nitrogen uptake)
Vegetation Growth	Calculation of potential and actual vegetation growth depending on limiting abiotic factors
Senescence	Senescence process and quantity of the remaining, living biomass
Litterfall	Process related to dead plant material (harvesting, litterfall and dead biomass)

Each namespace, in turn, is composed of several model components that each describe one concept involved in the PaL logical structure, for a total of 198 models that are logically consistent, self-contained and can run independently. The dependencies between models are defined at the purely logical level as concepts, and are resolved at the moment of execution by the k.LAB engine: if needed, the modeler can influence the choice using well-defined scoping rules. When dependencies cannot be satisfied within the same namespace or project, or within user-provided data and models, the k.LAB engine will look for ways to satisfy them by looking up models from the network and ranking them for appropriateness to the context. The ability to access the entire k.LAB semantic web enacts a fully distributed, interoperable chain of computation that minimizes the effort involved in producing results without compromising on quality, transparency or traceability.

In this particular implementation, all models are deterministic, using equations and look-up tables derived from the literature and expert knowledge. For example, the simplest namespace, the Radiation module (Table 2), is composed of the "Solar Radiation over Vegetation" model, which includes three different component models. Each of these sub-models generates an output and, at the same time, is interoperable with others to generate more complex models, such as the "Solar Radiation limiting factor causing Vegetation Growth" model (Fig 4).

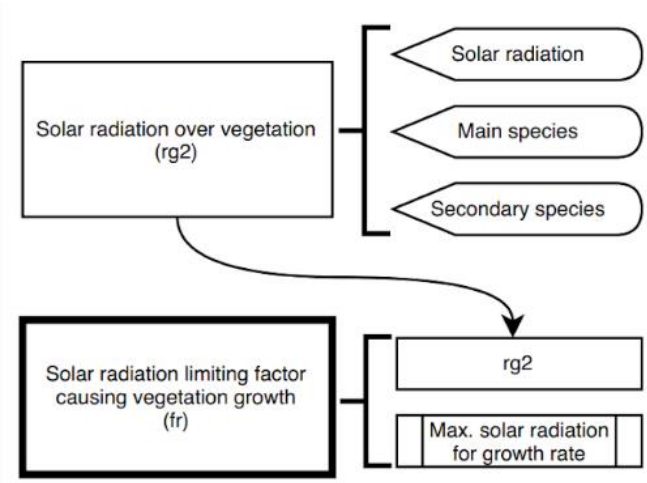


Figure 4 Workflows of "Solar Radiation over Vegetation" and "Solar Radiation limiting factor causing Vegetation Growth" (diagram on the left). The figure shows the interaction between them and the models that act as inputs. A total of six models are involved in this process.

In addition, each of these models interact with other namespaces. For example, Figure 5 shows the model of "*Nitrogen in living aboveground biomass caused by cattle solid manure*" from the 'Excretion' namespace (Table 2), which is composed of three different models that are developed within other namespaces. For example, "*Proportion of Living AboveGround Biomass in Cattle Digestion*" is located within the "*Livestock mass"* namespace while '*Proportion of Nitrogen in Living AboveGround Biomass* 'is in the "*Nitrogen"* namespace and '*Living AboveGround Biomass causing Cattle Ingestion'* in "*Ingestion.*"

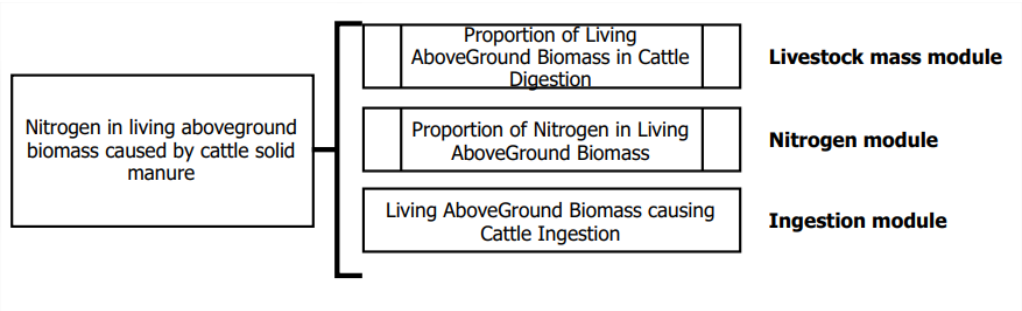


Figure 5 Workflow of "Nitrogen in living above ground biomass caused by cattle solid manure" model from excretion namespace composed of three models related to namespaces of livestock mass, nitrogen and ingestion.

In this way, each namespace is composed of models that can run independently, unlike Puerto's original monolithic structure. This semantic-driven interoperability allows each model to interoperate with models from the same namespace or from different ones, according to the projects available in the k.LAB resource network and ARIES project. For example, the nitrogen leaching model can interoperate with a runoff model from an independently developed hydrological modelling project, automatically connecting knowledge across these projects. Consistency is maintained through the semantic infrastructure, generating an integrated response to user queries and scenarios.

PaL namespaces use spatially explicit data (raster and vector) and look-up tables as input files. Most of the data come from field-validated expert knowledge, including for instance the raster dataset of main pastureland species. Open-source data from global to local scale with different temporalities can complement the model when local parameters are missing, such as the raster data describing soil texture. Based on the user-defined spatial and temporal context, k.LAB changes the spatial resolution and harmonizes the spatial reference of input data on the fly. Each input dataset can thus have different spatial and temporal resolution, which are automatically mediated by the system based on a given user query.

To use the model in dynamic mode, PaL requires climate data for the entire model timeline. The rest of the inputs are only needed at initialization, because PaL generates the transitions based on the declared algorithms.

Results

The main result of PaL, the k.LAB-compatible recoded version of Puerto, is the ability to calculate any of the 198 component models independently and quickly; making them reliably available to stakeholders with minimal work (depending on the model, from seconds to 6

minutes at 50 meters' spatial resolution). The results generate parameters with self-explanatory variable names, thanks to the k.IM semantic language (Table 1). Both the data sources and the algorithms used as inputs for the results are automatically generated, and are publicly available and downloadable, giving the users additional information to interpret and communicate model results and maintain quality control (see "End-user features" below).

In the following sections, we describe the main outputs of each PaL namespace for the Cantabrian Pas, Miera, and Ason watersheds, thus emphasizing the importance of taking a systems approach in agricultural modelling. The main outputs are temporally explicit raster data produced on demand for the context of analysis (including the selected spatial and temporal scales). As the graphical outputs of the Puerto model are limited, predetermined and based on a monolithic code structure, it is difficult to directly compare all the PaL model results with those of the original Puerto model. However, we can validate some of the PaL results that directly match the final Puerto outputs. For this, the Puerto results had to be postprocessed to give them spatial dimension, the R-generated outputs are not spatially explicit.

The PaL models outputs have been run at the default spatial resolution of 50 meters using mean climate values for May 2018. The entire list of the models is in the Supplementary Material 1 and the code in Bitbucket repository (https://bitbucket.org/integratedmodelling/im.ecology.grassland.livestock/).

Model outputs

Factors limiting Vegetation Growth

The "Factors limiting Vegetation Growth" model is composed of three main models: Moisture, Radiation, Temperature and Nitrogen (Fig. 6). These dynamic models quantify climatic and soil conditions' control of potential vegetation growth. Vegetation growth follows an annual cycle influenced by seasonal patterns and extreme weather events. These models thus depend on time and can help to forecast changes in vegetation behaviour with climate change, as seasons shift and extreme events become more frequent. Moreover, factors limiting vegetation growth are affected by the spatial distribution of vegetation, which is influenced for example by the presence of mountain ranges. These effects are complex: soil characteristics affect water content, aspect affects shade patterns and the incidence of radiation, and elevation affects the temperatures and precipitation levels to which plants are exposed.

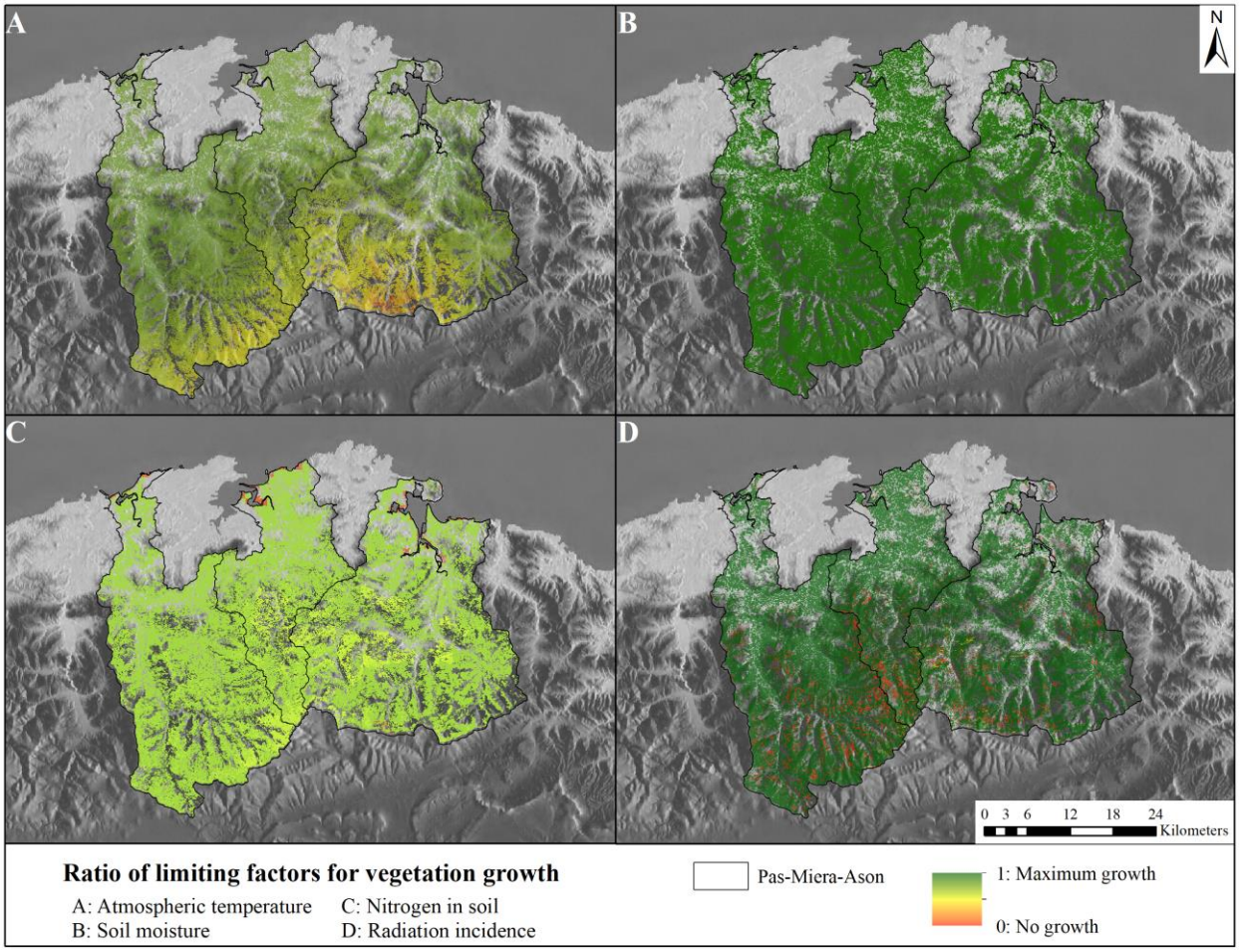


Figure 3 Modelled results of vegetation limiting factors for May 2018; all outputs range from 0 (no growth) to 1 (maximum growth). A) Atmospheric Temperature limitation. B Soil Moisture limitation. C) Soil Nitrogen limitation. D) Solar Radiation Incidence limitation.

Figure 6 shows the influence of each variable managed vegetation growth in May 2018. While soil moisture (Fig. 6B) and solar radiation incidence (Fig. 6D) positively affect vegetation growth (except in some shaded areas in the case of solar radiation incidence), temperature (Fig. 6A) has an increasing influence with elevation and nitrogen is the most uniformly limiting factor (Fig. 6C).

Puerto does not provide these results in spatial form. An expert in R can extract the R internal table (Table 3), which contains outputs of the limiting factor for climate. The table indicates:

- the observed plot ("IDMancha"),
- the code of the main (“com”) and overstory (“com2”) vegetation, in case there is one,
- the timeline, starting at the first of January of the year determined by the modeller,
- the mean parameter corresponding to Temperature (“FT”), Radiation (“FR”), Moisture (“FH”) and Nitrogen (“FN”) as vegetation limiting factor for each observed plot, vegetation type, time.

In this case, users can link the plot identification to a vector dataset to know where the plots are located. We do not know the distribution of vegetation within each plot.

Table 3 Sample Vegetation Limiting Factor output from R table of Puerto model.

IDMancha	com	com2	t	FT	FR	FH	FN
442	9	9	1	0.701909	0.164	1	0.5
442	14	14	1	0.701909	0.164	1	0.65
442	28	28	1	0.701909	0.164	1	0.65
458	7	7	1	0.701909	0.116	1	0.65
458	13	13	1	0.701909	0.116	1	0.5

Vegetation

The entire vegetation life cycle - including growth, senescence, and litterfall - is composed of three different namespaces which include 44 component models. Vegetation life cycle is affected not only by climate, but also by livestock activity, nutrient uptake and human intervention, in particular by harvesting or fertilization cycles. With PaL, we can estimate the evolution of the parameters in each grid cell over time, depending on the type of vegetation. This group of models can be run with or without human and animal influence.

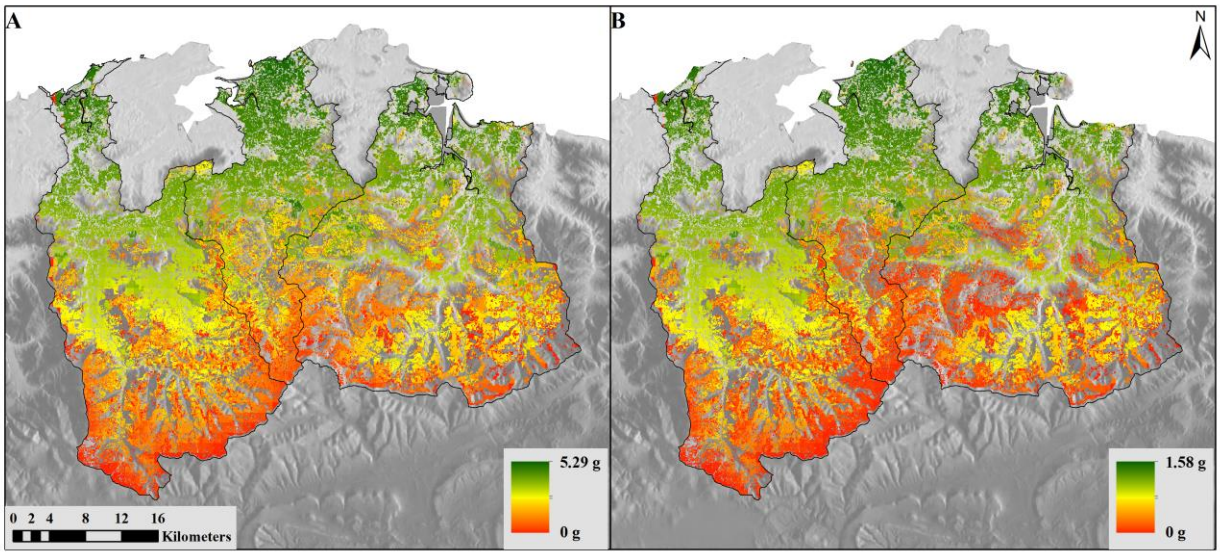


Figure 4 A) Potential Growth causing AboveGround Biomass model in grams/day and B) Growth causing AboveGround Biomass model in grams/day (Cantabrian case study, May 2018).

Figure 7A shows the potential vegetation growth under climatic factors (temperature, solar radiation and soil moisture). The results of Figure 7B are the actual growth model, based on potential growth but also taking into account nitrogen limitation and the influence of livestock on the grazing areas. Two notable trends emerge – first, that maximum potential daily vegetation growth is 5.29 grams per day, while actual growth is 1.58 grams per day. Second, the distribution

of vegetation growth is heterogeneous, decreasing in mountainous areas than flatter areas (Figure 7B).

Puerto vegetation growth outputs include tables in R or graphical bar and line graph outputs (Fig. 8). The information on monthly average vegetation growth (bars) and livestock ingestion (line) are shown for a period of years determined by the modeller, in this case, 5 years. Results are aspatial, as compared to the spatially explicit outputs for a flexible, user-defined time period in PaL.

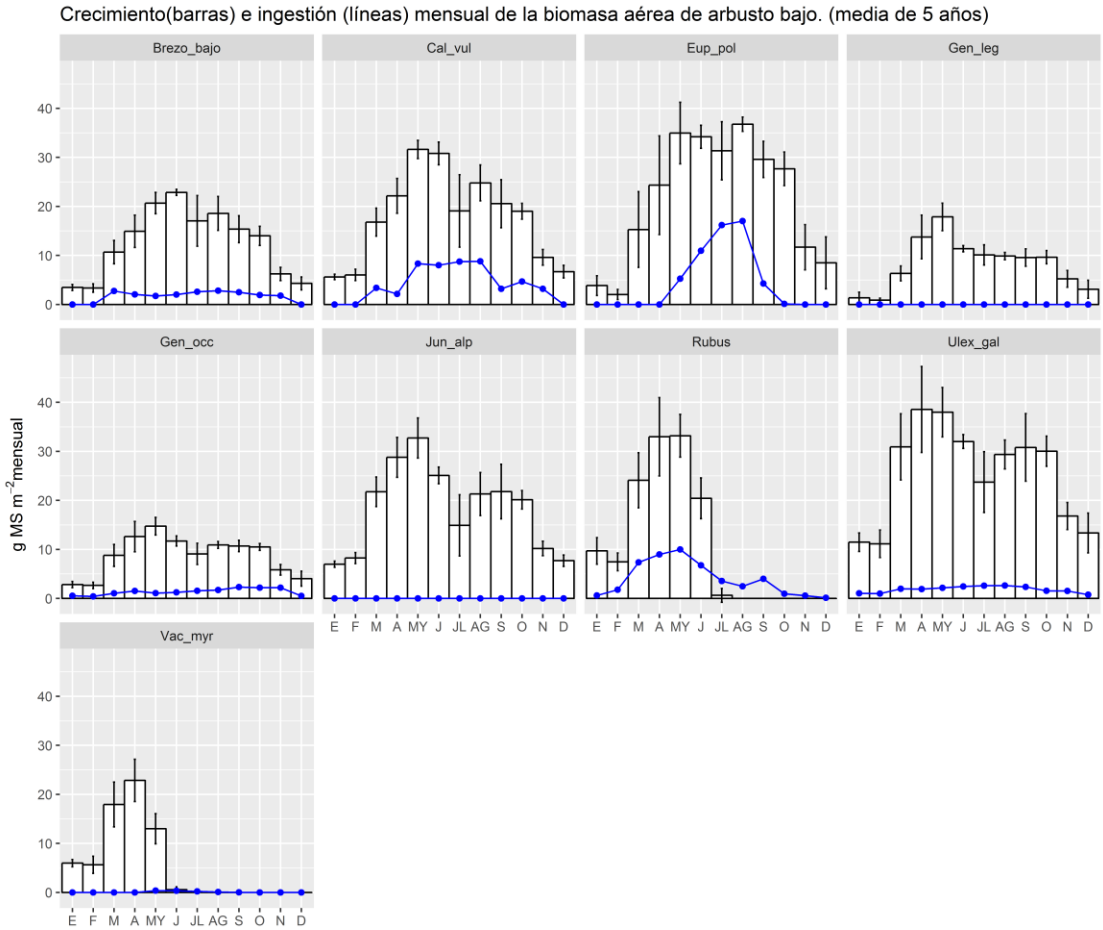


Figure 5 Puerto output (not spatially explicit). Mean monthly vegetation Growth and Ingestion model outputs of Puerto, for nine pasture types (see Fig. 2).

Livestock

The namespaces related to intake (Ingestion namespace), excretion (Excretion namespace) and variation of body mass (Livestock mass) of livestock include a total of 55 component models, including both cattle and mares. Key outputs include sustainability of the exploitation of pastures, biomass intake, the variation of livestock weight and the amount of excrement returned to the environment. Based on modelled livestock mass variation for cattle (Fig. 9A) and mares (Fig. 9B), cattle are more affected by altitude and vegetation availability than mares.

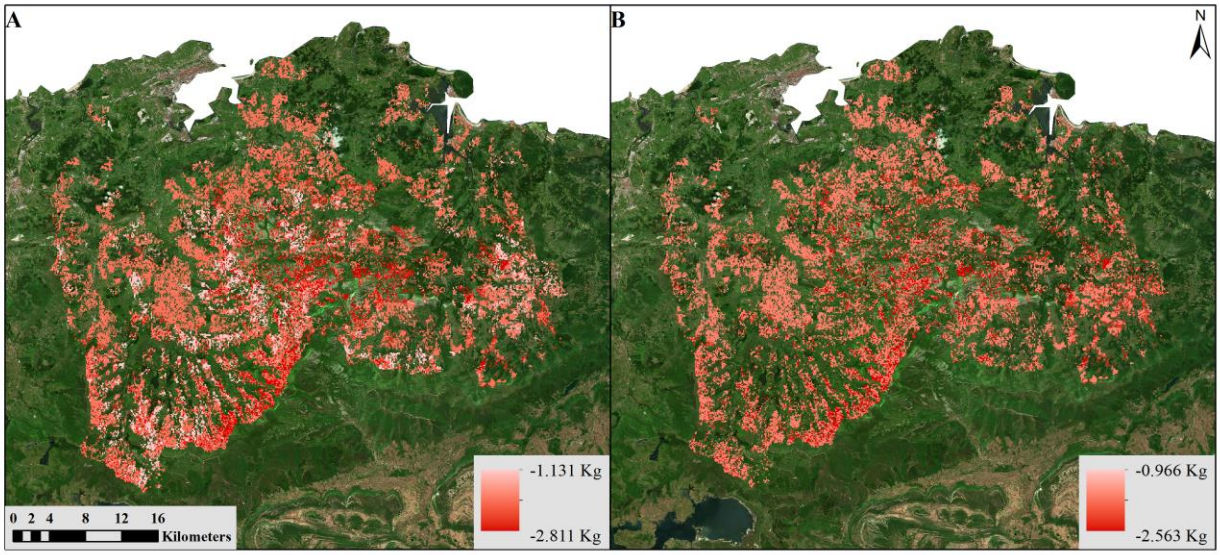


Figure 6 Livestock mass variation of (A) Cattle and (B) Mares in kg/day, May 2018.

Results depend not only on vegetation type and life cycle, but also on the estimated number of animals on each hectare of land, competition between them, accessibility to the vegetation, and topography, among other influences.

The Puerto version result for livestock (Figure 10) is the cumulative livestock mass variation per hectare and year for both mares ("Equino") and cattle ("Vacuno"). Results are aggregated by grazing unit but are not spatially distributed as in the PaL model.

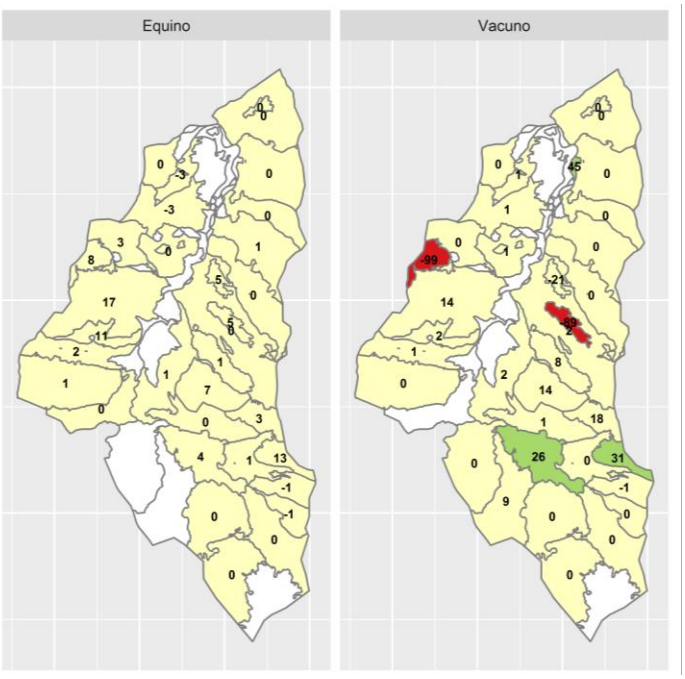


Figure 7 Cumulative livestock mass variation per hectare and year in Puerto output (no spatially explicit).

Nitrogen Cycle

The nitrogen cycle namespace includes all the models related to nitrogen in its different states and forms. The calculation of the nitrogen content in senesced leaves, mineral nitrogen present in the soil, nitrogen in livestock excrement and that used for plants are some of the models called on by this namespace. An interesting part of this namespace is the "Nitrogen leaching" model (Fig. 11), which can interact with the models related to the water cycle within k.LAB for future studies of water quality and pasture management. The output of Puerto is an internal R table as Table 3.

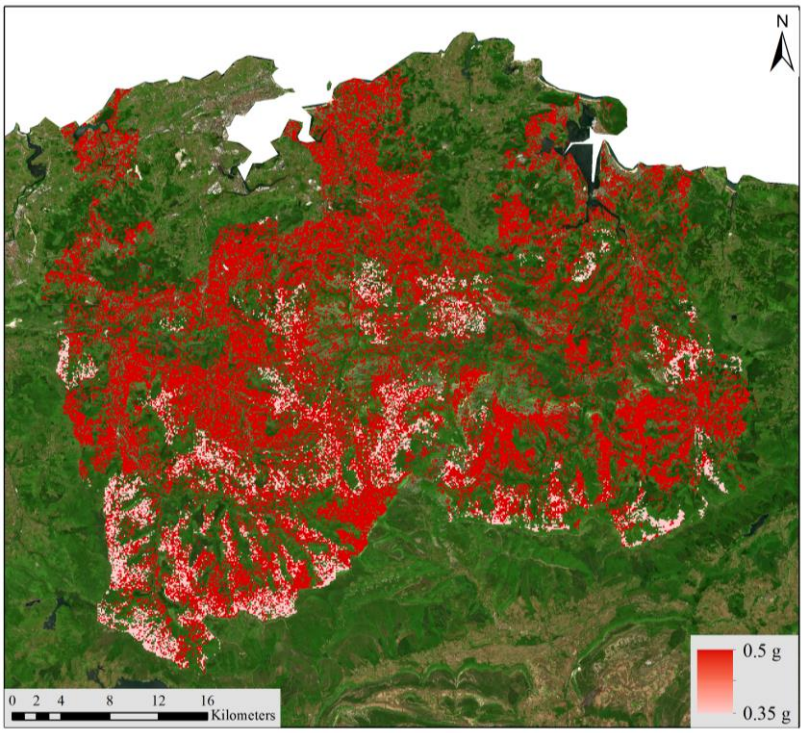


Figure 8 Nitrogen Leaching output model in grams of nitrogen mass.

<u>End-user features</u>

Output maps

The first set of outputs provided to the end-user is a series of temporally explicit maps. Temporally dynamic outputs can be viewed using the “play” button at the bottom of the menu on the left side of Figure 12. A user can also view all the models computed as dependencies of the requested model. All results (main model and dependent models) can be downloaded in geotiff format or as an image. In addition, basic information is provided such as total grid size, cell size, temporality, total observed model area, symbology and colour ramp style with labelling and a histogram for each of the model’s inputs and outputs (Fig. 13).

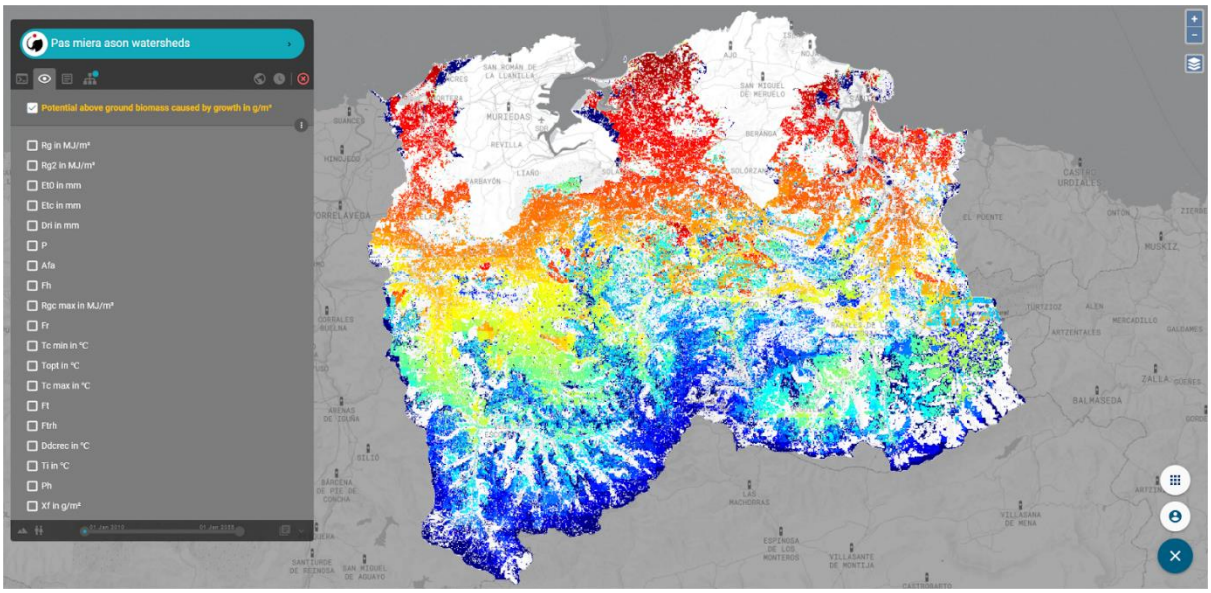


Figure 9 Output of the model "Potential above ground biomass caused by growth" and its model dependencies.

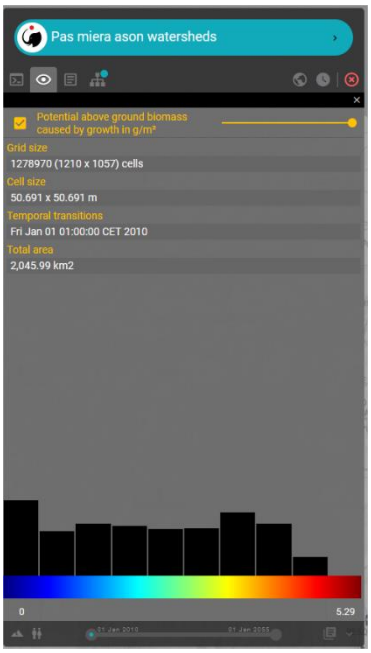


Figure 10 Information related to each model output or dependency.

Data flow

k.LAB creates an interactive data flow of the requested model that is built on the fly (Fig. 14). Thus, all the models and dependencies are shown. By clicking on each block of the data flow, more information is provided describing:

1) for resources (data sources), basic information about the data source. This is based on metadata contributed by users who have previously contributed data resources to the k.LAB network, including links back to the original data source; Fig. 15.A);
2) for tables, each table's composition (Fig. 15.B); and
3) for parameterised models, the expression or algorithm used (Fig. 15.C).

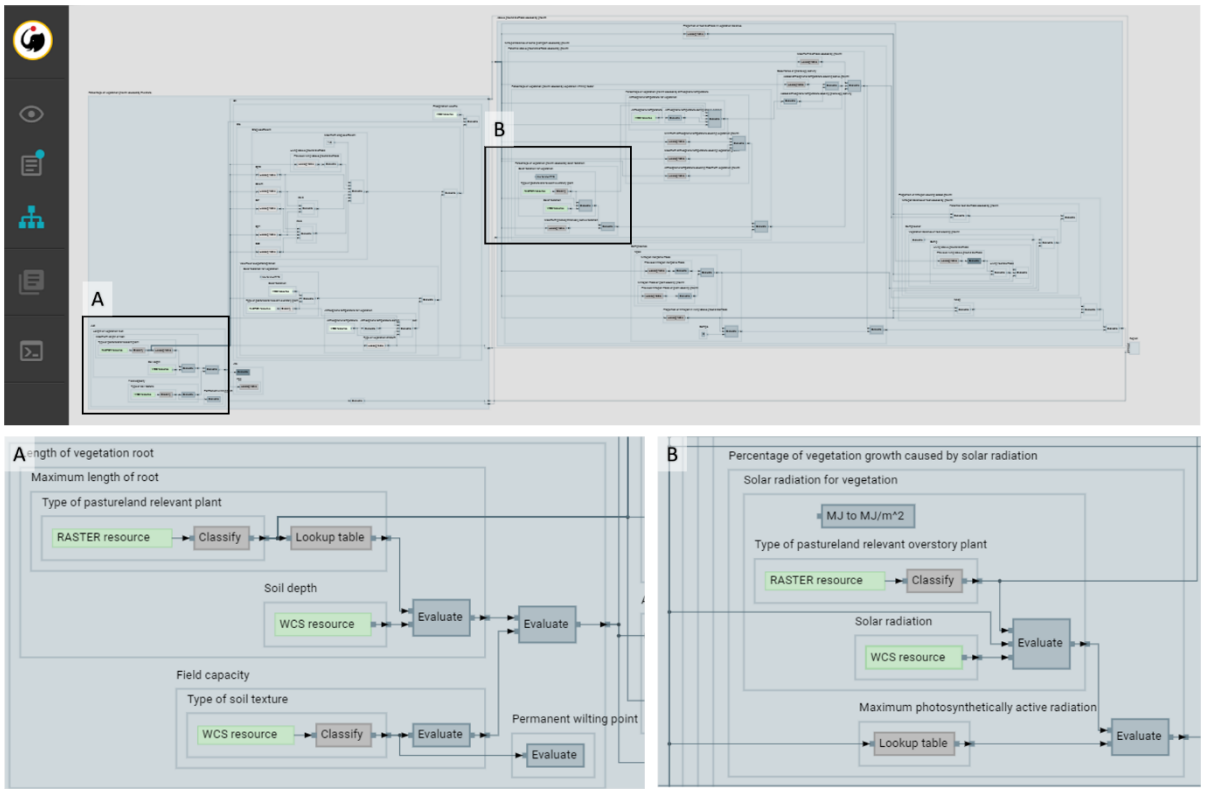


Figure 11 Workflow of "Above ground biomass caused by growth" model created on the fly as the model runs.

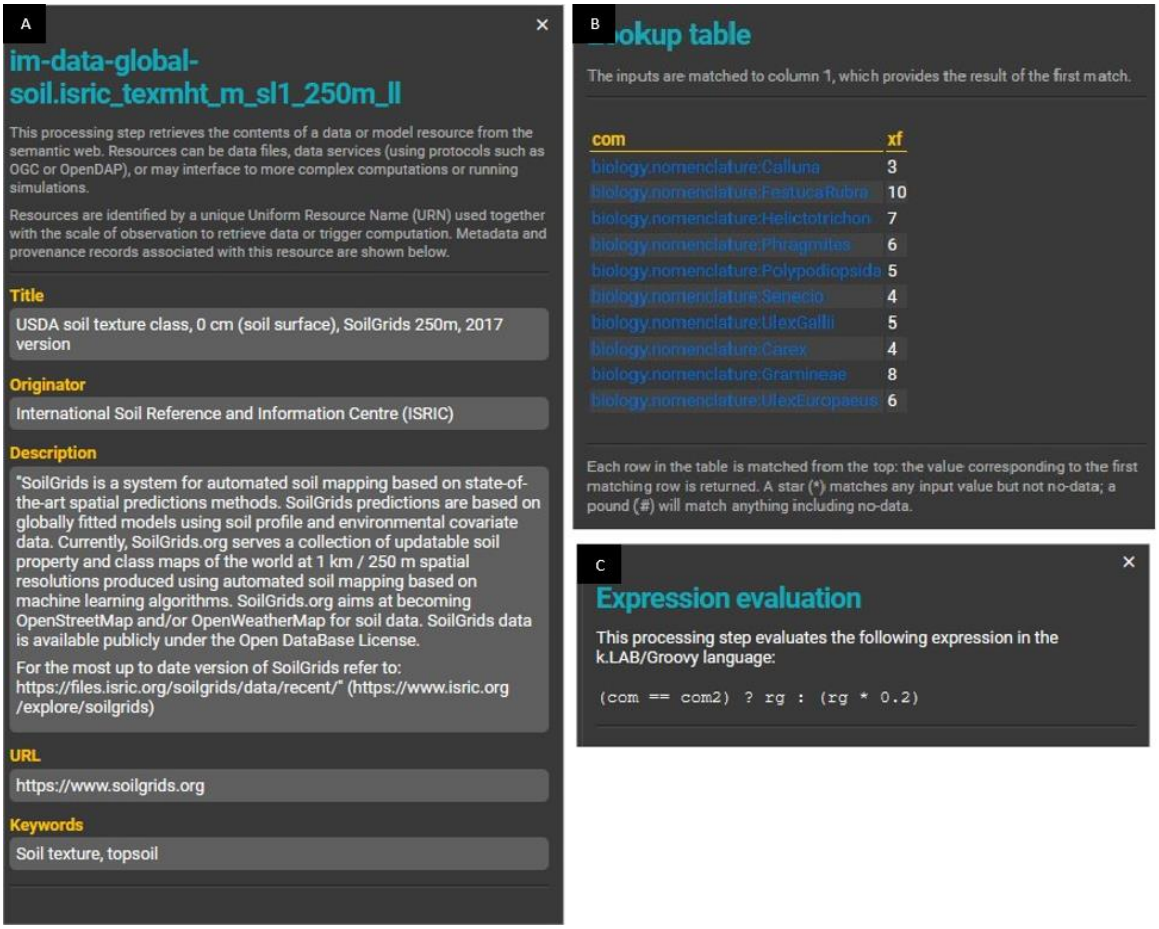
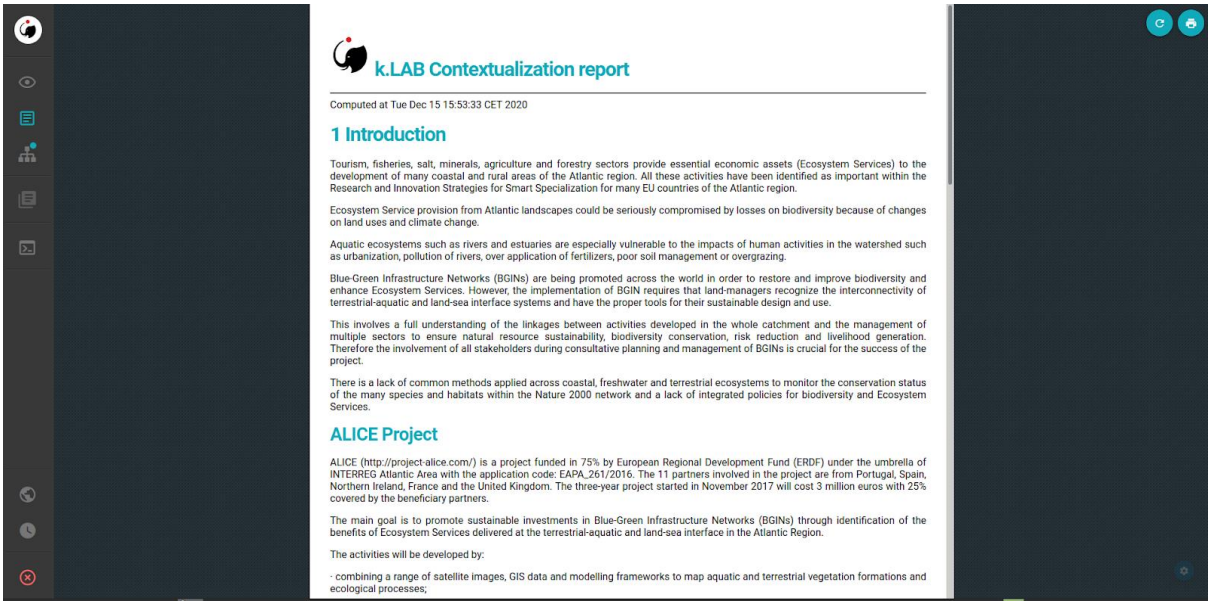


Figure 12 Additional workflow component views. A) Information related to resources (i.e., data), B) information related to a look-up table, C) information related to a model algorithm.

Report

A printable report (Fig.14) is also created on the fly, collecting documentation from each model being run and adapting it to the results being calculated. Basic documentation about each model component is entered by each model's contributor in k.LAB, which is called when the model is run and assembled into the report; the modellers' documentation uses a template language that makes it possible to "react" to the results. This reporting facility complements the workflow graph in making the system transparent and reliable. The report follows the standard structure of a scientific article (introduction, methods, results, discussion, conclusion and references). It can include tables, figures or other elements, depending on the model, and can be downloaded in .pdf format.



k.LAB Contextualization report

Computed at Tue Dec 15 15:53:33 CET 2020

1 Introduction

Tourism, fisheries, salt, minerals, agriculture and forestry sectors provide essential economic assets (Ecosystem Services) to the development of many coastal and rural areas of the Atlantic region. All these activities have been identified as important within the Research and Innovation Strategies for Smart Specialization for many EU countries of the Atlantic region.

Ecosystem Service provision from Atlantic landscapes could be seriously compromised by losses on biodiversity because of changes on land uses and climate change.

Aquatic ecosystems such as rivers and estuaries are especially vulnerable to the impacts of human activities in the watershed such as urbanization, pollution of rivers, over application of fertilizers, poor soil management or overgrazing.

Blue-Green Infrastructure Networks (BGINs) are being promoted across the world in order to restore and improve biodiversity and enhance Ecosystem Services. However, the implementation of BGIN requires that land-managers recognize the interconnectivity of terrestrial-aquatic and land-sea interface systems and have the proper tools for their sustainable design and use.

This involves a full understanding of the linkages between activities developed in the whole catchment and the management of multiple sectors to ensure natural resource sustainability, biodiversity conservation, risk reduction and livelihood generation. Therefore the involvement of all stakeholders during consultative planning and management of BGINs is crucial for the success of the project.

There is a lack of common methods applied across coastal, freshwater and terrestrial ecosystems to monitor the conservation status of the many species and habitats within the Nature 2000 network and a lack of integrated policies for biodiversity and Ecosystem Services.

ALICE Project

ALICE (http://project-alice.com/) is a project funded in 75% by European Regional Development Fund (ERDF) under the umbrella of INTERREG Atlantic Area with the application code: EAPA_261/2016. The 11 partners involved in the project are from Portugal, Spain, Northern Ireland, France and the United Kingdom. The three-year project started in November 2017 will cost 3 million euros with 25% covered by the beneficiary partners.

The main goal is to promote sustainable investments in Blue-Green Infrastructure Networks (BGINs) through identification of the benefits of Ecosystem Services delivered at the terrestrial-aquatic and land-sea interface in the Atlantic Region.

The activities will be developed by:

· combining a range of satellite images, GIS data and modelling frameworks to map aquatic and terrestrial vegetation formations and ecological processes;

Figure 13 Report describing the model, created on the fly as the model runs.

Discussion

A sustainable balance between agricultural production and healthy ecosystems in agricultural landscapes has been challenging to achieve. The main difficulties can be linked to population growth and people's increased demands for food, water and energy, the limited area of arable land to expand food production and increasing pressure on natural resources from various human activities (Zhang, Wang & Wang, 2002; Kitzes et al., 2008). These factors are further compounded by land degradation and water contamination, climate change, sub-optimal agricultural and land-use policies and market fluctuations (Kendall & Pimentel, 1994; Laurance, Sayer & Cassman, 2014). The PaL models developed in k.LAB can be used to improve the management of agricultural systems by:

- integrating all the components of agricultural systems modelling in one platform,
- simulating the effects of alternative resource use strategies,
- improving the efficiency of low-input and intensive agricultural systems, and
- improving accessibility and transparency of simulation models to stakeholders.

The divergence in the time scales between farmer choices and environmental goals is a substantial management challenge. While farmers often need or want to fulfil their financial and land management objectives in the short term (i.e., months and seasons in this and the following year), environmental goals may take much longer to be reached (potentially years to decades). The temporal flexibility in modelling plays a key role to quantify short- and long-term processes in both the agricultural system and the environment. As we show in this article, the k.LAB approach ensures semantic consistency in temporal data, from historical observations to future scenarios, to respond to these needs in different situations. Moreover, the PaL namespaces could be expanded to simulate environmental disturbances, disease spread, climatic change and simulated management plans to deal with such challenges, building on the existing PaL

namespaces and without having to change any of them and its models. For example, providing a model for "change in X" is all it takes to make a previously static model of concept X dynamic, as the k.LAB engine will automatically insert it in the workflow whenever the context is computed over multiple timesteps.

Because environmental modelling, including pasture and livestock simulation, tends to be driven by the need to address case-specific issues, data and model reuse recommendations are often unclearly defined. Moreover, the collected data are often not made available to other researchers; when they are placed in public repositories data are often findable and accessible but lag in their interoperability and reusability (Borycz & Carroll, 2020). As a result, in the best case substantial manual GIS processing is required before a user can work with previously generated data; in the worst case data may be lost entirely after the modelling results are published. In this article, we demonstrate a semantics-first approach to harmonize data and models of livestock and pastureland, in order to make them interoperable (Villa et al., 2014). Thus, PaL's modular approach allows models and data to be combined for specific purposes in one platform, making the simulation process more efficient by representing diverse pieces of knowledge in the same system, which is a common difficulty in agricultural modelling systems (Harrison et al., 2016). This is a significant improvement in dealing with the complex interdependencies between humans and nature in agricultural systems, where data come from different sources and knowledge domains as in the case study presented.

The models, algorithms, data sources, and results described in this article are accessible to non-technical users through a web browser application, k.Explorer – a substantial improvement from the previous edition of the Puerto model, which was only available to technical modelers proficient in the R programming language. As described in the "End-user features" section of the Results, this makes scientific information more easily understandable and accessible, bringing scientific research closer to society with greater transparency (Figs. 12-16). k.LAB is an open and collaborative technology aiming to expand and improve the availability of interoperable data and models across disciplines (Willcock et al., 2018; Martínez-López et al., 2019). This technology can be used to substantially improve agricultural data and models' accessibility, harmonize them in order to facilitate their wider reuse, improve their quality and consistency. PaL namespaces are made available to both farmers and policy makers as an open, reusable and efficient toolbox. Modellers can contribute new data and models and the knowledge to ensure their appropriate reuse through a dedicated interface (Villa et al., 2014) - a collective effort to provide stakeholders with the needed tools to face the new challenges in agriculture systems (Matthews et al., 2007; Verburg, Eickhout & van Meijl, 2008).

The versatility and flexibility of this approach encourages model reusability, which is particularly valuable to iteratively update assessments as newer or more reliable information becomes available. Data inputs made available in the k.LAB system can affect PaL modelling outputs and other ecosystem services models connected through semantics (Fig. 5). Both inputs

and outputs from the PaL namespaces can be automatically reused at different temporal and spatial scales, ranging from local analysis to national scales.

While this article offers an integrated and semantic modelling adaptation of the original Puerto model, we note three limitations and complexities for the benefit of future investigations. First, input data needed to run PaL outside the Cantabrian case study region are available on the k.LAB network but may not have the same quality or resolution due when relying on global data. This could affect the reliability of PaL outputs when run outside the Cantabrian region. Hence, we recommend further validation of model outputs in future applications. Second, the types of modelled pastureland vegetation and livestock are currently limited to certain classes (Figure 2). Third, some excessively complicated models (Sun et al., 2016) could be replaced by simpler ones. This would require more accessible cloud-hosted data, but would simultaneously decrease computational needs.

This article demonstrated how agricultural modelling can be made more transparent and accessible. In particular, we showed how to run and produce results from the Pasture and Livestock (PaL) namespaces in the k.LAB modelling platform, capitalizing on a semantics-first approach (Villa et al., 2017). We applied this set of models to a case study in the Cantabrian region of Spain, where complex interactions among vegetation, livestock, and nitrogen need to be disentangled for improved agroecosystem management. Additional agricultural models can be incorporated and connected with the currently available PaL namespaces in the future. Some of these models may expand on other ecological aspects, such as pest, weed and disease spread or carbon and phosphorus cycling, which are closely linked to nitrogen. Others might expand on the microeconomics of farm operations, taking into account the cost-efficiency of management activities given farmers' current economic status. Similarly, the existing namespaces can incorporate new input data related to vegetation and livestock species. Moreover, further research could analyse the interactions between PaL namespaces and other ecosystem service models, to fully capture the complex implications of pasture management patterns (Bagstad et al., 2014; Balbi et al., 2015; Martínez-López et al., 2019).

Conclusions

The evolution of agriculture and the challenges it faces, both in terms of productivity and ecological impacts, require focused efforts to design more sustainable agricultural systems. The case study in Cantabria addresses a set of environmental and agricultural management changes over the past decades. The current pressure of tourism and the trend of farmland abandonment are risking the balance between nature and society in these systems. One of the main challenges of this study was to combine, using a unified yet highly flexible and accessible approach, the biophysical, technical and management knowledge needed to analyse the current conditions and explore future trends.

In this article, we break down the original monolithic Puerto model, developed for managing rangelands in the Cantabrian region of Spain, into ten Pasture and Livestock k.LAB namespaces, composed of 198 models. We applied these a fine temporal and spatial scale over the case study area, the Pas, Miera and Ason watersheds in Cantabria, responding to the needs for modelling their extensive agricultural systems. To do so, we first provided insights into current and past agricultural trends derived from literature and expert knowledge regarding to the Cantabrian agroecosystem situation. Next, we developed an open and semantic modelling application for pasture and livestock modelling in the k.LAB platform. This provides stakeholders with an accessible and user-friendly web-browser with that better bridges the gap between technical scientific modelling and land managers. Accessible and context-dependent models can provide solutions for different needs, such as those of i) policy-makers, who can better monitor landscape performance and health, ii) farmers, who can simulate alternative management strategies and potential risks to farming production and devise adaptation strategies, and iii) scientists, who can contribute to greater knowledge reuse and application to on-the-ground decision making.

This article elaborated the importance of overall modelling strategy and design for interoperability and reusability, showing how to improve the ease of use of scientific models and their application to decision making. Within a collaborative modelling system like k.LAB, all models are enhanced through wider community testing, reuse, and application to different contexts. Through wider reuse, models can become increasingly realistic, reliable and useful. This approach is applicable for a wide range of environmental modelling problems, though it is especially suitable for agricultural systems, where underlying data are gathered from different sources and domains, as it facilitates a transdisciplinary scientific approach to complex modelling and management problems.

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