Anonymous Referee #1

Received and published: 19 December 2017

R1: The study by Baatz et al. assess the current status of the level of integration of models used by the LTER and CZO communities, and gives perspectives how the fusion of measurement and modelling communities could exploit the full strengths of observational networks to increase our understanding of Earth System Dynamics. In my opinion, this attempt is timely and deserves the presentation in a journal like Earth System Dynamics. There are many straightforward thoughts in this manuscript, and also the analysis of level of integration and the survey itself are useful instruments.

Thank you for taking the time to review and for your positive comments on our short communication manuscript.

R1: However, I see three major points that need thorough revision.

1. The utilization of terms (integration, incorporation, linkage of data model-usage, coupling) is not precise, and especially terms like model integration should be defined thoroughly and then remain reserved for the given used. One example is the abstract:

"Advancing our understanding of Earth System Dynamics (ESD) depends on the development of models and other analytical tools that integrate physical, biological and chemical data. This ambition of increased understanding and model development of ESD based on integrated site observations was at the origin of the creation of the networks of Long Term Ecological Research (LTER), Critical Zone Observatories (CZO), and others". If I understand it correctly, in the second sentence, "integrated site observations" means a set of measured variables that comprises both driving variables and target (mapped) variables that are necessary to run and validate a process based model. As the preceding sentence already uses integrated, I suggest rephrasing the next one, otherwise the readers will stumble already here. In addition, objective 3) (Line 10) suggests network integration. This needs to be specified, and distinguished from model integration. In addition, the difference between model coupling and integration is not clear, and the terms are used interchangeably (see section3.2), though they are not: Is integration of a new variable more pertinent or could these processes be used at the same time, or would model coupling be more efficient? Furthermore, it remains unclear what exactly the authors mean with data-model linkage, and how was it quantified?

Answer: Thank you for this specific suggestion which is shared by Referee #2. We admit that some terms were used ambiguously in several places. In the revised manuscript, we define each term upon first usage and remain consistent throughout. More specifically, we use data application instead of model-data linkage and associated terms. We use steering synergies of observation networks when we refer to the 'coupling' or 'integration' of observation networks. We use more specific and exact wording for model integration and model coupling. We explain the elements at first appearance, near the conceptual diagram that present the different steps and processes for which this paper brings new perspectives.

R1: 2. To this end, I suggest introducing a figure on how data assimilation, data integration and model coupling are related, where can they complement each other, and what are the differences?

Answer: Thank you, we agree that a visualization of the concepts and processes through a flow chart would be useful. In the revised manuscript, we added the Figure below.

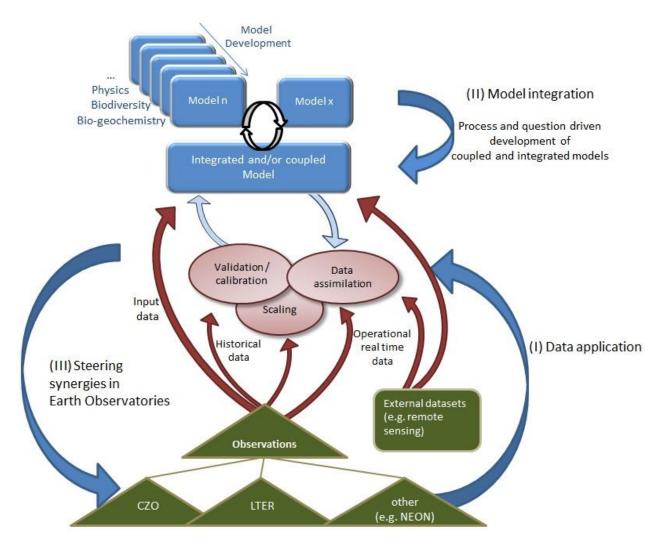


Figure 1: Flowchart of concepts, pathways and processes of applying terrestrial observatory network data to earth system dynamics models; identifying the three challenges of (I) data application, (II) model integration, and (III) steering synergies in observation networks.

R1: 3. The structure of the paper needs to be changed. A materials and methods section is required to give the reader an overview on the questions posed in the survey, and on the evaluation methods. The current Appendix structure (Appendix figures were missing) produces duplicate information which could be avoided when materials and methods section would follow the introduction.

Answer: Thank you for the suggestion. Your suggestion to bring the appendix into the main part of the manuscript was also made by Referee #2. In the revision of the manuscript, we follow your suggestion to bring information on Materials and Methods from the appendix into the main body of the manuscript.

R1: In general, the different paragraphs even in a section or sub section need to be linked in a more straightforward way, and the writing styles need to be harmonized.

Answer: In the revision of the manuscript, we specifically work on linking the paragraphs, one by one, in a harmonized manner to make the writing more consistent and easy to follow.

See for instance at page 3 L15, where we added: 'For these purposes, the '.

R1: See some more detailed comments below.

Title

ok

Highlights

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Abstract

L6: "we look for" sounds colloquial, I suggest changing to "The survey results identified gaps . . ."

Answer: Agreed. Changed as suggested.

L10: please specify complementarity. Unclear if you mean complementarity of networks or observations that occur at given sites, but are missing at the other.

Answer: We use complementarity to refer to both network topology and specific elements in terrestrial observation networks. We clarify this in the revised version: 'identifying complementarity in measured variables and spatial extent'

L13: functional topological network: Formulation unclear. Please specify.

Answer: Agreed. We now use the following formulation in the revised version: 'including co-location of sites of the existing networks and further formalizing these recommendations among these communities.'

Introduction

L20: this is an odd sentence, I don't think it's verbatim. What exactly do you refer to with "scientific and societal imperatives" which are paramount to improve our understanding? Please rephrase the sentence, and probably split it.

Answer: Scientific and societal imperatives refer to global change and the threats that it poses to Earth's habitability. We restructured the first three lines, and split the sentence as suggested:

'Complex interactions among 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 the Earth as habitable space, the scientific and societal demands require improved understanding of Earth System Dynamics (ESD).'

L30: exemplary is ambiguous here. I suggest to change to "are for instance networks . . . " **Answer: Agreed, changed as suggested.**

P3L2: ESD has been introduced before. **Answer: Yes, statement removed.**

P3L3: please rephrase sentence, it starts with "...range form...", but there is not "to".

Answer: Right, we rephrased the sentence.

P3L2-10: This section is fundamental in this contribution. It contains data assimilation, an attempt to define integrated/coupled models and calls for "more" integrated models.

The authors need to clearly define the borders what can be achieved with data assimilation, model integration and model coupling, work out what the differences are and to comment on if "more integrated" models are less or more efficient than coupled models. I also suggest having a figure here on how data assimilation, model integration and model coupling is connected or distinguished.

Answer: We think it is a great idea to add a figure to clarify these concepts. As outlined above, we expanded this paragraph, and added a figure linking concepts, connections and bottlenecks.

L11: how exactly are more integrated and coupled models different? For more integration, capabilities of a usually couples model need to be implemented in the parent (less) integrated model. There are also several ways of coupling, which should here described in detail.

Answer: We do prefer not to go into all details of different techniques and nuance of differentiating integration and coupling of models. We expanded this section by 1-2 sentences describing the ways of integration/coupling:

'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 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.'

L13: At this point the authors bring in another terminology: incorporation of measurements. I suppose, this is in no way different from data integration. Please be very clear at this point. Incorporation also contradicts the coupling approach promoted in the preceding sentence.

Answer: We now use data application throughout the manuscript. Here too, 'incorporation of measurements' was changed to 'data application'.

L17, and following two paragraphs come out of the blue. A connecting, introducing sentence is required at this point.

Answer: We agree and added a connecting introductory phrase: 'For these purposes, the '.

P4L6-9: The sentence seems too long for the part of the message I understand. I am not sure what your mean with organizing science questions. If I get it right, I suggest: "At the same time, the science questions, observed variables and associated measurement methods lead to . . ."

Answer: Thank you, we added the suggestion and shortened the sentence to focus more on the message.

L10: I suggest deleting the "Here".

Answer: Agreed. We used "For this study," instead.

L12: still at this point model integration and linkage of data-model usage remain vague.

Answer: We followed your suggestion, defined the terms 'model integration' early in the manuscript (as outlined above), and use the term consistently.

New formulation: 'Integrated models include cross-scale and cross-disciplinary processes that are needed to fully predict ESD responses to...'

We also use the term 'data application' to models now instead of data-model usage or linkage, or related expressions to be more consistent and clearer.

And

L17-28: Introduction could stop here. I find it very odd that you dive in section 2 directly into the Challenges without describing what was asked in the survey. I strongly advocate for a materials and methods section, as the neglect of the named section leads to duplicate information in the appendix.

Answer: We agree and, integrated this section with the newly introduced Materials and Methods section.

Materials and Methods (in appendix, unfortunately)

We introduced a Materials and Methods now by briefly presenting the survey setup and analysis of the responses. The results which were previously in the appendix, were now integrated into the 'Current status' sub sections of the three challenges.

Results

P5L1: How is data-model linkage defined? This needs to be explained in a preceding section (e.g., Materials methods or such like) P5L3: Appendix and supplement: quite vague. All appendix, all supplements? The fundamental data should occur in the main text body.

Answer: Thank you. We addressed the previous two comments by following your suggestion to place the Materials and Methods section between the Introduction and the Challenges in the main body of the paper.

L15: Does "used" mean that it is an input variable or a target variable. Please consider having the categories input and target variables at this point. It may be useful information if calibration/validation data has been determined at the site directly.

Answer: In our survey we asked about usage of the variables used as 'model input,' 'input or calibration/validation', or both. We now moved the following sentence to the more relevant position at the end of this paragraph:

'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).'

L20: I don't see the relation of this paragraph to the section head "data-model linkage". Please consider having another section head, or link figure one with (for instance) scales of the input data. This would be the link to your section head. In Figure 1 I suggest leaving the 0-values white.

Answer: We revised this text to clarify its meaning and emphasized its relevance to Figure 1 (now Figure 2). This figure delineates the character of current model usage and observations within the LTER and CZO networks based on results from the extensive survey. To make this more clear we added:

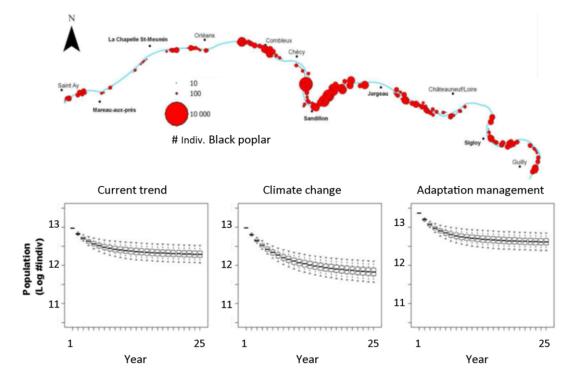
'This result stresses the relevance of both observation networks to ESD processes in terms of the spatial and temporal scales in CZO/LTER modelling activities. At the same time, Figure 2 reveals a lack of modelling activities at larger extent (continental and global) in both communities.' From our perspective and as stated, linking CZO/LTER observation data to ESD models is critical to addressing these scaling challenges.

Regarding the 0-values of Figure 2, we left the 0-values light-grey, because the survey relies on participants' answers and is not exclusive. Thus, the light-grey color stresses the light/dark contrast but not the values.

P6, section 2.2: I suggest reducing this section to one paragraph, i.e., only giving one example, but explain this properly. The corresponding figure is illegible, especially the river-like structure, the model structure? (seed rain model and some ellipses and arrows, without explanation), is it boxplots I am looking at, is the reference scenario "human impacted" only? Also after several readings it is not clear to me what the difference between data-model linkage and integrated modelling should be, especially if the Figure caption starts with "Integrated model . . ." and section 3 is on integrated modelling. The reference to the figure is missing.

Answer: We clarified this figure by reducing it to its key elements. We highlighted the relevance of the example to the Challenge 1 by stressing the huge number of diverse and site-specific types of observational data used in current LTER/CZO models:

'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.'



New caption 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).'

L24 "holistic integrated models". This class has not been defined before. Does this class comprise all the models used by the survey respondents?

Answer: We agree that the term holistic does not introduce new information, and therefore removed this term.

L25/26: unclear what "replaced" means. Would modellers prefer using other products than the directly measured ones, and what would be the reason? The following sentence claims that there is a need for on-site measurements, but would they be used?

Answer: Agreed. The term replaced is ambiguous. We reformulated:

'As the survey results demonstrated, for some themes (e.g., habitat/vegetation/crop), remotely sensed or existing database information was preferably used in contrast to potential data from on-site field measurements (Table A1).'

Furthermore, we argue that generally on-site measurements are more accurate than remotely sensed information.

P7L9-10: All disciplines and compartments should be subject to the main text.

Subsection 3.1: I don't fully understand how the level of integration was calculated exactly, and how the variables (L12, 14) find their way into this metric. Please specify. The metric "level of integration" is also not discussed in this section, but there is only a reference to the figure.

Answer: We agree that the level of integration needs to be clear. We moved our explanation of this metric from the appendix to the main text on page 5 lines 5 to 7:

'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.'

L30-31: According to the subsection head this section is about integrated modelling. In the named lines, it says "requires coupling of models. . .". This switch of model integration to coupling is really confusing, and inadequate.

Answer: We agree that it is confusing to use coupling and integration interchangeably. We now stick to the one term integration – that includes the 'coupling' of models through model couplers - for the revision and modified the passage accordingly:

'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).'

P8L1: RT-FluxPIHM: what is the purpose of this model?

Answer: Right, we clarified that this model integrates geochemistry and hydrology: '...RT-FluxPIHM, which integrates processes from a reactive transport (RT) with a land-surface and hydrologic model (FluxPIHM) ...' L10: I suggest stopping here (don't give the next example) and tell the reader what the preliminary results were. The figure suggests increased groundwater flow though now trees with a greater rooting depth are present. Please discuss this briefly, and what regional implications does it have?

Answer: We agree and omitted the second example. We clarified that the examples are presented not for their results, but to illustrate how the models are constructed. References are provided if the reader is interested in the specific results. We briefly discuss the results now in the text: 'The enhanced vertical macro-pore development through deeper roots of woody encroachment compared to grass led to higher groundwater flow (Figure 5b).'

P9L18: please add the appropriate reference to your analysis.

Answer: The reference to the Figure was added (Fehler! Verweisquelle konnte nicht gefunden werden.).

P10L18-20: Please rephrase sentence.

Answer: The sentence was rephrased to be more clear:

'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).'

P11L18-20: True, but this paper would be a chance to describe how this could be set into action.

Answer: Agreed, but we regret that describing frameworks is out of the scope of this paper. We rephrase:

'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.'

P12L29-30: Please finish this sentence.

Answer: Right, the ending of the sentence was reformulated to:

'Parsimonious 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.'

This section: what do the communities think of your two suggestions? Would a new network replace the old ones? Please also specify the term functional topological networks. What does it imply for the networks.

Answer: Thank you, we now removed the term 'topological' networks to avoid being ambiguous. We also reformulated the strategies proposed towards focusing more on steering synergies in the observation networks. This is reflected in the new title of the manuscript:

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

and detailed in section 6.3 Strategies for steering synergies in Earth observatory networks. The main strategies on steering synergies of observatory networks are to increase the interaction of observatory networks, focus on data harmonization, and co-locate sites of different networks:

'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.' and

'Furthermore, the interaction of observatory networks increase the spatial coverage of multicompartment observations, allowing ESD models to address research questions and testing hypothesis over larger scales gaining full benefit of multi-compartment CZO and LTER data.'

The reasons to focus on steering synergies are diverse:

'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.' and

'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.'

P13L19: here the term "more deeply-informed" comes into play as another model class. It is necessary for the authors to clarify how this translates to model coupling, integration in their opinion.

Answer: We agree that this may cause confusion. We avoided using the term 'deeply-informed' when talking about models informed by data/data assimilation and use the terminology that has already been introduced.

Anonymous Referee #2

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The manuscript discusses a very pertinent problem in Earth System Dynamics and for that reason merits consideration in principle. However, it does so without sufficient technical coherence and depth, transmitting the notion of a vague opinion paper than a thoroughly developed scientific study, which would be needed to provide solid grounds to the argumentation conducted in the manuscript.

The obstacles being already at a scientific language level, where there is no syntax unicity behind fundamental concepts. In practice, each and every term prone to cause confusion should be clearly defined in a rigorous manner, e.g. as the other reviewer pointed out "integration, incorporation, linkage of data model-usage, coupling". Otherwise this is not a scientific paper, but rather a soft-formulated style of manuscript tailored for a non-scientific audience (which has its merits but is outside the scope of ESD).

While articulate divagations with catchy phrases and buzzwords may be popular in some soft venues in environmental science (e.g. Water Resources Research, WRR) and outreach communication (EOS or general media), this sort of approach feels out of place at ESD. In fact, here a rigorous "hard-science" treatment and discussion of problems should rather be the norm. For every bold statement of opinion, a rigorous scientific argumentation is a fundamental requirement, and in many cases mathematics are actually extremely helpful for that purpose.

My recommendation is thus to restructure and strengthen the paper so that its true scientific DNA comes out and the formulation, methodologies, definitions and overall concepts are all clearly stated. To drop the fashionable WRR-style beauty without substance, and rather take a more sober, theoretical ecology or ESD style scientific construct. The ESD readers will highly appreciate your insightful rigour.

Moreover, a clearer distinction should be made between the known facts and insights, and the novel contributions brought on by this study. The strategies followed in the study should also be more explicitly and rigorous formulated and justified, alongside with their merits and caveats. At some stages, the reader is left to wonder what has actually been done in practice, and what are essentially suggestions and statements of purpose. The formal procedures belong to the main body of the manuscript, as they are fundamental to bring more substance to the eloquent argumentation.

In order to actually grasp some basic sense of the scientific work beneath the manuscript, the reader has to jump between the main body and the supporting/annex material, where hope begins to emerge that there might be something to this study beyond the vague statements typical of an opinion paper.

In conclusion, at this stage I cannot enter into specific technical recommendations because I see a profound lack of substance and consistency throughout the manuscript. I enjoyed reading it as a person, but felt utterly disappointed at the lack of substance as a scientist.

Notwithstanding my criticism, I do see potential for this paper to succeed in ESD. This is why, despite disappointed at its content after the initial excitement brought by the abstract, I do not recommend rejection at this stage. I believe in the purpose, I believe in the mission, and I hope that despite the limitations of my own review assessment, it will somehow contribute to help the authors reformulate and strengthen their message. However, for publication to happen at ESD, it is my firm understanding that it will need to be reformulated more scientifically. And at that stage, we can discuss whether the scientific and technic details will substantiate the author's eloquent argumentation.

We thank Referee #2 for his/her thoughtful and constructive review of our manuscript. The reviewer appears to have unmet expectations of reading a Research article, which was not the purpose of this manuscript. Rather, our manuscript is a Short Communication, describing and discussing results of a community survey to raise questions for future discussion and analysis. Bringing a high level of detail while at the same time a high level of abstraction, we thoroughly analyzed the survey's results, discussing the merits of the survey and the limitations of the analysis. The survey's outcome is described, synthesized and discussed in terms of information on synergies, challenges and perspectives to ESD modeling as seen by scientists of the CZO, LTER, NEON and ISMC networks. We do not understand the reviewers concerns about Water Resources Research, which is a fine journal publishing highly detailed and rigorous results from observational, theoretical, experimental and modeling studies. More fundamentally, we argue that our Short Communication falls squarely within the domain of ESD which is "dedicated to the publication and public discussion of studies that take an interdisciplinary perspective of the functioning of the whole Earth system and global change" and "accepts research articles, review articles, short communications, and commentaries."

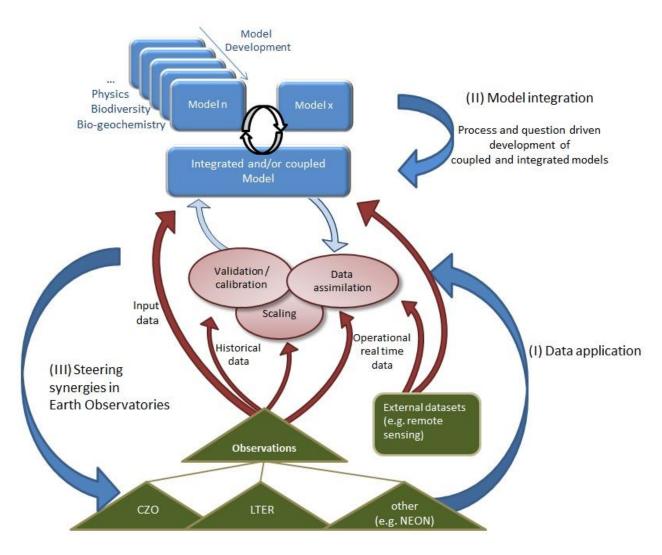
Many of the Referee #2's comments were consistent with those of Referee #1. We have made our use of terms more consistent and clear and have moved the materials and methods from the appendix to the main text. We point out the difference between integrating models and coupling models, e.g. here:

'For this 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.'

Where appropriate, we reformulated and strengthened statements and argumentation, adding e.g.: '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.' or:

'LTER sites answer specific ecological questions, for which specific data are gathered, e.g., Black poplar population persistence under climate change.'

With a conceptual graphical presentation of the flow between observation network data and model development, indicating the different aspects of data application, model integration, and steering synergies of observational networks, we believe the paper will grow to the strength and scientific DNA the reviewer refers to. We inserted:



Caption of Figure 2: '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. '

<u>Integration of Steering synergies in</u> terrestrial <u>observational observation</u> networks: opportunity for advancing Earth system dynamics modelling

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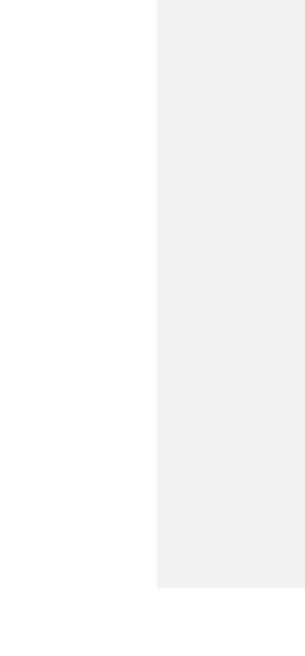
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Abstract. Advancing our understanding of Earth System Dynamics (ESD) depends on the development of models and other analytical tools that integrateapply both physical, biological and chemical data. This ambition of increased understanding and model developmentdevelop models of ESD based on integrated site observations was at the origin of the creation of stimulus for creating the networks of Long Term Ecological Research (LTER), Critical Zone Observatories (CZO), and others. We organized a survey-to identify, 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. With the survey results, we look for gaps between data collection, and ESD model development, to draw perspectives for the provide insights for improvement both in data collection and model integration.

From this <u>survey</u> overview of <u>modeldata</u> applications <u>gathered</u> in the context of LTER- and CZO research, we identified three challenges: 1) <u>Improving integrationwiden application</u> of <u>observational terrestrial observation network</u> data in Earth system modelling, 2) developing <u>eoupledintegrated</u> Earth system models that incorporate process representation and data of multiple disciplines, and 3) identifying complementarity, and ways to integrate in measured variables and spatial extent, and promoting <u>synergies in</u> the existing <u>observational networks</u>. These challenges lead to perspectives and recommendations for <u>strategic integration of observational nimproved dialogue between the observation</u> networks and <u>links to</u>—the ESD modelling community. We propose the further integration, including co-location of the <u>observational networks</u>, either by 1) making<u>sites in</u> the existing <u>site determined networks also functional topological networks with organising spread and coverage, and/or 2) thematically and geographically restructuring or co-locating the existing networks, networks and further formalizing these recommendations among these communities. <u>Such integration Developing these synergies</u> will enable cross-site <u>and cross-network</u> comparison and synthesis studies, which will <u>offer significant help produce the</u> insights <u>and extraction of around organizing principles</u>, classifications, and general rules of coupling processes <u>and with environmental conditions</u>.</u>

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1 Introduction

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In light of accelerating global change (e.g. IPCC, 2014; Camill, 2010), the scientific and societal imperatives are paramount to improve our understanding of Earth System Dynamics (ESD), which comprise complex interactions amongbetween rock, soil, water, air, and living organisms that 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 (Banwart et al., 2012; Aronova et al., 2010; Banwart et al., 2012; Reid et al., 2010). For this purpose, observationalthese purposes, observation networks have been developed the last decennia aiming in recent decades aimed at a temporal and multidisciplinary coverage of continental and global scale ecosystem observations. The Critical Zone Observatory network (BrantleyWhite et

al₋₁₂ 2015), the International Long Term Ecosystem Research network (Mirtl et al., 20172018), the US National Ecological Observatory Network of the US (Loescher et al₋₁₂ 2017, Schimel et al₋₁₂ 2001), the Chinese Ecosystem Research Network (Fu et al., 2010) and the Australian Terrestrial Ecosystem Research Network (Lindenmayer, 2017), are a few exemplaryexamples of networks that focus at the continental to global spatial scalesextent, and daily to decadal temporal scales.

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One overarching goal of these research and observational 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 Earth System Dynamics (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) as well as), to distributions and functional roles of organisms, land use practices, climate, and humans (Mirtl et al., 2013). However, the majority of these models focus on one or a few processes, while integrated or coupled models offer frontier opportunities to explore cross-scale and cross-disciplinary processes that are needed to fully predict ESD responses to perturbations in combined local to global driving forces. No single ESD model can accomplish the full representation of pressure and response functions. An improved understanding of. 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 guides the development of more integrated terrestrial Earth system models (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 reason, eoupled model developing integrated models dealing with different processes, such as Land Surface Models, or coupling existing process models in suites and frameworks (e.g. Duffy et al., 2014; Peckham et al., 2013; Duffy et al., 2014) are one optionoptions 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 incorporationapplication of hydrological, meteorological, biogeochemical and biodiversity measurements from within and across sites into such coupledintegrated model systems (Figure 1) is a key component to providing the multi-scale/multi-process understanding that is needed to advance predictions of ESD responses to land use and elimatic climate changes, and the ever-increasing demand for natural resource demandresources.

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 offer the lens through which examine the interactions among the lithosphere, pedosphere, hydrosphere, biosphere and atmosphere can be brought into focus (White et al., 2015, Banwart et al., 2012; Brantley et al., 2007; Banwart et al., 2012). 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 (Lin et al., 2015; 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 advance our-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 leadled 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 site-network, and long-term datasets necessary to document and analyze environmental change. Larger scale case study areas (In addition, Long-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. Parr et al., 2002; 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. 20172018).

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 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, although these networks were not specifically designed to promote it, the nature of the organizing science questions, Earth systemobserved variables being characterized, and associated measurement methods used for measuring those variables, 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 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?

HereFor 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 linkage of data-model usage application. ISMC envisions 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 modelmodeling approaches that use data from the LTER and CZO sites.

With the survey, we examined the complementarity and disparity among the models used in the two networks, identified gaps in current data collection and how those data are used in models, and propose a path forward to bridge these gaps for improving both novel data collection and model integration in ESD science. Details on the survey results and analyses can be found in the Appendix, while survey questions and responses on model applications are found in the Supplement. We note that the survey was completed on a voluntary basis, which implies that not all modellers working with LTER/CZO data and models responded; thus, we acknowledge the list of models used in LTER and CZO communities is far from complete. However, more than 70 responses to the survey allowed exploration of the availability and use of observational data for modellers. Moreover, the survey informs the scientific community on the status of evolving and optimizing the monitoring networks, and communicates individual and common values of these networks for the Earth system modelling community. The survey listed 52 variables (see Appendix Table 1) based on the common measurements in the LTER and CZO networks. The respondents were asked to identify the source of the data used, being data measured at sites (LTER and/or CZO) or obtained from other sources such as remotely sensed, modelled, or literature.

Based on the results of the survey, we come to definedescribe challenges and perspectives implications for 1) usage of observatory data in integrated ESD models, 2) model integration in relation to specific disciplines, and 3) complementarity

and possibilities for network integration.steering network synergies (Figure 1).

Material and Methods

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The survey was addressed to the principal investigators (PIs) of individual CZOs, to the larger Critical Zone Exploration 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

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

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(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.

5 3 Challenge I: Observatory data application to ESD modelling

3.1 Current status

2 Challenge 1: Data-model linkage

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.

15 2.11.1 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 Current status

In response to the survey (see Appendix and Supplement for details), the 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 CO₂), 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. The average model used 14 variables of the supplied list, ~2/3 of Model applications affiliated with the CZO were more focused on the variables for model inputlithosphere and ~1/3 for calibration/validation (Appendix Table 1)-cryosphere, while biodiversity was addressed only in models of the LTER community (Figure A1e). While the CZO model applications use variables and data of 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 (FisherFisher's exact test, p<0.05) more data of based on eddy flux measurements (evapotranspiration and CO₂), root density, soil water content, soil

temperature, bedrock, and soil texture and physics compared to models associated with LTER. Models using data of related to habitat mapping, biotic and biodiversity elements were associated much stronger with the LTER community.

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 include snowpack distribution and duration.

Figure 1 presents

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There is a large congruence in the spatial and temporal scales modelled with the density of model applications. There is a large congruence in spatial and temporal scale between both modelling communities. Spatially, the model applications extend mostly from Spatial scales of models were primarily site- to catchment scales, with few occurrences models at them acro pore, lab or global scale; (Figure 2). The high density in the center of Figure 1 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 time scaleresolution. 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 macroporemacro-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. This also lines well (Figure A1d). These scales of modelling are consistent with the focus on management and predictive process and system understanding of both network's model applications for LTER associated responses, while CZO applications focusthe management and prediction aspect is more strongly on the description of embraced by LTER model applications in the interplay between various processes.survey results (Figure A1c).

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2.23.2 Example of data-model linkage application from an LTER site

Next to the common, cross-site measurements, observation networkCZO and LTER datasets often alsogenerally include some site-specific elements for individual sites, types of observations gathered from the perspective of prediction and model development, to deal with answer site-specific scientific questions of on model development, ecosystem responses response to global change. An 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.

2.33.3 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 into enhance predictive modellingcapacity provides a strong opportunity 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—holistic 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 have—shown_demonstrated, for some themes (e.g., habitat/vegetation/crop)—potential_data_from on-site_field measurements are often replaced by), remotely sensed or existing database information (Appendix was preferably used in contrast to potential data from on-site field measurements (Table A1). This suggests a strong need of on-site measurements for these data for modelling site-specific processes because). 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 absence of harmonized measurements, and the time and personnel-consuming requirements for data_gathering-collection, and the absence of

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harmonized measurement protocols. The strong complementarity identified in data sources and model applications, in terms of biotic vs abiotic and above vs below ground 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.

In line with the observatory missions, models using LTER data more strongly embrace management and predictive applications (Stoll et al., 2015) ranging predominantly from site and sub-catchment to region, from days to decades, compared to CZO models that focus more on process/system understanding and are more geophysical and subsurface oriented with a wider range of scales from lab to global, from seconds to millennia (Appendix Figure 6). The biotic theme in the survey is only covered by applications of LTER, whereas petrology and mineralogy are only covered by CZO model applications (Supplement). The results reveal the strong complementarity of models used in the CZO community addressing below ground processes while for LTER the focus lies more on above ground processes.

34 Challenge 211: Model integration

4.1 Current status

15 3.11.1 Current status

To answer the question how data-rich LTER and CZO sites are used in holistic, integrated models, a 'level of integration' was calculated for each model by normalizing to the scale 0 (low) to 1 (high) the number of disciplines (e.g., atmospheric circulation, biodiversity, biogeochemistry, and others, see Appendix Figure 6) and compartments (e.g., Atmosphere, Hydrosphere Lithosphere, and others) indicated by the respondents, and equally weighing them. The models using data from the LTER and CZO networks cover a wide range of integration, from very specific singular process models (little integration and variables), to highly integrated models that cover many disciplines and compartments, and have large numbers of variables. On average, models had a rather high level of integration is present for the models, meaning that the ; CZO and LTER and CZO data model applications cover on average multiple disciplines (mean=3.6; sd=±2.1 standard deviation) and ecosystem compartments (mean=2.7; sd=1.6). Models using data from both networks were in the higher data use range. Highest integration of data and disciplines in models is present in hydrological and geophysical disciplines.±1.6), Model 'level of integration' iswas strikingly similar in LTER and CZO data applications andCZO (mean=0.37±0.18) and LTER (mean=0.34±0.17). The richness in variables was positively related to the number of disciplines (R² = 0.29), and to compartments (R² = 0.4). However, unifying compartments and disciplines to the 'level of integration' measure correlated most strongly to the number of variables (R² = 0.47) (Figure 4).

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3.24.2 Example of integrated modelling

Plant-soil interactions are changing across the globe, whether it beby the encroachment of woody species into polar, alpine and temperate grassland areas (Archer et al., 1995; Jackson et al., 2002), the increase in atmospheric CO₂ 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 injection introduction (spatial distribution) of organic carbon into the ground, controlling microbial productivity and respiration, macroporemacro-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 CO₂; (Jones, 1998)). These factors will impact infiltration of meteoric water charged with carbonic acid (H₂CO₃), 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 coupling integration of modelsprocesses from twodifferent scientific fields, a reactive transport 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 to the RT-[FluxPIHM-Model] (Figure 5) (Bao et al., 2017; Li et al., 2017a2017). To further understand how these systems evolve in response to land cover change, we can couple these models with ecosystem models, such as Biome BGC (Thornton et al, 2005). One limitation to such complex 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. For example, 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) altersalter groundwater flow patterns, and thus stream water discharge and solute behaviour. The enhanced vertical macropore 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. As another example, the Dhara model resolves coupled soil-vegetation dynamics affecting water and biogeochemical processes. It has been used to examine the impact of tile drains on nutrient transport in agricultural watersheds (Woo and Kumar) and potential impact of ecohydrologic response to climate change on spatial hydrologic patterns (Le and

3.34.3 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 localsites to continental scales continents (Grimm et al., 2013). Simple In our survey, 10% of the models, also called parsimonious already used data from both LTER and CZO networks in model applications. This implies that these models, are models which aim at predictions using as few variables as possible and limitting process representation to the necessary minimum. Parsimonious models can provide good conceptual frameworks, also for already integrated questions. At the same time, parsimonious models processes of interest to the two communities. However, inclusion of multiple disciplines and ecosystem compartments may not increase model complexity and data requirements. Hence, integrated modelling may be spatially explicitlimited by data availability, but developed for highly specialized process representations and particular purposes. Therefore, parsimonious models stand in contrast to the desired prediction capability of models for nonlinear environmental system responses to global change. However, the development and use of parsimonious models is advantageous for targeted processes within disciplinary boundaries, yet, the allows for more general applicability of conclusions drawn is highly limited (Basu et al., 2010; Li et al., 2017b). It is an interesting question whether data access limits model integration, or whether a lack of integration is mainly caused by the model development side. Model integration is data demanding. 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. 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. It does not necessarily mean that the data are co-measured. Where CZOs mainly focus on understanding near surface structure and dynamics, integrationdeveloping 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 a minimal level of integration, fundamental process understanding, with using specific parsimonious models, nevertheless remains integrated models remain an essential part of the mission. Model integration does not necessarily require an increase in model complexity. Parsimonious 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,

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45 Challenge 3III: Complementarity and/or disciplinary segregation

5.1 Current status

4.11.1 Models Current status

In an ordination of the model variables (see Appendix), models that usedincluded data offrom both LTER and CZO sites cluster in the center of the ordination of the surveyed models ((Figure 6)), which indicates that those models use a fairly similar and large group of variables. A significant number of The models are co-located in the center, focusing of the ordination focus mostly on hydrology and geophysical processes. The Group A models Models clustered in group A are associated with CZOs concentrate, are mostly located in the second quadrant, and are distinguished by thea focus on modelling processprocesses in the petrologysoil profile, regolith, and bedrock. The Group-Models clustered in group B modelsare associated with LTER dataLTERs, are mostly located in the first and fourth quadrants (Figure 5) resorting under the ecology discipline, and focus on processes related to habitatecosystems and biota. Disciplines separate from The horizontal axis of the ordination separates physics-oriented to from biotic-oriented models, along with compartments from and below-ground (negative) to above-ground (positive). The vertical axis distinguishes stronglyhighly integrated models, mainly hydrology-based, which contain a number of processes, from specific models, such as those focusing only on rock weathering models focusing only petrology/mineralogy.

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4.25.2 Open issues and implications to join the networks and communities' expertise

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. Although few up to
now, these examples show the opportunity these observation network data offer to integrate a larger number of compartments
in models. Biotic data are applied in models of the CZO community (for instance, see Data Integration example), but they are
few in number. Nevertheless, there is strong evidence for the important role of biota in coupled processes such as energy,
carbon and nutrient cycling, and weathering (Filser et al., 2016;Richter and Billings, 2015;Wall et al., 2015). The (Figure 4).

However, the outlier position of models focussing on biota and habitat variables in the ordination (Figure 6) indicates the need
for integration of to integrate the biotic compartment in model development (Vereecken et al., 2016b). Therefore,
harmonization and standardization of biotic observations is particularly important for those biotic variables related to models
of coupled processes such as energy, carbon and nutrient cycling, and feedbacks with the hydrologic and biogeochemical
eyeles-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 data application formodels 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

Available data sets provide the opportunity to integrate a larger number of compartments into ESD models, but the ordination

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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 the terrestrial Earth system science and models (Key to Soil Organic Matter Dynamics and Modelling – Keysom-Biolink project, Filser et al., 2016), along withand the provision of substantial datasets on soil biota and biodiversity (global soil biodiversity database, Ramirez et al., 2015). Models 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 the often discipline specific data, as well as 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.

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56 Outlook

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5.16.1 Satisfying cross-disciplinary data demand forby ESD models

The relationship of models and data is a relationship of mutual benefits. Data are collected in tremendous efforts for serving Data enable scientists to develop and test hypotheses (e.g. Braud et al., 2014; Clark et al., 2011). Models, but models may also help scientists to better design data collection strategies and tactics infor 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 answertest hypotheses. Stochastic analyses can be used to identify key physical processes and their impacts if variables are subject to change. Models Thus, models can feed back to data through evaluation of improved improve observation network strategies including by quantifying process sensitivity to observation observed variables, and parameters, as well as measurement frequency, orand resolution/extent_needs in space and time (Lin, 2010). ConsideringModel-based assessments of observability, predictability, and the impact of heterogeneity on processes at the relevant scales through modelling could reduce resources spent on specific could improve network data gathering collection efficiency and benefit the gain in observing complementary data sets. Another aspect brought by merging complementarity. Merging data and modelling through data assimilation is the potential facilitation of upscale cascading of knowledgealso may enable testing predictions from smallersmall-scale process understanding toin larger-scale, simplified representation, patterns and parameterization (Heffernan et al., 2014; Vereecken et al., 2016a). In this way, models can feed back to data and even drive observation requirements for maximum benefits for the model-representations (Heffernan et al., 2014; Vereecken et al., 2016a),

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In particular, the reanalysis concept addresses the benefits of a strong model data linkage. Frequently application in ESD modeling. Although it is widely used in meteorological models (e.g., Compo et al., 2011; Dee et al., 2011), reanalysis is not has

only sparingly been used in terrestrial Earth system science, especially or ecology, yet, as it is in atmospheric science. 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 observation, model and forcing uncertainty, in observations, model structure, initial states and forcings. Application of reanalysis in Earth system models could generate gap filled, holistiemulti-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 observational 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 bio geochemical concepts, hypothesis, and observations, and explore historical developments in the context of Earth system science. However, such ecosystem reanalysis depends on the quality of the observational data and needs to be physically coherent. Many challenges such as the optimal 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 need to be addressed for generating ecosystem reanalysis data encompassing variables characterizing biological processes and biodiversity.

Where there

1994; Richter and Billings, 2015), there is nevertheless a general knowledge gap for biotic elements in integrated ESD models. More specifically, a clearer (Deruiter et al., 1994; Richter and Billings, 2015). Such efforts must be based on improved understanding of the physicalbiotic-abiotic interactions, feedbacks, and chemical processes that shape the environment in which biota respond to climate forcing and shape the physical environment themselves is required based on a solid observational basis to detect and predict thresholds, since small changes in temperature and precipitation may cause a non-linear and irreversible response in ecosystem structure and function (e.g., forest die-back Breshears et al., 2005). The emphasis of CZOs on geophysical processes reduces the focus on biotic and ecological dynamics that drive much of the dynamic responses of the Earth system. Phenomena Integrated ESD models must include phenomena such as community assembly, evolution, the emergence of pests and pathogens, and colonizationinvasion by invasive species has important effects on ESD, but, which are not well represented currently included in most CZO studies models. New initiatives have been launched recently to integrate the biotic component in Earth system science and models (Filser et al., 2016). Measurements, including, for example, modelling the roles of biota in the subsurface (e.g., bacteria, fungi, roots), especially at depth, is expecting strong developments in the coming decade as is the modelling) in the subsurface (Grandy et al., 2016). As explained in the section on network integration, harmonization and standardization of biotic observations could better facilitate access to biotic observations related to processes and feedbacks with the At the same time, improved representation of processes such as

A related challenge is strong evidence for how to represent the specific roleroles of biota in ESD processes (Deruiter et al.,

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hydrologic and geochemical cycles. Network may improve the integration would feed the of LTER need for a deeper geoscience emphasis models.

5.26.2 Integration of models

- Integrated models covering different disciplines and compartments are needed to objectively raiseincrease 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, but is challenged by. 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.
- Yet, integration does not necessarily mean that individual models need to increase in complexity. In the realm of higher integration for inter disciplinary understanding of feedback mechanisms across disciplines and scales, parsimonious models can be integrated in a larger model platform (e.g. Peckham et al., 2013; Duffy et al., 2014) to investigate these feedback mechanisms over climatic and geographic gradients. A model platform was also a clear demand issued by the majority (80%) of the surveyed modellers. The respondents were less unified as to
- 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. Development of those models often requires 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). Such insights also can be gained through
 cross-site comparison and synthesis studies of observation data across different sites under gradients of climate, earthEarth
 surface characteristics (e.g., soil type, lithology, topography, vegetation), and human impact (e.g., pristine, agriculture, pristine,
 urban) conditions, which observation networks are well positioned to carry out. In turn, the need for calibration/validation data
 of integrated models can only be achieved when a well constructed network of biotic and abiotic observations make interdisciplinary data sets available to the model community.

30 5.36.3 Strategies for network integrationsteering synergies in Earth observatory networks

With respect to investigating specific aspects of ESD, the interactions of biotic and abiotic processes as well as below-ground and above-ground processes are key links, where geosphere focussed research by CZO and ecology focussed research by

LTER-could benefit observation and model integration wise. This also counts for the highlighted lack of integration of underground biotic elements, although the underground biota performs a crucial ecosystem functioning role (Deruiter et al., 1994; Wall et al., 2015). Data harmonization could be achieved based upon the concept of blending the conceptual frameworks of Ecosystem Integrity (Müller et al., 2000) and the Essential Biodiversity Variables (Pereira et al., 2013) as suggested Haase et al. (2018) and the Critical Zone approach (Chorover et al., 2015 and Brantley et al., 2016) 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 (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 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,

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integration efforts in several regions around the globe, basically aiming at the joint use of resource intensive observatories by more than one research community. The integration of existing research and observation networks can be accomplished by either 1) making the existing networks also functional topological networks (Brantley et al., 2017), or 2) thematically and geographically restructuring the available networks. For the first option, both LTER and CZO need to reconsider their existing topological structure in view of filling knowledge and observation gaps to their relevant large scale scientific questions crossing climatic, geographic and disciplinary gradients. For the second option, a new network can be proposed optimizing the thematic and geographic setting to answer the fundamental questions at the basis of the individual research sites' and observatories' conceptual models, as well as answering the Earth surface evolution and formation questions in their full spatial and geographical context over biomes and continents. The design aim of network restructuring would ideally be a controlled site selection process to cover climatic, geographic and disciplinary.

Drawing from the requirements of ESD modelling, and the apparent complementarities and synergies already lead to network

30 As indicated above, the situation of LTER and CZO research as well as the level of network integration and collaboration vary strongly between countries and continents around the globe. The challenges ahead for US-LTER, US-CZO and NEON are as specific as those for the European efforts to establish one joint research infrastructure. Considerations about network integration also

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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 levelsdegree of implementation and formalization rangeof observatory networks also varies with geography, ranging from regions with well-established networks (US-LTER, US CZO and NEON), to countries and regions where research and observation networks are based on the initiative of individual sites, observatories or projects.

Existing Some existing Earth observation networks such as NEON already are more systematic in topographicalspatial coverage and constitution, offering opportunities for the proposed advanced geographical integration ESD analysis. A notable European initiative is the Integrated European Ecosystem, Critical Zone and Socio-Ecological Research Infrastructure (eLTER RI), which comprises the definition of overall research challenges, includes the focal aspect of CZO research and requirements of widely ecosystem models. In order to successfully restructure the existing observatory networks, a dialog is necessary with the demand side of the ESD modelling community and to the need for integration of data with respect to the calibration/validation of current integrated models (e.g., Coupled Model Intercomparison Project, Mechl et al., 2005). This will help troubleshoot some essential missing parameters or problems with spatio temporal resolution and measurement accuracy. Furthermore, this interaction is necessary to construct the topology of an integrated research and observatory network, based on basic questions in ESD process understanding over larger scales and model calibration/validation needs to be answered by observatory network dataincludes 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.

67 Concluding recommendations

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The CZO and LTER networks should act as synthesizers of could promote interdisciplinary research approaches that lead to emergent understanding and ultimately result in more deeply informedimproves process-based models (Brantley et al., 2017; Rasmussen et al., 2011), in particular crossingspanning the boundary of geoscience that guides CZO and bioscience that guides LTER.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 for this objective, a stronger dialog is needed between the observatory networks. With the modelling communities, better communicationMore work is needed to enhance integration of apply CZO and LTER data in modellingESD models and thus strengthen the crucial role of the observatory networks in raising understanding of ESD processes and derive predictionderiving predictive capabilities for drivers, impacts and responses to global change. Additionally, there is a need for more conversation/coordination between modellers and empiricists to develop strategies for observation networks. The role of discussion amongst stakeholders, decision makers, funding agencies, observatory networks, and the broader scientific community cannot be over-stressed. The rapidly increasing technological

capabilities in computational power, ground based instrumentation, and unmanned automated remote sensing technologies 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/targets within allocated resources thanks to towards cross-community harmonized methods and data sets. The communication and exchange about services, and tools for making data-model linking available through web platforms offers obvious opportunities in this sense.

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

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20 7 Appendix

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7.1 Methods: Survey method and results

Questionnaires are a useful approach to derive opinion in a structured way from communities through individual responses (e.g. Blume et al., 2017;Reiners et al., 2013;Steel et al., 2004). In order to investigate the use of models and linkage of models to data in the CZO and LTER communities, a questionnaire was set up with multiple response questions. The communities were addressed by e-mail to principal investigators (PIs) of the CZOs through the Critical Zone Exploration Network (approximately 1200 individuals), and the PIs of the ILTER network (approximately 400 individuals) with the request to forward the survey to respective modellers. The first part of the questionnaire characterizes the computational model used in respects such as associated network, geographic region, purposes of the modelling activity, spatial and time scale, compartments, disciplines and model structure. The second set of question inquired the type of variables/data used, purpose of the data usage (model input or calibration), and the source of the data used in the model (measurements at sites, remotely sensed, database, modelled or literature). The third part of the questionnaire investigated whether and for which specific purpose the respondents would desire a model integration platform. Except Yes/No questions, all questions were answerable

with multiple responses by simple ticks. The questions were designed through iterative feedback loops together with leading scientists of earth system disciplines.

7.2 Methods: LTER and CZO variables

The specificities, purpose and scientific origin of the LTER and CZO networks accumulated to the design of a suite of variables and parameters desirable and common to be measured at the respective sites. In total 52 variables were surveyed in this survey. based upon the ecosystem integrity concept (Müller et al., 2000), the essential biodiversity variables (Pereira et al., 2013; Haase et al., 2018), the common CZO measurements (Chorover et al., 2015 and Brantley et al., 2016), and variables for energy and matter balances at the catchment scale. The ecosystem integrity concept formulated conceptual requirements to evaluate the 10 state and integrity of an ecosystem (Andreasen et al., 2001). The intention of ecosystem integrity assessments was to provide information for knowledge based policy and management decisions for improved ecosystem integrities. Haase et al. (2018) linked the ecosystem integrity concept with the essential biodiversity variables framework (Pereira et al., 2013) to formulate the most recent set of biotic and abiotic variables which are desirable to be measured at LTER sites around the globe. The list of common CZO measurements (Chorover et al., 2015) was formulated to allow for a site-wise comparison of infrastructure and measurements at the ten CZOs in the United States (Chorover et al., 2015). Each observatory was funded based upon very site specific questions, hypothesis and therefore set of measurements. With the common set of CZO measurements and protocols, a foundation is laid to develop concepts how a network of CZOs can be established to address scientific questions across scales. Variables regarding mass and energy fluxes were in common by all three concepts, some biogeochemical parameters were specific to the common CZO measurements and some variables of the biota were specific to the biodiversity 20 indicators list. The set of variables in this survey entails variables from all three concepts and was gathered with regard to the potential use, opportunities, complementarities and synergies of the variables and both networks.

7.3 Methods: Statistical analysis

For analysis of the survey data, three statistical methods were used. Fisher's exact test (Agresti, 2002) was applied for testing whether variables or model characteristics were independent of the network associated with the respondent. The null hypothesis of the Fisher's exact test was that the variable occurs independent whether the response is associated with CZO or LTER. Hence, it was tested whether particular variables or model characteristics can be associated for a specific network (rejection of null hypothesis) or if they are equally distributed over models of both networks to a significance level indicated (0.95% or 0.99%). The Mann-Whitney U test (Bauer, 1972) was applied for testing whether the distribution of model complexity (range: 0.1) and number of variables (range: 0.52) across the responses was distributed independently of the associated networks (CZO, LTER or both). For analysis of trends in the variable space, the detrended correspondence analysis (DCA) (Hill and Gauch, 1980) was performed using the DECORANA package implemented in R and Fortran (Oksanen and

Minchin, 1997). DCA ordinates presence absence data, in this case, the response whether a variable was used in the model application (1) or not (0). First, a correspondence analysis is done by iteratively calculating the scores for the model responses as weighted average of the total variable abundance. Second, the scores are detrended and rescaled by cutting the axis scores of the correspondence analysis into segments and moving the residuals into a secondary axis. As usual, only the first two axes will be used as those yield the strongest correspondences.

7.4 Results on model characteristics

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118 surveys were returned with information on model application. 70 out of 118 surveys provided full information related to model characterization and variables. Nearly half of the respondents (47 %) reported CZO observational data application, two-thirds (66 %) associated LTER data to their model and 12 % model applications used data of both networks (Appendix Figure 6a). 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 purposes of models were representatively distributed; however, LTER model applications were more strongly oriented to management/prediction, compared to CZO model applications that were relatively more focused on process and system understanding. In terms of the modelled time scales, the long time scales over centuries to millions of years are mostly covered by models employed in the CZO community (Figure 6d). Spatially, the model applications extend mostly from site—to catchment scale, with few occurrences at the lab (n = 3) or global (n = 5) scale. Compartment wise, CZO model responses worked more the lithosphere and cryosphere (Figure 6e). Except for biodiversity, the modelled disciplines are rather evenly distributed. Biodiversity is exclusively covered in models of the LTER community. Although models employed for CZO may include biota, this was not the case for the 22 models associated with CZOs in this survey. Since only few models were used by more than one respondent, the survey responses indicate the application of a large variety of models in terms of disciplines and scales (Figure 6).

The measured variables used most frequently in the models were from the atmospheric compartment (295 times in total), respectively: precipitation, air temperature, incoming shortwave radiation, humidity, wind speed/ direction, and eddy flux of ET and CO2. The next most frequently used variables were soil structure (soil depth, layers), above groundbiomass, instantaneous discharge, texture and physical characterization, soil water content, and vegetation structure and dynamics. In contrast to these, individual variables associated with biodiversity (60 times in total), and saprolite and bedrock properties (50 times in total) were much less used in the models. Most likely, this is because they are much more sampling intensive in terms of time and resources compared to atmospheric variables (e.g. a weather station). The variables used reflect also the current most frequent model applications in terrestrial Earth system science. CZO and LTER data are mostly applied for coupled hydrological geophysical models being the most data intensive types of models, which may as well be reflected in these statistics. Biogeochemistry, petrology and biology communities appear as less data intensive.

As could be expected, the CZO models most frequently apply variables of saprolite and bedrock (54%, plus 26% joint CZO and LTER model applications) while variables associated with biodiversity appear more frequently in LTER model applications (91.7%, plus 8.3% joint models). The following variables are significantly (Fisher test, p<0.05) more frequently applied in CZO site modelling: 'eddy flux of ET and CO2', 'root density', 'soil water content', 'soil temperature', 'bedrock soil texture and physics'. Models using data of 'habitat mapping', and 'vascular plant diversity' were associated with the LTER community.

The majority of variables used in the models are sourced from on-site measurements (55% on average). 45% of the data is sourced from other sources, including remotely sensed, modelled, external database, or literature. The fraction of on site measured data use is slightly higher for the variables in the atmospheric compartment (58%) compared to, for example, the fraction of variables represented by habitat/vegetation/crop. Compartment wise, the fractional use of empirical, site based measurements is highest for the variables belonging to the surface waters (68%). The most commonly remotely sensed data in the survey were variables of the biosphere, especially 'habitat mapping', 'leaf area index', 'vegetation structure (height) and dynamics', 'above-groundbiomass', 'snowpack distribution and duration', 'eddy flux of evapotranspiration', and 'CO2'. Model wise, the average model used 14 variables, 9 of those as model input and 5 of those for calibration/validation (Appendix Table 1).

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The model 'level of integration' was calculated by normalizing the model wise number of disciplines and compartments indicated by the responses to a scale of 0 to 1 (high) and equally weighing both to obtain the 'level of integration' between 0 and 1. On average, a rather high level of integration is present for the models; meaning that the CZO and LTER data model applications cover on average multiple disciplines (mean=3.6 \pm 2.1 standard deviation) and ecosystem compartments (mean=2.7 \pm 1.6). Model 'level of integration' is strikingly similar in CZO and LTER data applications. The richness in variables was positively correlated to the number of disciplines (R² = 0.29), and to compartments (R² = 0.4). However, unifying compartments and disciplines to the 'level of integration' measure correlated most strongly to the number of variables (R² = 0.47) (Figure 3). The level of integration for models used at CZO and LTER sites raises with the number of variables used. Models using data from both networks were in the higher data use range. In terms of purpose, models used to gain 'process understanding' were described by a significantly higher median of both level of integration and number of variables. The time scale of 'days' was also indexed by a high number of variables and level of integration.

The question whether the CZO and LTER modelling communities would benefit from a model platform providing data-model linking services, was answered affirmative by a large majority (80%) of the surveyed modellers. The respondents were less unified as to what services should be provided on such a platform. Most saw it primarily as a 'marketplace' with links to data platforms, some advocate that the model platform could even distribute software tools and models. With the promising observation that 10% of the models already integrated data from both networks, the need for more integration between the CZO and LTER communities is also underpinned by this expressed desire for an integrated model platform.

8 References

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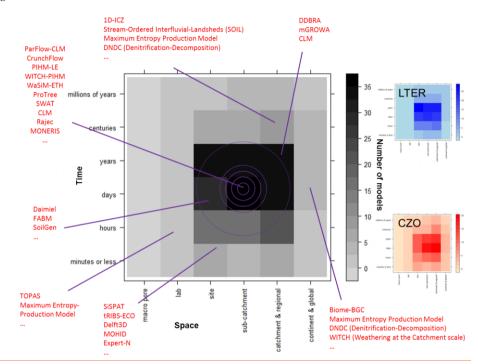
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Figures and Tables



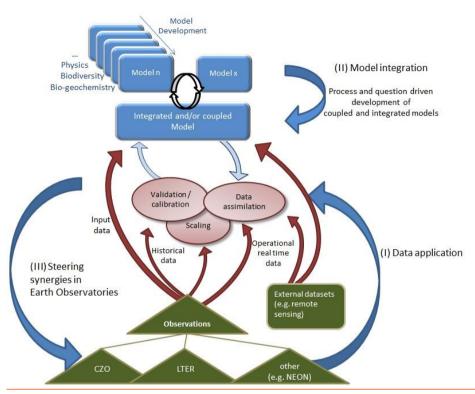


Figure 1: Flowchart of concepts, pathways and processes of applying terrestrial observatory network data to earth system dynamics models; identifying the three challenges of (I) data application, (II) model integration, and (III) steering synergies in observation networks.

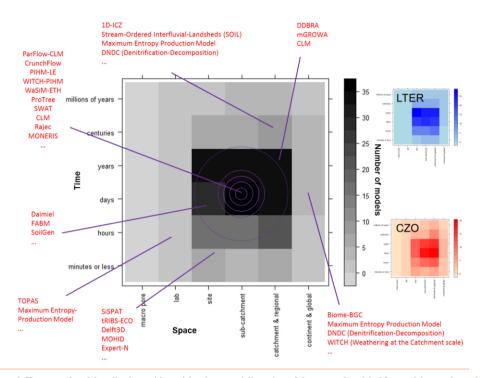
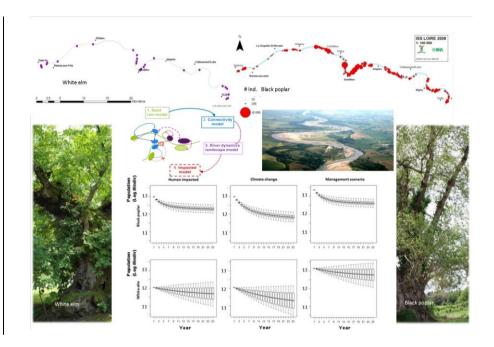


Figure 2: Heat map of model applications, with spatial and temporal dimensions of the surveyed models. Most models were denoted using several temporal and spatial scales. For visualization, we present some individual models at one exemplary instance. On the right, CZO and LTER model applications are presented separately.



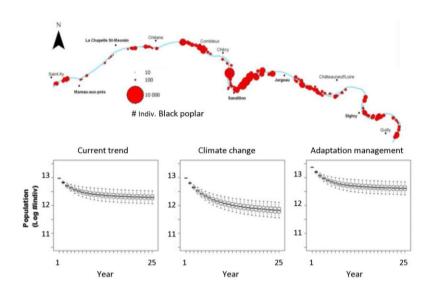


Figure 3: Integrated model of vegetation dynamics (with population dynamics and landscape dynamics modules) in the French Loire LTER, constructed with data of tree individuals, flow regime, sedimentation and climatic conditions. Outcome presenting the total Loire basin population (logarithms number individuals) for 25 year in a baseline scenario (human impacted), projected climate change, and adaptation management for Black poplar and White elm: 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),

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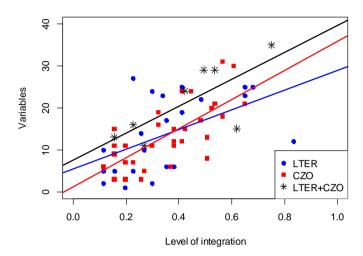
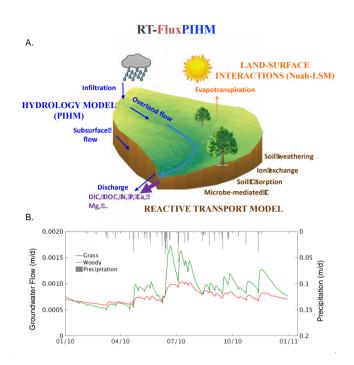
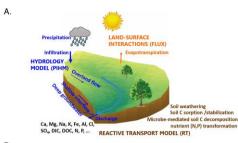


Figure 4: Model-wise 'level of integration' calculated from the summed scientific disciplines and modelled compartments for the corresponding model. Trend lines corresponding to the models associated with LTER (blue), and CZO (red), and models associated with data from both networks (black) are presented.





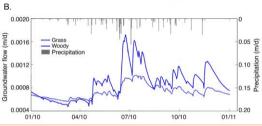


Figure 5: A. Representative processes from different disciplines (different colours) in different modules that can be integrated into one model suite or a coupled reactive transport-land surface-hydrologic model RT-Flux-PIHM (Bao et al., 2017). The integration among processes from mechanistic bases in the model will allow systematic understanding at the watershed scale, B. Simulated Model result of simulated difference in groundwater flow for a grassland (reddotted line) and woody encroached (greensolid line) watershed (N04D), at the Konza Prairie, KS (USA). Grassland simulations are parameterized with a 0.3 m rooting depth and enhanced horizontal macroporemacro-pore development, while woody encroached simulations have a rooting depth that extends to 1.0 m deep with the enhanced vertical macropore development, all other parameters are the same between the simulations.

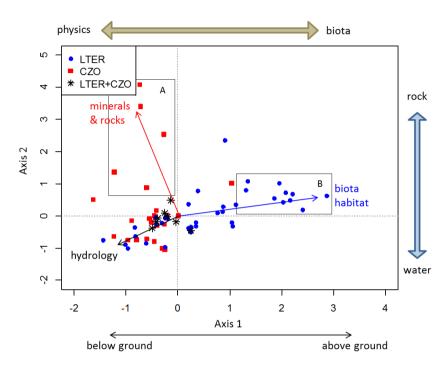
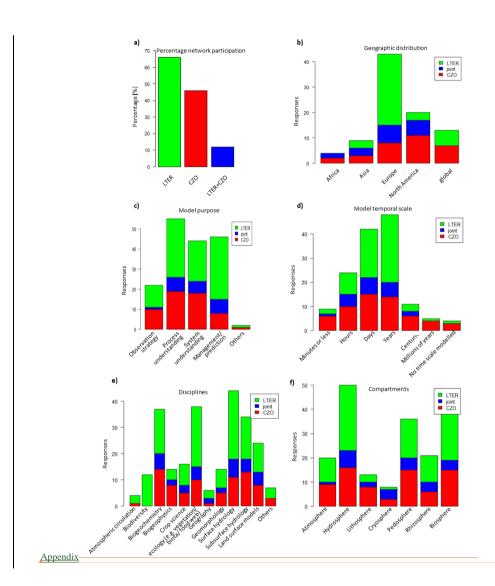


Figure 6: Ordination of the models and data in the survey; clusters show significant differences for models of LTER and CZO. CZO cluster A focuses on variables of the saprolite and bedrock, LTER cluster B focusses on the variables of biota/biodiversity.



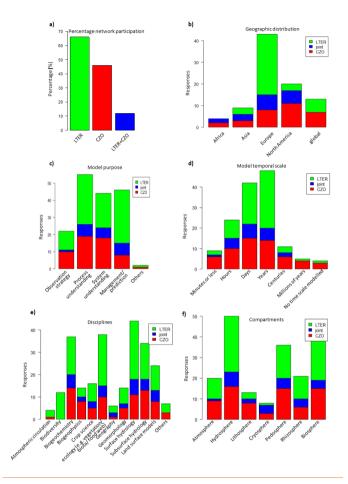


Figure 641: Distribution of respondents associated with either LTER, CZO, or both sites (a) to geographic region modelled (b), purpose of the modelling (c), time scale modelled (d), disciplines (e) and compartments (f) integrated.

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Table $\underline{\blacktriangle}$ 1: 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.

			Sum of all		
Ecosystem	Subcategory / theme	Variable	instances	Source:sites	Source:others
compartment			nr.	[%]	[%]
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