Steering operational synergies in terrestrial observation networks: opportunity for advancing Earth system dynamics modelling

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Abstract. Advancing our understanding of Earth System Dynamics (ESD) depends on the development of models and other analytical tools that apply both physical, biological and chemical data. This ambition to increase understanding and develop models of ESD based on site observations was the stimulus for creating the networks of Long Term Ecological Research (LTER), Critical Zone Observatories (CZO), and others. We organized a survey, the results of which identified pressing gaps in data availability from these networks, in particular for the future development and evaluation of models that represent ESD processes, and provide insights for improvement both in data collection and model integration.

From this survey overview of data applications in the context of LTER- and CZO research, we identified three challenges: 1) widen application of terrestrial observation network data in Earth system modelling, 2) developing integrated Earth system models that incorporate process representation and data of multiple disciplines, and 3) identifying complementarity in measured variables and spatial extent, and promoting synergies in the existing observational networks. These challenges lead to perspectives and recommendations for an improved dialogue between the observation networks and the ESD modelling community, including co-location of sites in the existing networks and further formalizing these recommendations among these communities. Developing these synergies will enable cross-site and cross-network comparison and synthesis studies which will help produce the insights around organizing principles, classifications, and general rules of coupling processes with environmental conditions.

1   Introduction

Complex interactions between rock, soil, water, air, and living organisms regulate the natural habitat and determine the availability of life-sustaining resources for human well-being (MEA, 2005). In the light of accelerating global change (e.g. Camill, 2010; IPCC, 2014) and safeguarding Earth as habitable space, the scientific and societal demands require improved understanding of Earth System Dynamics (ESD). Understanding and modelling of Earth system processes and interactions among Earth system compartments can be enhanced by accessing a wider range of both observational and experimental data (Aronova et al., 2010; Banwart et al., 2012; Reid et al., 2010). For these purposes, observation networks have been developed in recent decades aimed at temporal and multidisciplinary coverage of continental and global scale ecosystem observations. The Critical Zone Observatory network (White et al., 2015), the International Long Term Ecosystem Research network (Mirtl et al., 2018), the US National Ecological Observatory Network (Loescher et al., 2017, Schimel et al., 2001), the Chinese Ecosystem Research Network (Fu et al., 2010) and the Australian Terrestrial Ecosystem Research Network (Lindenmayer, 2017) are examples of networks that focus at the continental to global spatial extent, and daily to decadal temporal scales.

One overarching goal of these research and observation networks is to use measurement data to improve the predictive capabilities of current models (Loescher et al., 2017). The growing availability of data (Hampton et al., 2013) and an

improved representation and resolution of modelled processes drive the development of ESD models with ever increasing sophistication (Wood et al., 2011) and novel validation and assimilation techniques (Penny and Hamill, 2017). Terrestrial Earth system models represent a large range of processes, from tracking the fluxes and storage of energy, water, sediments, carbon, and other elements (scalars), to distributions and functional roles of organisms, land use practices, climate, and

5   humans (Mirtl et al., 2013). However, the majority of these models focus on one or a few processes. In contrast, we define integrated models as terrestrial Earth system models which include interactions and feedbacks among water, energy and weathering cycles with biota, ecosystem functions and services (Vereecken et al., 2016b). Integrated models include cross-scale and cross-disciplinary processes that are needed to fully predict ESD responses to perturbations from driving forces at local to global scales. No single ESD model can accomplish the full representation of driver and response functions. For this

10   reason, developing integrated models dealing with different processes, such as Land Surface Models, or coupling existing process models in suites (e.g. Duffy et al., 2014; Peckham et al., 2013) are options to expand our current modelling capability to incorporate cross-disciplinary processes for improved prediction of whole ESD system-level understanding, as well as for policy and management decisions. The application of hydrological, meteorological, biogeochemical and biodiversity measurements from within and across sites into such integrated model systems (Figure 1) is a key component to

15   providing the multi-scale/multi-process understanding that is needed to advance predictions of ESD responses to land use and climate changes, and the ever-increasing demand for natural resources.

For these purposes, the Critical Zone Observatories (CZOs) provide essential data sets and a coordinated community of researchers that integrate hydrologic, geochemical and geomorphic processes from soil grain to watershed scales (Brantley et al., 2017). CZOs examine the interactions among the lithosphere, pedosphere, hydrosphere, biosphere and atmosphere

20   (White et al., 2015, Banwart et al., 2012; Brantley et al., 2007). CZOs examine how scalar mass and energy fluxes interact with life and lithology over geological timescales that see the transformation of bedrock into soils, and how the same coupled processes enact feedbacks with changing climate and changing land use (Brantley et al., 2016; Lin et al., 2015; Sullivan et al., 2016). The US Long Term Ecological Research (LTER) network was created with the aim to provide the data and information needed for long-term, integrative, cross-site, nation-wide principle investigator (PI)-based research to

25   advance ecological literacy and act upon solving societal grand challenges (Callahan, 1984). This US project quickly gained attention, and sparked the foundation of other national and regional LTER networks (e.g. China, Europe, Australia). This led to the foundation of the global International LTER network in 1993 (ILTER) (Kim, 2006; Mirtl, 2010; Vanderbilt and Gaiser, 2017), which currently comprises 44 formal national LTER networks. ILTER provides the scientific expertise, a global-scale network, and long-term datasets necessary to document and analyze environmental change. In addition, Long-

30   term Socio-Ecological Research Platforms (LTSER) are designed to support research on long-term human-environment interactions and transdisciplinary approaches. Recognizing that the value of long-term data extends beyond use at any individual site, the global ILTER network aims at making data collected by all (I)LTER sites broadly accessible to other investigators (e.g. Breda et al., 2006; Parr et al., 2002; Vihervaara et al., 2013), enhanced by the standardized documentation

of measurements and sites (Haase et al., 2016), and a proposal to unify abiotically and biotically oriented concepts (Haase et al., 2018). Site metadata and data are increasingly accessible via the DEIMS-SDR web-service (Mirtl et al. 2018).

As the above review illustrates, each of these networks was created in an effort to address recognized science questions and knowledge gaps in specific disciplines that led their creation (e.g., ecology, geology). The collection of data within each
5   network – the variables measured, the methods by which they were measured, and associated campaign activities leveraging these networks – have been designed to address these specific questions and knowledge gaps. At the same time, the science questions, observed variables and associated measurement methods lead to opportunities for across-network synthesis and co-production of knowledge across these networks and disciplines. Moreover, there is great potential to advance the development of ESD models, especially integrated ones, by providing site-level observations for calibration, validation, and
10   data assimilation. However, the question remains – to what degree do modeling efforts use observatory network data, and how do those efforts fit within the broader activities of the networks?

For this study, the International Soil Modelling Consortium (ISMC, https://soil-modelling.org/) conducted a survey with participation from the ILTER and the global CZO network (Critical Zone Exploration Network) to identify knowledge and functional gaps in data availability and in our ability to integrate models and the data application. ISMC envisions
15   integration of models from different disciplines of hydrology, biogeochemistry and ecology, to increase the understanding and awareness of ESD processes, especially when these processes underpin other processes (e.g., carbon cycling, biological activities, soil formation, global and regional climate) (Vereecken et al., 2016b). To this end, the survey brings quantitative information on the level of integration of modeling approaches that use data from the LTER and CZO sites. Based on the results of the survey, we describe challenges and implications for 1) usage of observatory data in integrated ESD models, 2)
20   model integration in relation to specific disciplines, and 3) complementarity and possibilities for steering network synergies (Figure 1).

2   Material and Methods

The survey was addressed to the principal investigators (PIs) of individual CZOs, to the larger Critical Zone Exploration
25   Network (approximately 1600 individuals), and to the PIs of the ILTER network (approximately 400 individuals) with the request to forward the survey to associated modelers. The first part of the survey collected information on the model used, the geographic region, purposes of the modelling activity, spatial and temporal scale, compartments, disciplines, and model structure. The second part of the survey identified the type of variables/data used, data application (model input or calibration/validation), and the source of data used in the model (measurements at sites, remotely sensed, database, modelled
30   or literature).

As the purpose and scientific origin of the LTER and CZO networks differ, the respondents were asked about a diverse set of variables and parameters. In total, 52 variables were included in the survey (Table A1) based on the common measurements

in the LTER and CZO networks (Chorover et al., 2015 and Brantley et al., 2016). Survey results were tabulated and analyzed to address several questions. Examining both networks separately and analyzing them together, we tested (1) the degree to which variables or model characteristics were associated with a specific network, (2) the relationship between model integration (range between 0 to 1) and number of variables (range: 0 to 52) used in the model, and (3) a correspondence analysis for the data application across the models. The model 'level of integration' (an index ranging from 0 [low] to 1 [high]) was calculated by normalizing the model-wise number of disciplines and compartments indicated by the responses to a scale of 0 (none) to 1 (many) and averaging these two indices. The survey variables were combined in an ordination using detrended correspondence analysis (Hill and Gauch, 1980) implemented in R and Fortran (Oksanen and Minchin, 1997). The ordination was designed to identify common features among the models used.

3   Challenge I: Observatory data application to ESD modelling

3.1   Current status

The survey revealed a wide variety of models in terms of disciplines and scales (Figure A1). 70 out of 118 completed surveys provided full information on model characterization and variables. Nearly half of the respondents (47 %) reported on use of CZO observational data, two-thirds (66 %) used LTER data and 12 % reported model applications using data from both networks (Figure A1a). Geographically, the majority of model applications came from Europe (63 %), followed by North America (27 %), global (18 %), Asia (12 %), and Africa (5 %). Particularly in Europe, a large fraction of respondents were associated with LTER, while in North America the CZO community was the most responsive.

The average model used 14 variables of the supplied list of 52, ~2/3 of the variables for model input and ~1/3 for calibration/validation (Table A1). The majority of variables used in the models are sourced from on-site measurements (55% on average). The rest of the data (45 %) is derived from other sources, mostly remote sensing (e.g., MODIS), to a lesser extent modelled (e.g., North American Land Data Assimilation System), external database (e.g., FluxNet), or literature sources. The most common remotely sensed variables were of the biosphere, especially habitat mapping, leaf area index, vegetation structure and dynamics, above-ground biomass, but also snowpack distribution and duration. Variables used most frequently in models applied by CZO and LTER communities were from the atmospheric compartment (precipitation, air temperature, incoming shortwave radiation, humidity, wind speed/direction, and eddy flux of evapotranspiration and CO_2), followed by soil characterization (structure, texture, water content), above-ground biomass, and vegetation structure and dynamics. This reflects the current most frequent model requirements and applications in terrestrial Earth system science for coupled hydrological-biogeophysical models. Model applications affiliated with the CZO were more focused on the lithosphere and cryosphere, while biodiversity was addressed only in models of the LTER community (Figure A1e). While the CZO model applications use variables and data related to saprolite and bedrock mineralogy, data on biotic and

biodiversity variables were used more frequently in models associated with LTER. Models associated with CZOs applied significantly (Fisher's exact test, $p < 0.05$) more data based on eddy flux measurements (evapotranspiration and CO_2), root density, soil water content, soil temperature, bedrock, and soil texture and physics compared to models associated with LTER. Models using data related to habitat mapping, biotic and biodiversity elements were associated with the LTER community.

There is a large congruence in the spatial and temporal scales between both communities. Spatial scales of models were primarily site- to catchment scales, with few models at macro pore, lab or global scale (Figure 2). The high density in the center of Figure 2 shows the focus for sub-catchment scale modelling, and time scales of days to years, potentially decades, which is in line with the aims and conceptual basis of both LTER and CZOs. This result stresses the relevance of both observation networks to ESD processes in terms of the spatial and temporal scales in CZO/LTER modelling activities. At the same time, Figure 2 reveals a lack of modelling activities at larger extent (continental and global) in both communities. The specific inset diagrams show that for LTER, the prevailing yearly, potentially decadal, time span is mostly covered at the site scale, whereas CZO associated responses work pre-dominantly at the catchment scale and incorporate daily resolution. Some CZO models seem to cover a larger range of spatial scales since the models indicated in the survey cover the full spatial range from macro-pore to continental and global scales. In terms of the modelled time scale, the long-time scales (centuries to millions of years) are mostly covered by models employed in the CZO community (Figure A1d). These scales of modelling are consistent with the focus on process and system understanding of both network's model applications, while the management and prediction aspect is more strongly embraced by LTER model applications in the survey results (Figure A1c).

3.2   Example of data application from an LTER site

Next to the common, cross-site measurements, CZO and LTER datasets generally include site-specific types of observations gathered to answer site-specific scientific questions on model development, ecosystem response to global change and prediction. One example is the vegetation dynamics modelling in the French LTER Zone Atelier Loire (Van Looy and Piffady, 2017), which uses predicted hydrological changes in river flow regimes and droughts to predict changes in land use and vegetation in the Loire floodplain (Figure 3). It enables the construction of population dynamics models for characteristic tree species Black poplar and White elm for the LTER site where count data of the species populations is present. The proposed adaptation management scenario of water retention and restoration of flow regime and floodplain inundation proved successful according to the model to mitigate predicted climate change impacts on population dynamics.

Another example of vegetation dynamics modelling using observation network data concerns forest dieback under climate change (Breshears et al., 2005). At an intensively studied site of the Drought-Induced Regional Ecosystem Response

Network, after 15 months of depleted soil water content, > 90% of the dominant overstory tree species died. This combination of detailed spatial-temporal observational data on tree condition, soil water content, precipitation and atmospheric conditions (temperature) allowed for data-driven development and validation of a regional model on drought-induced vegetation changes.

3.3 Open issues and implications

The LTER/CZO network sites monitor a wide range of environmental variables with long-term or at least regularly repeated measurements, expected to provide more reliable and robust results than single measurements that produce 'snap-shot' information only. The application of long-term monitoring data to enhance predictive capacity provides a strong opportunity

10   in the era of ESD modelling (Parr et al., 2002). Application of the rich data collected at LTER/CZO network sites should improve process understanding and enable the scientific community to address the challenges of validating Earth system models that integrate coupled processes. Although integrated models at LTER and CZO sites *are* used to raise understanding of the coupled processes, cases are mostly restricted to individual sites and too limited in numbers. As the survey results demonstrated, for some themes (e.g., habitat/vegetation/crop), remotely sensed or existing database information was

15   preferably used in contrast to potential data from on-site field measurements (Table A1). As on-site measurements generally are more accurate than remotely sensed or modelled data, this suggests a strong need for on-site measurements for modelling site-specific processes. Plausible causes for the lack of on-site measurements relating to vegetation and biota are the time and personnel-consuming requirements for data collection, and the absence of harmonized measurement protocols. The strong complementarity identified in data sources and model applications, in terms of biotic vs abiotic and above vs below ground

20   in LTER and CZO networks (respectively), does suggest strong potential benefits and gains in process understanding if data from both observatory networks can be applied simultaneously to integrated models at regional, continental and global scales.

4 Challenge II: Model integration

25   ### 4.1 Current status

On average, models had a rather high level of integration; CZO and LTER data model applications cover on average multiple disciplines (mean=3.6±2.1 standard deviation) and ecosystem compartments (mean=2.7±1.6). Model 'level of integration' was strikingly similar in CZO (mean=0.37±0.18) and LTER (mean=0.34±0.17). The richness in variables was positively related to the number of disciplines ($R^2 = 0.29$), and to compartments ($R^2 = 0.4$). However, unifying compartments

30   and disciplines to the 'level of integration' measure correlated most strongly to the number of variables ($R^2 = 0.47$) (Figure 4).

4.2   Example of integrated modelling

Plant-soil interactions are changing across the globe, whether by the encroachment of woody species into polar, alpine and temperate grassland areas (Archer et al., 1995; Jackson et al., 2002), the increase in atmospheric CO_2 concentrations that potentially alter the depth penetrations of roots (Bond and Midgley, 2012; Van Auken, 2000), or changing land cover (agriculture, forest plantations; (Van Minnen et al., 2009)). Subsurface changes to the root system architecture (root function, density and depth) alters the introduction (spatial distribution) of organic carbon into the ground, controlling microbial productivity and respiration, macro-pore location, distribution and evolution, controlling the transport of most water that moves through soil (Beven and Germann, 1982), and spatial distribution of organic acids and root respiration (generation of CO_2; (Jones, 1998)). These factors will impact infiltration of meteoric water charged with carbonic acid (H_2CO_3), influencing the breakdown of minerals and the redox conditions under which metals can be mobilized.

To explore the larger scale consequences of changes in root system architecture on soil water and riverine chemistry requires integration of processes from different scientific disciplines into an integrated or coupled model. Here we show the example of RT-FluxPIHM, which integrates processes from a reactive transport (RT) with a land-surface and hydrologic model (FluxPIHM) (Figure 5) (Bao et al., 2017; Li et al., 2017). RT-FluxPIHM is being used to examine the hydrologic and biogeochemical ramifications of woody encroachment into grasslands at the Konza Biological Station (KS, USA), a well characterized and monitored LTER site. Preliminary numerical experiments explore how differences in rooting depth and macro-porosity distribution (vertically and horizontally) alter groundwater flow patterns, and thus stream water discharge and solute behaviour. The enhanced vertical macro-pore development through deeper roots of woody encroachment compared to grass led to higher groundwater flow (Figure 5b). One limitation to such complex integrated numerical models is the numerous datasets needed for parameterization. However, working with datasets derived from LTER, CZOs and NEON allows evaluation of model performance against data that characterizes key processes embedded within integrated models. These types of coupled models (see also Dhara model by Le and Kumar (2017)) offer a way to explore plant-water-biogeochemical feedbacks at the watershed scale and help guide future field experiments.

4.3   Open issues and implications

Fragmentation and lack of integration has limited our abilities to understand the formation and function of ESD at various spatial scales, and to predict system response to global change and interaction of processes and parameters from sites to continents (Grimm et al., 2013). In our survey, 10% of the models already used data from both LTER and CZO networks in model applications. This implies that these models already integrated processes of interest to the two communities. However, inclusion of multiple disciplines and ecosystem compartments may increase model complexity and data requirements. Hence, integrated modelling may be limited by data availability, but allows for more general applicability of conclusions

(Basu et al., 2010; Li et al., 2017b). The numerical model applications necessary to test LTER and CZO conceptual model assumptions are integrated, process-based, spatially explicit models at the watershed scale that predict emergent behavior. The high level of multidisciplinary model inputs requires numerically expensive models and more importantly a sharp learning curve of the users. It does not necessarily mean that the data are co-measured. Where CZOs mainly focus on

5   understanding near surface structure and dynamics, developing synergies with LTER might fill many of the ecological gaps in CZO studies by providing the scientific expertise, research platforms, and datasets necessary to analyze environmental change with a particular focus on ecological driven processes. Whereas the conceptual models for LTER and CZO sites orient to fundamental process understanding using specific parsimonious models, nevertheless integrated models remain an essential part of the mission. Model integration does not necessarily require an increase in model complexity. Parsimonious

10 models can be integrated in a larger model platform (e.g. Duffy et al., 2014; Peckham et al., 2013) to investigate feedbacks over climatic and geographic gradients, and across disciplines.

5   Challenge III: Complementarity and disciplinary segregation

5.1   Current status

Models that included data from both LTER and CZO sites cluster in the center of the ordination (Figure 6), which indicates
15 that those models use a fairly similar group of variables. The models located in the center of the ordination focus mostly on hydrology and geophysical processes. Models clustered in group A are associated with CZOs, are mostly located in the second quadrant, and are distinguished by a focus on modelling processes in the soil profile, regolith, and bedrock. Models clustered in group B are associated with LTERs, are mostly located in the first and fourth quadrants, and focus on processes related to ecosystems and biota. The horizontal axis of the ordination separates physics-oriented from biotic-oriented models,
20 and below-ground (negative) to above-ground (positive). The vertical axis distinguishes highly integrated models, mainly hydrology-based, which contain a number of processes, from specific models, such as those focusing only on rock weathering.

5.2   Open issues and implications

25 Available data sets provide the opportunity to integrate a larger number of compartments into ESD models, but the ordination reveals that this integration has not progressed very far. The survey revealed that models using data from both CZO and LTER networks generally cover a larger range of variables compared to models applied to only one network (Figure 4). However, the outlier position of models focussing on biota and habitat variables in the ordination (Figure 6) indicates the need to integrate the biotic compartment in models of coupled processes such as energy, carbon and nutrient
30 cycling, and weathering (Filser et al., 2016; Richter and Billings, 2015; Vereecken et al., 2016b; Wall et al., 2015). In this survey, many biotic models were opposed to below-ground compartments in the ordination (Figure 6). This result

demonstrates the lack of models of biotic processes in the subsurface, e.g., the representation of the weathering microbiome or root system architecture and dynamics (Smithwick et al., 2014), despite the fact that the underground biota performs a crucial ecosystem functioning role (Deruiter et al., 1994; Wall et al., 2015). Therefore, it is particularly important to harmonize and standardize observations of biotic variables related to processes and feedbacks with hydrologic and biogeochemical cycles. Recent initiatives address the missing integration of below-ground biota in terrestrial Earth system science and models (Key to Soil Organic Matter Dynamics and Modelling – Keysom-Biolink project, Filser et al., 2016), and the provision of substantial datasets on soil biota and biodiversity (global soil biodiversity database, Ramirez et al., 2015). Some models are being developed that are capable of estimating the role of biotic activity in soil formation, decomposition/mineralization processes, and predicting the carbon and nutrient cycles in specific soil types (Komarov et al., 2017; Wieder et al., 2017). Nevertheless, joining discipline-specific data with the largely site-to-catchment based but discipline-specific modelling expertise of the CZO and LTER communities would lay the ground for new findings.

6 Outlook

6.1 Satisfying cross-disciplinary data demand by ESD models

The relationship of models and data is a relationship of mutual benefits. Data enable scientists to develop and test hypotheses (e.g. Braud et al., 2014; Clark et al., 2011), but models may also help scientists to better design data collection strategies and tactics for observation networks (Brantley et al., 2016). With the increase in computational capabilities, stochastic methods such as data assimilation, global sensitivity analysis, and optimization algorithms are becoming more widely used. Commonly, these methods are used for parameter and state estimation. Additionally, stochastic analyses open the way to determine the observation requirements to reduce model uncertainties and test hypotheses. Stochastic analyses can be used to identify key physical processes and their impacts if variables are subject to change. Thus, models can improve observation network strategies by quantifying process sensitivity to observed variables and parameters, as well as measurement frequency, and resolution/extent needs in space and time (Lin, 2010). Model-based assessments of observability, predictability, and the impact of heterogeneity on processes at the relevant scales could improve network data collection efficiency and complementarity. Merging data and modelling through data assimilation also may enable testing predictions from small-scale process understanding in larger-scale, simplified model representations (Heffernan et al., 2014; Vereecken et al., 2016a).

In particular, the reanalysis concept addresses the benefits of data application in ESD modeling. Although it is widely used in meteorological models (e.g., Compo et al., 2011; Dee et al., 2011), reanalysis has only sparingly been used in terrestrial Earth system science or ecology. For performing reanalysis, a physics-based model is fed with observations through a data assimilation scheme over a sufficiently long time period to update model states and parameters over time. Model states and

parameters are optimized with the data assimilation method based on the observation, considering uncertainty in observations, model structure, initial states and forcings. Application of reanalysis in Earth system models could generate gap filled, multi-compartment, and coherent physics-based time series of terrestrial states, fluxes and parameters including variables characterizing biological processes and biodiversity. Based on often non-continuous and sparse in-situ observations from long term observation networks such as CZOs and LTER networks, critical zone- or ecosystem reanalysis would need to specifically target biological and biodiversity related processes in Earth system models. The generated continuous reanalysis data could inform further modelling processes or be used to test existing hypotheses. However, to undertake reanalysis for ESD, many questions need to be resolved, including the choice of the Earth system model, the data assimilation method, model parameterization and forcing data, validation data, and ultimately the representation of biotic and abiotic processes.

A related challenge is how to represent the roles of biota in integrated ESD models (Deruiter et al., 1994; Richter and Billings, 2015). Such efforts must be based on improved understanding of biotic-abiotic interactions, feedbacks, and thresholds (e.g., forest die-back Breshears et al., 2005). Integrated ESD models must include phenomena such as community assembly, evolution, the emergence of pests and pathogens, and invasion by invasive species, which are not currently included in CZO models. New initiatives have been launched recently to integrate the biotic component in Earth system science and models (Filser et al., 2016), including, for example, modelling the roles of biota (e.g., bacteria, fungi, roots) in the subsurface (Grandy et al., 2016). At the same time, improved representation of processes such as hydrologic and geochemical cycles may improve the integration of LTER models.

6.2   Integration of models

Integrated models covering different disciplines and compartments are needed to objectively increase process understanding and develop predictive capabilities on the effects of climate and land use changes on ESD. In our survey, the few land surface-atmosphere integrated process-oriented models like PIHM and Parflow-CLM were exceptional in the level of integration and application of observation network data. Along with a few other examples (e.g., Boone et al., 2009; Lafaysse et al., 2017), land surface models are rarely used to model processes with an integrated approach embracing biotic and abiotic variables using LTER and CZO data. A stronger communication between land surface modellers and LTER/CZO communities would enhance the integration of in-situ observations in models. However, this communication must overcome the disparity in scales of analysis between the continental-to-global focus of land surface models versus the site-to-region focus of LTER/CZO observatories.

A majority (80%) of the surveyed modellers also supported the idea of creating a model platform, but they were divided about what services should be provided on such a platform. Integration of parsimonious models into an integrated process-

based model could be one service under such a model platform. A model platform could promote the understanding of organizing principles, classifications, and general rules of coupling processes and environmental conditions (Sawicz et al., 2011; Sivapalan, 2003; Sivapalan et al., 2003). Insights also can be gained through cross-site comparison and synthesis studies of observation data across different sites under gradients of climate, Earth surface characteristics (e.g., soil type, 5 lithology, topography, vegetation), and human impact (e.g., pristine, agriculture, urban) conditions, which observation networks are well positioned to carry out.

6.3   Strategies for steering synergies in Earth observatory networks

With respect to investigating specific aspects of ESD, the interactions of biotic and abiotic processes as well as below-10 ground and above-ground processes are key links, where geosphere focused research by CZO and ecology focused research by LTER could benefit observation and model integration, optimizing the joint use of resource intensive observatories by more than one research community. Leveraging the CZO and LTER data across networks and scales implicates enhanced ESD modelling capabilities. Desirable data harmonization across networks could be achieved based upon blending conceptual frameworks such as the Ecosystem Integrity (Muller et al., 2000) and the Essential Biodiversity Variables 15 (Pereira et al., 2013) as suggested by Haase et al. (2018), and the Critical Zone approach (Chorover et al., 2015 and Brantley et al., 2016). Data harmonization between networks and co-location of sites by different networks allow for more efficient allocation of resources and increases multi-compartment datasets at co-located sites. Co-location is the joint use of individual research sites by two or more networks. The merger of data from different networks to calibrate/validate ESD models, following the example of the Coupled Model Intercomparison Project (Meehl et al., 2005), may help existing networks to 20 identify missing variables and potential additional observation sites in a resource efficient manner. Continued efforts to integrate ESD models and data will help advance ESD process understanding. Furthermore, the interaction of observatory networks increase the spatial coverage of multi-compartment observations, allowing ESD models to address research questions and testing hypothesis over larger scales gaining full benefit of multi-compartment CZO and LTER data.

25 Considerations about steering observatory network synergies need to consider differences in the organizational structure, where CZOs have been mainly based on scientific networks and projects, while LTER has established formal governance structures in regional groups and globally. The degree of implementation and formalization of observatory networks also varies with geography, ranging from regions with well-established networks (US-LTER, US CZO and NEON), to regions where research and observation networks are based on the initiative of individual sites, observatories or projects. Some 30 existing Earth observation networks such as NEON already are more systematic in spatial coverage and constitution, offering opportunities for advanced geographical ESD analysis. A notable European initiative is the Integrated European Ecosystem, Critical Zone and Socio-Ecological Research Infrastructure (eLTER RI), which includes the focal aspect of CZO

research and requirements of widely used ecosystem models. In these attempts to steer synergies, the role of discussion amongst stakeholders, decision makers, funding agencies, and the broader scientific community cannot be over-stated.

7   Concluding recommendations

5   The CZO and LTER networks could promote interdisciplinary research that improves process-based models spanning the geosciences and biosciences (Brantley et al., 2017; Rasmussen et al., 2011), and modelling efforts may feed back to help improve observation network design. To be effective, a stronger dialog is needed between the observatory networks. More work is needed to apply CZO and LTER data in ESD models and thus strengthen the crucial role of the observatory networks in raising understanding of ESD processes and deriving predictive capabilities for drivers, impacts and responses to

10   global change. The rapidly increasing technological capabilities in computational power, ground based instrumentation, and unmanned automated remote sensing require all stakeholders to decide on which aspects the future observational requirements shall focus. Given today's grand challenges, the communities need to focus on expanding observation efforts towards cross-community harmonized methods and data sets. The communication and exchange about services and tools for making data available through web platforms offers obvious opportunities in this sense.

15   Finally, there is an essential need to educate and train the next generation of Earth system scientists for modelling across disciplines. This indicates the need for dedicated Earth system science university courses, online teaching materials on model usage, and a coordinated, community driven modelling platform.

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8   References

Agresti, A.: Categorical data analysis, Second edition, New York, Wiley, 91–101, 2002.

Archer, S., Schimel, D. S., and Holland, E. A.: Mechanisms of Shrubland Expansion - Land-Use, Climate or Co-2, Climatic Change, 29, 91-99, 1995.

Aronova, E., Baker, K. S., and Oreskes, N.: Big Science and Big Data in Biology: From the International Geophysical Year through the International Biological Program to the Long Term Ecological Research (LTER) Network, 1957-Present, Hist Stud Nat Sci, 40, 183-224, 2010.

Banwart, S., Menon, M., Bernasconi, S. M., Bloem, J., Blum, W. E. H., Souza, D. M., Davidsdotir, B., Duffy, C., Lair, G. J., Kram, P., Lamacova, A., Lundin, L., Nikolaidis, N. P., Novak, M., Panagos, P., Ragnarsdottir, K. V., Reynolds, B., Robinson, D., Rousseva, S., de Ruiter, P., van Gaans, P., Weng, L. P., White, T., and Zhang, B.: Soil processes and functions across an international network of Critical Zone Observatories: Introduction to experimental methods and initial results, Cr Geosci, 344, 758-772, 2012.

Bao, C., Li, L., Shi, Y. N., and Duffy, C.: Understanding watershed hydrogeochemistry: 1. Development of RT-Flux-PIHM, Water Resour Res, 53, 2328-2345, 2017.

Basu, N. B., Rao, P. S. C., Winzeler, H. E., Kumar, S., Owens, P., and Merwade, V.: Parsimonious modelling of hydrologic responses in engineered watersheds: Structural heterogeneity versus functional homogeneity, Water Resour Res, 46, Artn W04501 10.1029/2009wr007803, 2010.

Beven, K. and Germann, P.: Macropores and Water-Flow in Soils, Water Resour Res, 18, 1311-1325, 1982.

Bond, W. J. and Midgley, G. F.: Carbon dioxide and the uneasy interactions of trees and savannah grasses, Philos T R Soc B, 367, 601-612, 2012.

Boone, A., de Rosnay, P., Balsamo, G., Beljaars, A., Chopin, F., Decharme, B., Delire, C., Ducharne, A., Gascoin, S., Grippa, M., Guichard, F., Gusev, Y., Harris, P., Jarlan, L., Kergoat, L., Mougin, E., Nasonova, O., Norgaard, A., Orgeval, T., Ottle, C., Poccard-Leclercq, I., Polcher, J., Sandholt, I., Saux-Picart, S., Taylor, C., and Xue, Y. K.: The Amma Land Surface Model Intercomparison Project (Almip), B Am Meteorol Soc, 90, 1865-1880, 2009.

Brantley, S. L., DiBiase, R. A., Russo, T. A., Shi, Y. N., Lin, H., Davis, K. J., Kaye, M., Hill, L., Kaye, J., Eissenstat, D. M., Hoagland, B., Dere, A. L., Neal, A. L., Brubaker, K. M., and Arthur, D. K.: Designing a suite of measurements to understand the critical zone, Earth Surf Dynam, 4, 211-235, 2016.

Brantley, S. L., Goldhaber, M. B., and Ragnarsdottir, K. V.: Crossing disciplines and scales to understand the Critical Zone, Elements, 3, 307-314, 2007.

Brantley, S. L., McDowell, W. H., Dietrich, W. E., White, T. S., Kumar, P., Anderson, S., Chorover, J., Lohse, K. A., Bales, R. C., Richter, D., Grant, G., and Gaillardet, J.: Designing a network of critical zone observatories to explore the living skin of the terrestrial Earth, Earth Surf. Dynam. Discuss., 2017, 1-30, 2017.

Braud, I., Ayral, P. A., Bouvier, C., Branger, F., Delrieu, G., Le Coz, J., Nord, G., Vandervaere, J. P., Anquetin, S., Adamovic, M., Andrieu, J., Batiot, C., Boudevillain, B., Brunet, P., Carreau, J., Confoland, A., Didon-Lescot, J. F., Domergue, J. M., Douvinet, J., Dramais, G., Freydier, R., Gerard, S., Huza, J., Leblois, E., Le Bourgeois, O., Le Boursicaud, R., Marchand, P., Martin, P., Nottale, L., Patris, N., Renard, B., Seidel, J. L., Taupin, J. D., Vannier, O., Vincendon, B., and Wijbrans, A.: Multi-scale hydrometeorological observation and modelling for flash flood understanding, Hydrology and Earth System Sciences, 18, 3733-3761, 2014.

Breda, N., Huc, R., Granier, A., and Dreyer, E.: Temperate forest trees and stands under severe drought: a review of ecophysiological responses, adaptation processes and long-term consequences, Ann Forest Sci, 63, 625-644, 2006.

Breshears, D. D., Cobb, N. S., Rich, P. M., Price, K. P., Allen, C. D., Balice, R. G., Romme, W. H., Kastens, J. H., Floyd, M. L., Belnap, J., Anderson, J. J., Myers, O. B., and Meyer, C. W.: Regional vegetation die-off in response to global-change-type drought, P Natl Acad Sci USA, 102, 15144-15148, 2005.

Callahan, J. T.: Long-Term Ecological Research, Bioscience, 34, 363-367, 1984.

Camill, P.: Global Change. Nature Education Knowledge 3(10), 49, 2010.

Chabbi, A., H. W. Loescher, M. Tye and D. Hudnut: Integrated experimental research infrastructures as a paradigm shift to face an uncertain world. In: Terrestrial Ecosystem Research Infrastructures: Challenges and Opportunities. Eds. A. Chabbi, H.W. Loescher. CRC Press, Taylor & Francis Group, Boca Raton, FL,. pp. 3-23. ISBN 9781498751315, 2017.

Chorover, J., Anderson, S., Aufdenkampe, A. K., Bales, R. C., Brantley, S. L., Dietrich, W., Kumar, P., K. A. Lohse, McDowell, W., Richter, D., and White, T.: Common Critical Zone Observatory (CZO) Infrastructure and Measurements. A Guide Prepared By CZO PIs, 2015.

Clark, M. P., Kavetski, D., and Fenicia, F.: Pursuing the method of multiple working hypotheses for hydrological modeling, Water Resour Res, 47, 2011.

Compo, G. P., Whitaker, J. S., Sardeshmukh, P. D., Matsui, N., Allan, R. J., Yin, X., Gleason, B. E., Vose, R. S., Rutledge, G., Bessemoulin, P., Bronnimann, S., Brunet, M., Crouthamel, R. I., Grant, A. N., Groisman, P. Y., Jones, P. D., Kruk, M. C., Kruger, A. C., Marshall, G. J., Maugeri, M., Mok, H. Y., Nordli, O., Ross, T. F., Trigo, R. M., Wang, X. L., Woodruff, S. D., and Worley, S. J.: The Twentieth Century Reanalysis Project, Q J Roy Meteor Soc, 137, 1-28, 2011.

5 Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U., Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L., Healy, S. B., Hersbach, H., Holm, E. V., Isaksen, L., Kallberg, P., Kohler, M., Matricardi, M., McNally, A. P., Monge-Sanz, B. M., Morcrette, J. J., Park, B. K., Peubey, C., de Rosnay, P., Tavolato, C., Thepaut, J. N., and Vitart, F.: The ERA-Interim reanalysis: configuration and performance of the data assimilation system, Q J Roy Meteor Soc, 137, 553-597, 2011.

10 Deruiter, P. C., Neutel, A. M., and Moore, J. C.: Modeling Food Webs and Nutrient Cycling in Agroecosystems, Trends Ecol Evol, 9, 378-383, 1994.

Duffy, C., Shi, Y. N., Davis, K., Slingerland, R., Li, L., Sullivan, P. L., Godderis, Y., and Brantley, S. L.: Designing a Suite of Models to Explore Critical Zone Function, Proced Earth Plan Sc, 10, 7-15, 2014.

15 Filser, J., Faber, J. H., Tiunov, A. V., Brussaard, L., Frouz, J., De Deyn, G., Uvarov, A. V., Berg, M. P., Lavelle, P., Loreau, M., Wall, D. H., Querner, P., Eijsackers, H., and Jiménez, J. J.: Soil fauna: key to new carbon models, SOIL, 2, 565-582, 2016.

Fu, B. J., Li, S. G., Yu, X. B., Yang, P., Yu, G. R., Feng, R. G., and Zhuang, X. L.: Chinese ecosystem research network: Progress and perspectives, Ecol Complex, 7, 225-233, 2010.

Grandy, A. S., Wieder, W. R., Wickings, K., and Kyker-Snowman, E.: Beyond microbes: Are fauna the next frontier in soil 20 biogeochemical models?, Soil Biol Biochem, 102, 40-44, 2016.

Grimm, N. B., Chapin, F. S., Bierwagen, B., Gonzalez, P., Groffman, P. M., Luo, Y. Q., Melton, F., Nadelhoffer, K., Pairis, A., Raymond, P. A., Schimel, J., and Williamson, C. E.: The impacts of climate change on ecosystem structure and function, Front Ecol Environ, 11, 474-482, 2013.

Haase, P., Frenzel, M., Klotz, S., Musche, M., and Stoll, S.: The long-term ecological research (LTER) network: Relevance, current status, 25 future perspective and examples from marine, freshwater and terrestrial long-term observation, Ecol Indic, 65, 1-3, 2016.

Haase, P., Tonkin, J. D., Stoll, S., Burkhard, B., Frenzel, M., Geijzendorffer, I. R., Häuser, C., Klotz, S., Kühn, I., McDowell, W. H., Mirtl, M., Müller, F., Musche, M., Penner, J., Zacharias, S., and Schmeller, D. S.: The next generation of site-based long-term ecological monitoring: Linking essential biodiversity variables and ecosystem integrity, Sci Total Environ, 613-614, 1376-1384, 2018.

30 Hampton, S. E., Strasser, C. A., Tewksbury, J. J., Gram, W. K., Budden, A. E., Batcheller, A. L., Duke, C. S., and Porter, J. H.: Big data and the future of ecology, Front Ecol Environ, 11, 156-162, 2013.

Heffernan, J. B., Soranno, P. A., Angilletta, M. J., Buckley, L. B., Gruner, D. S., Keitt, T. H., Kellner, J. R., Kominoski, J. S., Rocha, A. V., Xiao, J. F., Harms, T. K., Goring, S. J., Koenig, L. E., McDowell, W. H., Powell, H., Richardson, A. D., Stow, C. A., Vargas, R., and Weathers, K. C.: Macrosystems ecology: understanding ecological patterns and processes at continental scales, Front 35 Ecol Environ, 12, 5-14, 2014.

Hill, M. O. and Gauch, H. G.: Detrended Correspondence-Analysis - an Improved Ordination Technique, Vegetatio, 42, 47-58, 1980.

IPCC: Climate Change 2014: Synthesis Report. Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team, R.K. Pachauri and L.A. Meyer (eds.)]. IPCC, Geneva, Switzerland, 151 pp, 2014.

40 Jackson, R. B., Banner, J. L., Jobbagy, E. G., Pockman, W. T., and Wall, D. H.: Ecosystem carbon loss with woody plant invasion of grasslands, Nature, 418, 623-626, 2002.

Jones, D. L.: Organic acids in the rhizosphere - a critical review, Plant Soil, 205, 25-44, 1998.

Kim, E. S.: Development, potentials, and challenges of the International Long-Term Ecological Research (ILTER) Network, Ecol Res, 21, 788-793, 2006.

45 Komarov, A., Chertov, O., Bykhovets, S., Shaw, C., Nadporozhskaya, M., Frolov, P., Shashkov, M., Shanin, V., Grabarnik, P., Priputina, I., and Zubkova, E.: Romul_Hum model of soil organic matter formation coupled with soil biota activity. I. Problem formulation, model description, and testing, Ecological Modelling, 345, 113-124, 2017.

Lafaysse, M., Cluzet, B., Dumont, M., Lejeune, Y., Vionnet, V., and Morin, S.: A multiphysical ensemble system of numerical snow modelling, Cryosphere, 11, 1173-1198, 2017.

50 Le, P. V. V. and Kumar, P.: Interaction Between Ecohydrologic Dynamics and Microtopographic Variability Under Climate Change, Water Resour Res, doi: 10.1002/2017WR020377. n/a-n/a.

Li, L., Bao, C., Sullivan, P. L., Brantley, S., Shi, Y. N., and Duffy, C.: Understanding watershed hydrogeochemistry: 2. Synchronized hydrological and geochemical processes drive stream chemostatic behavior, Water Resour Res, 53, 2346-2367, 2017.

Li, L., Maher, K., Navarre-Sitchler, A., Druhan, J., Meile, C., Lawrence, C., Moore, J., Perdrial, J., Sullivan, P., Thompson, A., Jin, L. X., 55 Bolton, E. W., Brantley, S. L., Dietrich, W. E., Mayer, K. U., Steefel, C. I., Valocchi, A., Zachara, J., Kocar, B., Mcintosh, J.,

Tutolo, B. M., Kumar, M., Sonnenthal, E., Bao, C., and Beisman, J.: Expanding the role of reactive transport models in critical zone processes, Earth-Sci Rev, 165, 280-301, 10.1016/j.earscirev.2016.09.001, 2017b.

Lin, H.: Earth's Critical Zone and hydropedology: concepts, characteristics, and advances, Hydrology and Earth System Sciences, 14, 25-45, 2010.

5   Lin, H. S., McDonnell, J. J., Nimmo, J. R., and Pachepsky, Y. A.: Hydropedology: Synergistic integration of soil science and hydrology in the Critical Zone Preface, Hydrol Process, 29, 4559-4561, 2015.

Lindenmayer, D.: Save Australia's ecological research, Science, 357, 557-557, 2017.

Loescher, H.W., Kelly, E., Lea, R.: National Ecological Observatory Network: Beginnings, Programmatic and Scientific Challenges, and Ecological Forecasting. In Terrestrial Ecosystem Research Infrastructures: Challenges and Opportunities, Chabbi, A., Loescher,

10   H.W., Eds., CRC Press, Taylor & Francis Group: Boca Raton, FL, pp. 27–48, ISBN 9781498751315, 2017.

MEA, Millennium Ecosystem Assessment: Ecosystems and Human Well-being: Synthesis. Island Press, Washington, DC (USA), 2005.

Meehl, G. A., Covey, C., McAvaney, B., Latif, M., and Stouffer, R. J.: Overview of the Coupled Model Intercomparison Project, B Am Meteorol Soc, 86, 89-93, 2005.

Mirtl, M.: Introducing the Next Generation of Ecosystem Research in Europe: LTER-Europe's Multi-Functional and Multi-Scale

15   Approach, Long-Term Ecological Research: Between Theory and Application, doi: 10.1007/978-90-481-8782-9_6, 2010. 75-93, 2010.

Mirtl, M., Orenstein, D. E., Wildenberg, M., Peterseil, J. and Frenzel, M.: Development of LTSER Platforms in LTER-Europe: Challenges and Experiences in Implementing Place-Based Long-Term Socio-ecological Research in Selected Regions. Long Term Socio-Ecological Research, S. J. Singh, H. Haberl, M. Chertow, M. Mirtl, and M. Schmid, Eds., Springer, 409-442, 2013.

20   Mirtl, M., Borer, E., Burns, E., Djukic, I., Forsius, M., Haubold, H., Hugo, W., Jourdan, J., Lindenmayer, D., McDowell, W.H., Muraoka, H., Orenstein, D., Pauw, J., Peterseil, J., Shibata, H., Wohner, C., Yu, X. and Haase, P.: Genesis, Goals and Achievements of Long-Term Ecological Research at the global scale: A critical review of ILTER and future implications Science of the Total Environment. Ref.Nr. STOTEN-D-17-06809, accepted, 2018.

Muller, F., Hoffmann-Kroll, R., and Wiggering, H.: Indicating ecosystem integrity - theoretical concepts and environmental requirements,

25   Ecol Model, 130, 13-23, 2000.

Oksanen, J. and Minchin, P. R.: Instability of ordination results under changes in input data order: Explanations and remedies, J Veg Sci, 8, 447-454, 1997.

Parr, T. W., Ferretti, M., Simpson, I. C., Forsius, M., and Kovacs-Lang, E.: Towards a long-term integrated monitoring programme in Europe: Network design in theory and practice, Environ Monit Assess, 78, 253-290, 2002.

30   Peckham, S. D., Hutton, E. W. H., and Norris, B.: A component-based approach to integrated modeling in the geosciences: The design of CSDMS, Comput Geosci-Uk, 53, 3-12, 2013.

Penny, S. G. and Hamill, T. M.: Coupled Data Assimilation for Integrated Earth System Analysis and Prediction, B Am Meteorol Soc, 98, Es169-Es172, 2017.

Pereira, H. M., Ferrier, S., Walters, M., Geller, G. N., Jongman, R. H. G., Scholes, R. J., Bruford, M. W., Brummitt, N., Butchart, S. H. M.,

35   Cardoso, A. C., Coops, N. C., Dulloo, E., Faith, D. P., Freyhof, J., Gregory, R. D., Heip, C., Hoft, R., Hurtt, G., Jetz, W., Karp, D. S., McGeoch, M. A., Obura, D., Onoda, Y., Pettorelli, N., Reyers, B., Sayre, R., Scharlemann, J. P. W., Stuart, S. N., Turak, E., Walpole, M., and Wegmann, M.: Essential Biodiversity Variables, Science, 339, 277-278, 2013.

Ramirez, K., Döring, M., Eisenhauer, N., Gardi, C., Ladau, J., Leff, J., Lentendu, G., Lindo, Z., Rillig, M., Russell, D., Scheu, S., St. John, M., de Vries, F., Wubet, T., van der Putten, W., and Wall, D.: Toward a global platform for linking soil biodiversity data,

40   Frontiers in Ecology and Evolution, 3, 2015.

Rasmussen, C., Troch, P. A., Chorover, J., Brooks, P., Pelletier, J., and Huxman, T. E.: An open system framework for integrating critical zone structure and function, Biogeochemistry, 102, 15-29, 2011.

Reid, W. V., Chen, D., Goldfarb, L., Hackmann, H., Lee, Y. T., Mokhele, K., Ostrom, E., Raivio, K., Rockstrom, J., Schellnhuber, H. J., and Whyte, A.: Earth System Science for Global Sustainability: Grand Challenges, Science, 330, 916-917, 2010.

45   Richter, D. D. and Billings, S. A.: 'One physical system': Tansley's ecosystem as Earth's critical zone, New Phytol, 206, 900-912, 2015.

Sawicz, K., Wagener, T., Sivapalan, M., Troch, P. A., and Carrillo, G.: Catchment classification: empirical analysis of hydrologic similarity based on catchment function in the eastern USA, Hydrology and Earth System Sciences, 15, 2895-2911, 2011.

Schimel, D., Keller, M., Berukoff, S., Kao, R., Loescher, H. W., Powell, H., Kampe, T., Moore, D. and Gram, W.: NEON Science Strategy; Enabling continental-scale ecological forecasting. Pub. NEON Inc., Boulder CO. pp 55, 2011.

50   Sivapalan, M.: Process complexity at hillslope scale, process simplicity at the watershed scale: is there a connection?, Hydrol Process, 17, 1037-1041, 2003.

Sivapalan, M., Bloschl, G., Zhang, L., and Vertessy, R.: Downward approach to hydrological prediction, Hydrol Process, 17, 2101-2111, 2003.

Smithwick, E. A. H., Lucash, M. S., McCormack, M. L., and Sivandran, G.: Improving the representation of roots in terrestrial models,

55   Ecol Model, 291, 193-204, 2014.

Sullivan, P. L., Ma, L., West, N., Jin, L., Karwan, D. L., Noireaux, J., Steinhoefel, G., Gaines, K. P., Eissenstat, D. M., Gaillardet, J., Derry, L. A., Meek, K., Hynek, S., and Brantley, S. L.: CZ-tope at Susquehanna Shale Hills CZO: Synthesizing multiple isotope proxies to elucidate Critical Zone processes across timescales in a temperate forested landscape, Chem Geol, 445, 103-119, 2016.

5   Van Auken, O. W.: Shrub invasions of North American semiarid grasslands, Annu Rev Ecol Syst, 31, 197-215, 2000.

Van Looy, K. and Piffady, J.: Metapopulation modelling of riparian tree species persistence in river networks under climate change, Journal of Environmental Management, 202, 437-446, 2017.

Van Minnen, J. G., Goldewijk, K. K., Stehfest, E., Eickhout, B., van Drecht, G., and Leemans, R.: The importance of three centuries of land-use change for the global and regional terrestrial carbon cycle, Climatic Change, 97, 123-144, 2009.

10   Vanderbilt, K. and Gaiser, E.: The International Long Term Ecological Research Network: a platform for collaboration, Ecosphere, 8, 2017.

Vereecken, H., Pachepsky, Y., Simmer, C., Rihani, J., Kunoth, A., Korres, W., Graf, A., Franssen, H. J. H., Thiele-Eich, I., and Shao, Y.: On the role of patterns in understanding the functioning of soil-vegetation-atmosphere systems, J Hydrol, 542, 63-86, 10.1016/j.jhydrol.2016.08.053, 2016a.

15   Vereecken, H., Schnepf, A., Hopmans, J. W., Javaux, M., Or, D., Roose, D. O. T., Vanderborght, J., Young, M. H., Amelung, W., Aitkenhead, M., Allison, S. D., Assouline, S., Baveye, P., Berli, M., Bruggemann, N., Finke, P., Flury, M., Gaiser, T., Govers, G., Ghezzehei, T., Hallett, P., Franssen, H. J. H., Heppell, J., Horn, R., Huisman, J. A., Jacques, D., Jonard, F., Kollet, S., Lafolie, F., Lamorski, K., Leitner, D., McBratney, A., Minasny, B., Montzka, C., Nowak, W., Pachepsky, Y., Padarian, J., Romano, N., Roth, K., Rothfuss, Y., Rowe, E. C., Schwen, A., Simunek, J., Tiktak, A., Van Dam, J., van der Zee, S. E. A. T. M.,

20   Vogel, H. J., Vrugt, J. A., Wohling, T., and Young, I. M.: Modeling Soil Processes: Review, Key Challenges, and New Perspectives, Vadose Zone J, 15, 10.2136/vzj2015.09.0131, 2016b.

Vihervaara, P., D'Amato, D., Forsius, M., Angelstam, P., Baessler, C., Balvanera, P., Boldgiv, B., Bourgeron, P., Dick, J., Kanka, R., Klotz, S., Maass, M., Melecis, V., Petrik, P., Shibata, H., Tang, J. W., Thompson, J., and Zacharias, S.: Using long-term ecosystem service and biodiversity data to study the impacts and adaptation options in response to climate change: insights from

25   the global ILTER sites network, Curr Opin Env Sust, 5, 53-66, 2013.

Wall, D. H., Nielsen, U. N., and Six, J.: Soil biodiversity and human health, Nature, 528, 69-76, 2015.

White T., Brantley S., Banwart S., Chorover J., Dietrich W., Derry L., Lohse K., Anderson S., Aufdendkampe A., Bales R., Kumar P., Richter D., McDowell B.: Chapter 2 – The Role of Critical Zone Observatories in Critical Zone Science, Developments in Earth Surface Processes, 19, 15–78, 2015.

30   Wieder, W. R., Knowles, J. F., Blanken, P. D., Swenson, S. C., and Suding, K. N.: Ecosystem function in complex mountain terrain: Combining models and long-term observations to advance process-based understanding, J Geophys Res-Biogeo, 122, 825-845, 2017.

Wood, E. F., Roundy, J. K., Troy, T. J., van Beek, L. P. H., Bierkens, M. F. P., Blyth, E., de Roo, A., Doll, P., Ek, M., Famiglietti, J., Gochis, D., van de Giesen, N., Houser, P., Jaffe, P. R., Kollet, S., Lehner, B., Lettenmaier, D. P., Peters-Lidard, C., Sivapalan,

35   M., Sheffield, J., Wade, A., and Whitehead, P.: Hyperresolution global land surface modeling: Meeting a grand challenge for monitoring Earth's terrestrial water, Water Resour Res, 47, 2011.

Figures
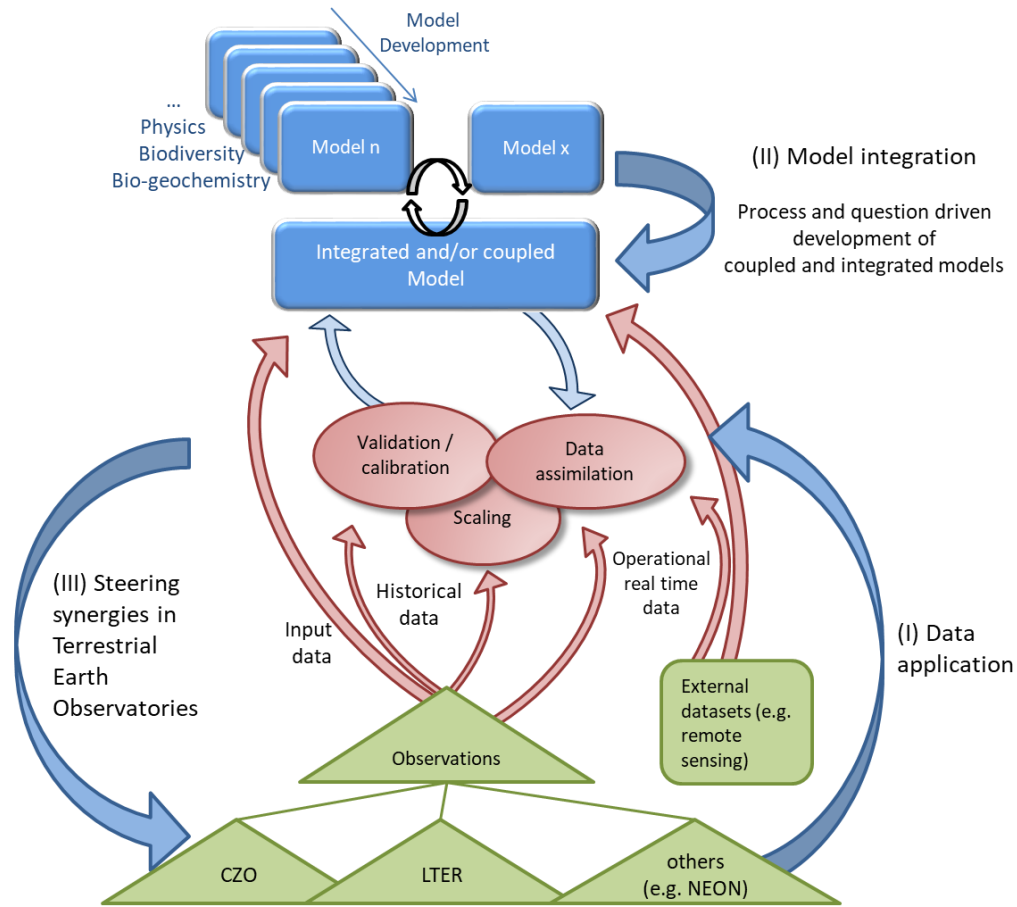
Figure 1: Flowchart of concepts, pathways and processes of applying terrestrial observatory network data to earth system dynamics models; identifying the three challenges of (I) data application, (II) model integration, and (III) steering synergies in observation networks.
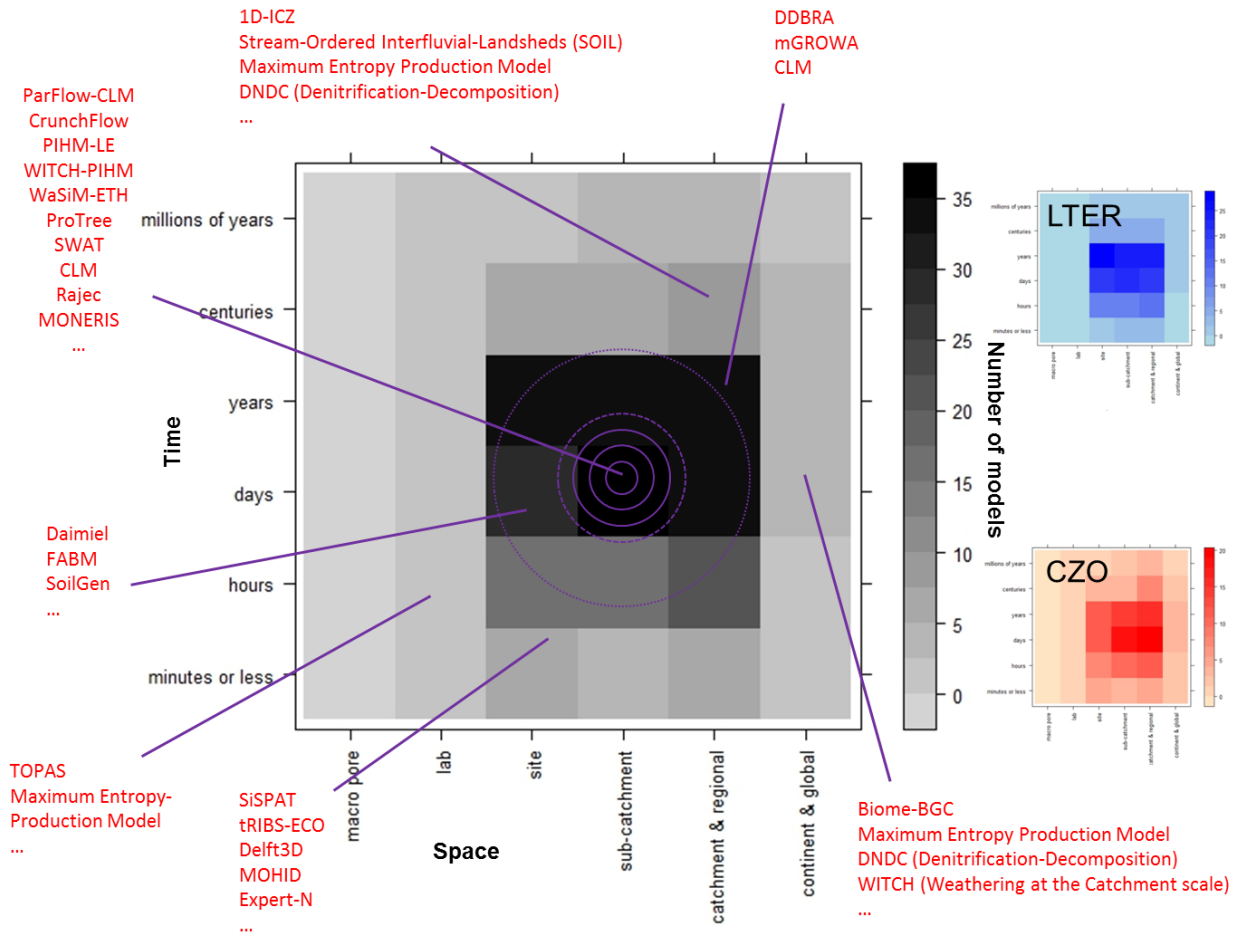
Figure 2: Heat map of model applications, with spatial and temporal dimensions of the surveyed models. Most models were denoted using several temporal and spatial scales. For visualization, we present some individual models at one exemplary instance. On the right, CZO and LTER model applications are presented separately.
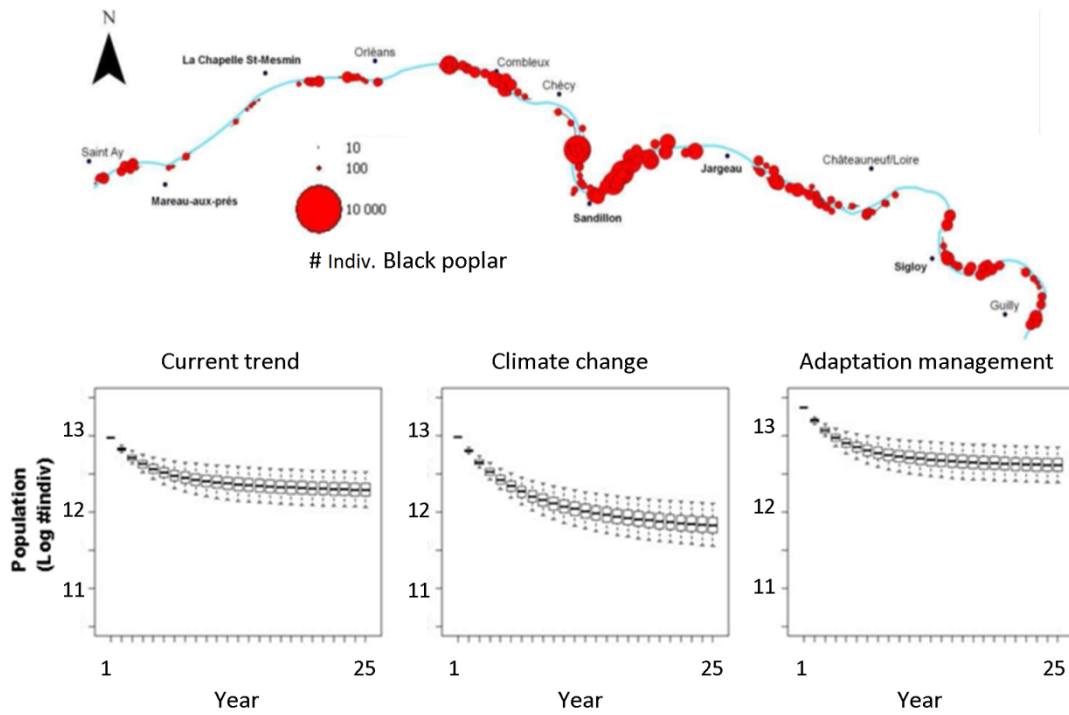
Figure 3: LTER sites answer specific ecological questions, for which specific data are gathered, e.g., Black poplar population persistence under climate change. Black poplar population strength along the French Loire River section (top), and model projections under current, climate change and adaptation management scenarios (Van Looy and Piffady, 2017).
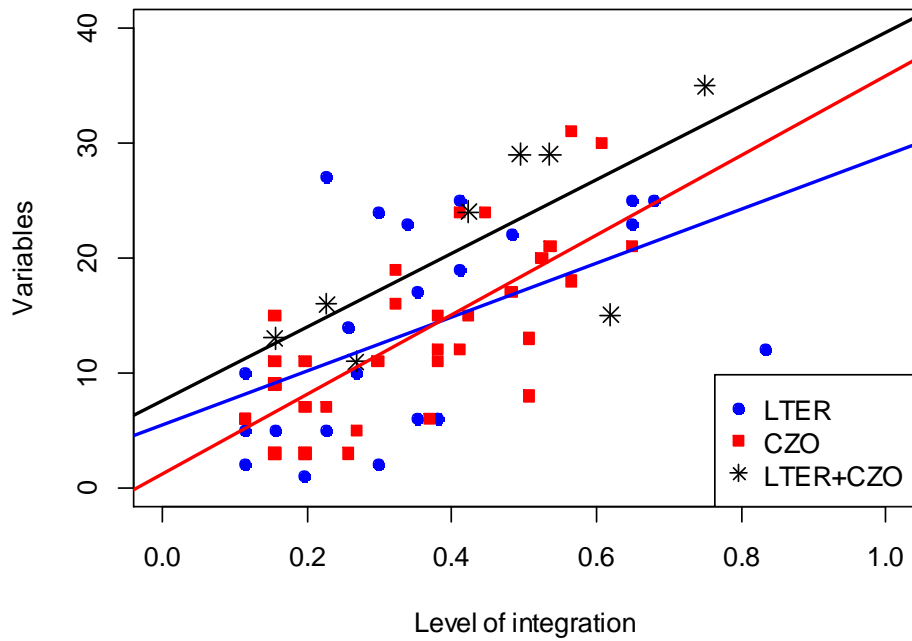
Figure 4: Model-wise 'level of integration' calculated from the summed scientific disciplines and modelled compartments for the corresponding model. Trend lines corresponding to the models associated with LTER (blue), and CZO (red), and models associated with data from both networks (black) are presented.

A.

B.
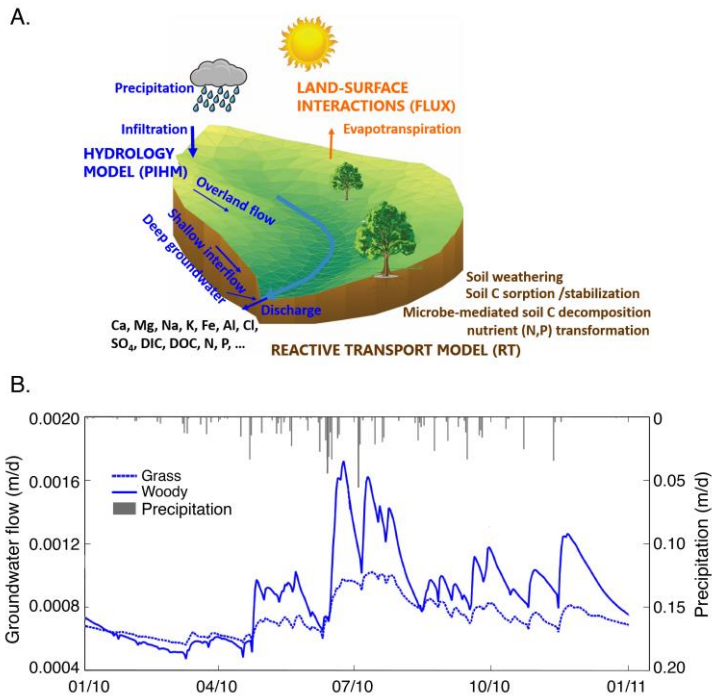
Figure 5: A. Representative processes from different disciplines (different colours) in different modules that can be integrated into one model suite or a coupled reactive transport-land surface-hydrologic model RT-Flux-PIHM (Bao et al., 2017). The integration among processes from mechanistic bases in the model will allow systematic understanding at the watershed scale. B. Model result of simulated difference in groundwater flow for a grassland (dotted line) and woody encroached (solid line) watershed (N04D), at the Konza Prairie, KS (USA). Grassland simulations are parameterized with a 0.3 m rooting depth and enhanced horizontal macro-pore development, while woody encroached simulations have a rooting depth that extends to 1.0 m deep.
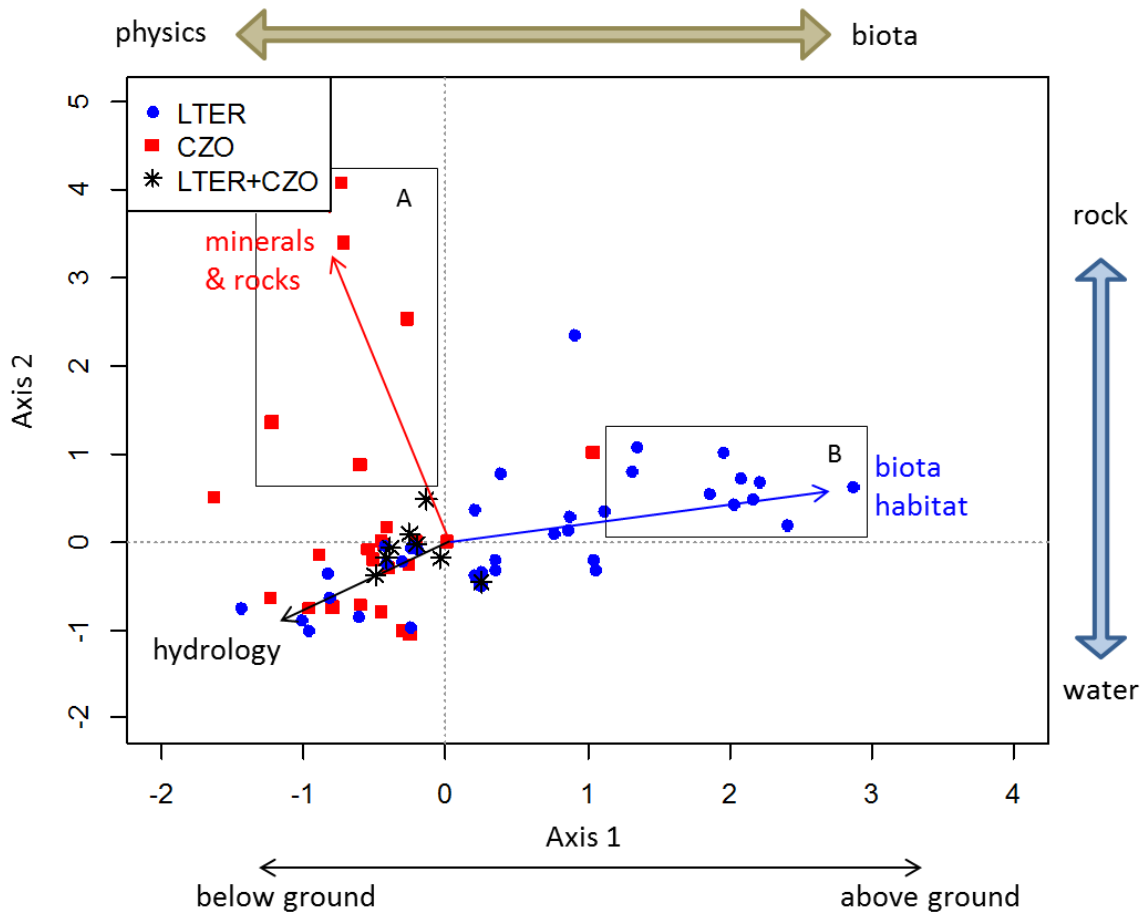
Figure 6: Ordination of the models and data in the survey; clusters show significant differences for models of LTER and CZO. CZO cluster A focuses on variables of the saprolite and bedrock, LTER cluster B focusses on the variables of biota/biodiversity.

Appendix
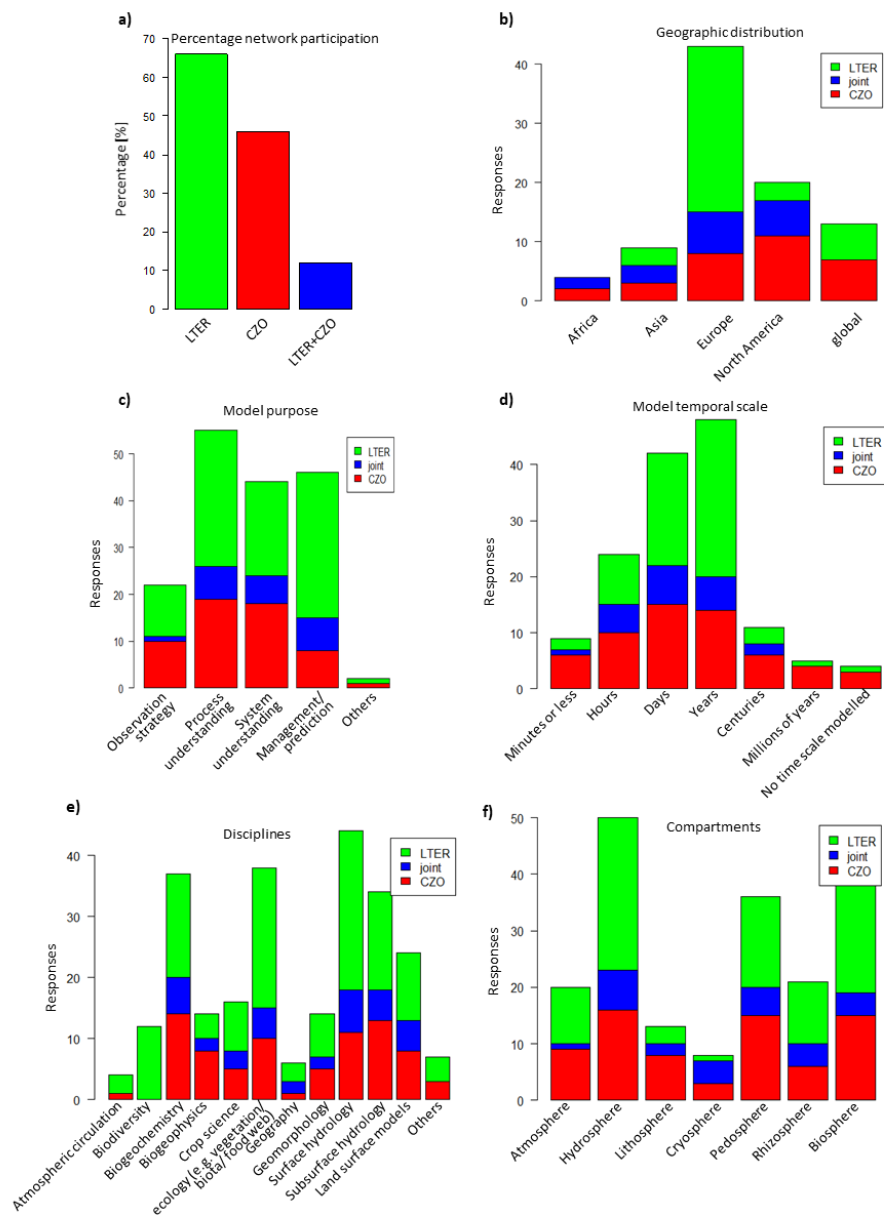
Figure A1: Distribution of respondents associated with either LTER, CZO, or both sites (a) to geographic region modelled (b), purpose of the modelling (c), time scale modelled (d), disciplines (e) and compartments (f) integrated.

Table A1: Summary table of variables, associated ecosystem compartment, the times it was associated with a model, the source for the data being either from site observation or from another source: i.e. remotely sensed, modelled, external database, literature.

Ecosystem compartment	Subcategory / theme	Variable	Sum of all instances nr.	Source:sites [%]	Source:others [%]
Atmosphere		Eddy flux of ET, CO_2	35	52	48
		Air temperature	47	62	38
		Humidity	38	65	35
		Incoming shortwave radiation	42	62	38
		Wind speed / -direction	37	66	34
		Precipitation	49	61	39
		Throughfall	25	41	59
		Snowpack distribution and duration	22	56	44
Vadose zone	Solid phase	Elemental composition and mineralogy	12	60	40
		Texture and physical characterization	33	59	41
		Structure (soil depth, layers)	35	61	39
		Organic Carbon	24	61	39
		Radiogenic isotope composition	2	50	50
	Litter	Litter composition and biomass	19	48	52
		Soil respiration	15	50	50
		Microbial biomass above-belowground	10	36	64
		Root density	21	31	69
	Liquid phase	Soil moisture	32	57	43
		Soil temperature	24	62	38
		Hydraulic head	20	44	56
		Matric potential, specific conductivity	24	45	55
		Water chemistry	19	54	46
Saprolite and bedrock	Solid phase	Texture and physics/structure	18	45	55
		Element composition/organic matter	8	67	33
		Petrology/mineralogy	7	43	57
		Age or rate constraints (radionuclides)	3	25	75
	Liquid phase	Potentiometric head, temperature	7	38	63
		Groundwater chemistry	5	38	63
		Gas chemistry	2	100	0
Surface water	Hydraulics	Instantaneous discharge	34	54	46
		Sediments	17	62	38
	Water quality	Water temperature, Electrical Conductivity, pH	25	69	31

		Water quality – Spectral Absorption Coefficient (DOC)	20	68	32
		Water Quality (nutrients, major cations / anions, others)	29	63	37
		Stable isotopes	9	90	10
Biosphere	Habitat/ vegetation/ crop	Habitat mapping	27	42	58
		Structure (height) and dynamics	32	43	57
		Above-groundbiomass	35	52	48
		Leaf area index	27	46	54
		Photosynthesis (Chlor a)	16	45	55
	Biota, diversity	Birds	4	80	20
		Ground beetles/spiders	5	57	43
		Soil invertebrates/gastropods	7	56	44
		Soil microbial diversity	5	60	40
		Benthic invertebrates/fish	6	57	43
		eDNA (environmental DNA; species detection)	2	50	50
		Food web diversity (e.g. AMMOD)	7	67	33
		Vascular plant diversity	11	53	47
		Lower plant diversity	7	50	50
		Fungi	4	50	50
		Biofilm	1	100	0