Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access

Realized ecological forecast through interactive Ecological Platform for Assimilating Data into model (EcoPAD)

Yuanyuan Huang[1,2], Mark Stacy[3], Jiang Jiang[1,4], Nilutpal Sundi[5], Shuang Ma[1,6], Volodymyr Saruta[1,6], Chang Gyo Jung[1,6], Zheng Shi[1], Jianyang Xia[7,8], Paul J.Hanson[9], Daniel Ricciuto[9], Yiqi Luo[1,6,10]

1, Department of Microbiology and Plant Biology, University of Oklahoma, Norman, Oklahoma

2, Laboratoire des Sciences du Climat et de l'Environnement, 91191 Gif-sur-Yvette, France

3, University of Oklahoma Information Technology, Norman, Oklahoma, USA

4, Key Laboratory of Soil and Water Conservation and Ecological Restoration in Jiangsu Province, Collaborative Innovation Center of Sustainable Forestry in Southern China of Jiangsu Province, Nanjing Forestry University, Nanjing, Jiangsu, China

5, Department of Computer Science, University of Oklahoma, Norman, Oklahoma, USA

6, Center for Ecosystem Science and Society, Northern Arizona University, Flagstaff, AZ, USA

7, Tiantong National Forest Ecosystem Observation and Research Station, School of Ecological and Environmental Sciences, East China Normal University, Shanghai 200062, China.

8, Research Center for Global Change and Ecological Forecasting, East China Normal University, Shanghai 200062, China

9, Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

10, Department of Earth System Science, Tsinghua University, Beijing 100084 China

Correspondence: Yuanyuan Huang (yuanyuanhuang2011@gmail.com) and Yiqi Luo (Yiqi.Luo@nau.edu)

Abstract. Predicting future changes in ecosystem services is not only highly desirable but also becomes feasible as several forces (e.g., available big data, developed data assimilation (DA) techniques, and advanced cyberinfrastructure) are converging to transform ecological research to quantitative forecasting. To realize ecological forecasting, we have developed an Ecological Platform for Assimilating Data (EcoPAD) into models. EcoPAD is a web-based software system that automates data transfer and processes from sensor networks to ecological forecasting through data management, model simulation, data assimilation, and visualization. It facilitates interactive data-model integration from which model is recursively improved through updated data while data is systematically refined under the guidance of model. EcoPAD relies on data from observations, process-oriented models, DA techniques, and web-based workflow.

We applied EcoPAD to the Spruce and Peatland Responses Under Climatic and Environmental change (SPRUCE) experiment at North Minnesota. The EcoPAD-SPRUCE realizes fully automated data transfer, feeds meteorological data to drive model simulations, assimilates both manually measured and automated sensor data into Terrestrial ECOsystem (TECO) model, and recursively forecast responses of various biophysical and biogeochemical processes to five temperature and two CO_2 treatments in near real-time (weekly). The near real-time forecasting with EcoPAD-SPRUCE has revealed that uncertainties or mismatches in forecasting carbon pool dynamics are more related to model (e.g., model structure, parameter, and initial value) than forcing variables, opposite to forecasting flux variables. EcoPAD-SPRUCE quantified acclimations of methane production in response to warming treatments through shifted posterior distributions of the CH_4:CO_2 ratio and temperature sensitivity (Q_{10}) of methane production towards lower values. Different case studies indicated that realistic forecasting of carbon dynamics relies on appropriate model structure, correct parameterization

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

and accurate external forcing. Moreover, EcoPAD-SPRUCE stimulated active feedbacks between experimenters and modelers so as to identify model components to be improved and additional measurements to be made. It becomes the first interactive model-experiment (ModEx) system and opens a novel avenue for interactive dialogue between modelers and experimenters.

EcoPAD also has the potential to become an interactive tool for resource management, to stimulate citizen science in ecology, and transform environmental education with its easily accessible web interface.

Key words:

Data assimilation, SPRUCE, carbon, global change, real time, acclimation, forecast

1. Introduction

One ambitious goal of ecology as one science discipline is to forecast future states and services of ecological systems. Forecasting futures in ecology is not only desirable for scientific advances in this discipline but also has practical values to guide resource management and decision-making toward a sustainable planet earth. The practical need for ecological forecasting is particularly urgent in this rapidly changing world, which is experiencing unprecedented natural resource depletion, increasing food demand, serious biodiversity crisis, accelerated climate changes, and widespread pollutions in the air, waters, and soils [*Clark et al.*, 2001; *Mouquet et al.*, 2015]. As a result, a growing number of studies have been reported in the last several decades on forecasting of phenology [*Diez et al.*, 2012], carbon dynamics [*Gao et al.*, 2011; *Luo et al.*, 2016; *Thomas et al.*, 2017], species dynamics [*Clark et al.*, 2003; *Kearney et al.*, 2010], pollinator performance[*Corbet et al.*, 1995], epidemics [*Ong et al.*, 2010], fishery [*Hare et al.*, 2010], algal bloom [*Stumpf et al.*, 2009], crop yield [*Bastiaanssen and Ali*, 2003], biodiversity [*Botkin et al.*, 2007], plant extinction risk [*Fordham et al.*, 2012], and ecosystem service [*Craft et al.*, 2009]. Despite its broad applications, ecological forecasting is still sporadically practiced and lags far behind demand due to the lack of infrastructure that enables timely integration of models with data. This paper introduces the fully interactive infrastructure, the Ecological Platform for Assimilating Data (EcoPAD) into models, to inform near-time ecological forecasting with iterative data-model integration.

Ecological forecasting relies on both models and data. However, currently the ecology research community has not yet adequately integrated observations with models to inform best forecast. Forecasts generated from scenario approaches are qualitative and scenarios are often not based on ecological knowledge [*Coreau et al.*, 2009; *Coreau et al.*, 2010]. Data-driven forecasts using statistical methods are generally limited for extrapolation and sometimes contaminated by confounding factors [*Schindler and Hilborn*, 2015]. Recent emergent mechanism-free non-parametric approach, which depends on the statistical pattern extracted from data, is reported to be promising for short-term forecast [*Sugihara et al.*, 2012; *Perretti et al.*, 2013; *Ward et al.*, 2014], but has limited capability in long-term prediction due to the lack of relevant ecological mechanisms. Process-based models provide the capacity in long term prediction and the flexibility in capturing short term dynamics on the basis of mechanistic understanding [*Coreau et al.*, 2009; *Purves et al.*, 2013]. Wide applications and tests of process-based models are limited by their often complicated numerical structure and sometimes unrealistic parameterization [*Moorcroft*, 2006]. The complex and uncertain nature of ecology precludes practice of incorporating as many processes as possible into mechanistic models. Our current incomplete knowledge about ecological systems or unrepresented processes under novel conditions is partly reflected in model parameters which are associated with large uncertainty. Good forecasting therefore requires effective communication between process-based models and data to estimate realistic model parameters and capture context-dependent ecological phenomena.

Data-model fusion, or data-model integration, is an important step to communicate model with data. But previous data-model integration actvities have mostly been done in an *ad hoc* manner instead of being interactive. For example, data from a network of eddy covariance flux tower sites across United States and Canada was compared with gross primary productivity (GPP) estimates from different models [*Schaefer et al.*, 2012]. *Luo and Reynolds* [1999] used a model to examine ecosystem responses to gradual as in the real world vs. step increases in CO_2 concentration as in elevated CO_2 experiments. *Parton et al.* [2007] parameterized CO_2 impacts in

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

an ecosystem model with data from a CO_2 experiment in Colorado. Such model-experiment interactions encounter a few issues: 1) Models are not always calibrated for individual sites and, therefore, not accurate; 2) It is not very effective because it is usually one-time practice without many iterative processes between experimenters and modelers [*Dietze et al.*, 2013; *Lebauer et al.*, 2013]; 3) It is usually one-directionary as data is normally used to train models while the guidance of model for efficient data collection is limited; and 4) It is not streamlined and could not be disseminated with common practices among the research community [*Dietze et al.*, 2013; *Lebauer et al.*, 2013; *Walker et al.*, 2014].

A few research groups have developed data assimilation systems to faciliate data-model integration in a systematic way. For example, data-model integration systems, such as the Data Assimilation Research Testbed - DART [*Anderson et al.*, 2009], the General Ensemble Biogeochemical Modeling System - GEMS [*Tan et al.*, 2005] and the Carbon Cycle Data Assimilation Systems - CCDAS [*Scholze et al.*, 2007; *Peylin et al.*, 2016], combine various data streams (e.g., FLUXNET data, satellite data and inventory data) with process-based models through data assimilation algorithms such as the Kalman filter [*Anderson et al.*, 2009] and variational methods [*Peylin et al.*, 2016]. These data assimilaiton systems automate model parameterization and provided an avenue to systematically improve models through combining as much data as possible. Model improvements normally happen after the ending of an field experiment and the interactive data-model intergration is limited as feedbacks from models to ongoing experimetal studies are not adequately realized. In addtion, wide applications of these data assimilation systems in ecological forecasting are constrained by limited user interactions with its steep learning curve to understand these systems, especially for exmperimenters who have limited training in modeling.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Realizing interactive ecological forecasting requires web-based technology to faciliate scientific workflow, the sequence of processes through which a piece of work passes from initiation to completion. Web-based modeling, which provides user-friendly interfaces to run models in the background, is uaully supported by scientific workflow. For example, TreeWatch.Net has recently been developed to make use of high precision individual tree monitoring data to parameterize process based tree models in real-time and to assess instant tree hydraulics and carbon status with online result visualization [*Steppe et al.*, 2016]. Although the web portal of TreeWatch.Net is currently limited to visualization purposes, it largely broadens the application of data-model integration and strengthens the interaction of modeling results with the general public. The Predictive Ecosystem Analyzer (PEcAn) is a scientific workflow that wraps around different ecosystem models and manages the flows of information coming in and out of the model [*Lebauer et al.*, 2013]. PEcAn enables web-based model similations. Such a workflow has advantages, for exmaple, making ecological modeling and analysis convenient, transparent, reproducible and adaptable to new questions [*Lebauer et al.*, 2013], and encouraging user-model interactions. PEcAn uses the Bayesian meta-analysis to synthesize plant trait data to estimate model parameters and associated uncertanties. Parameter uncertainties are propogated to model uncertanties and displayed as outputs. It is still not fully interactive in the way that states are not updated iteractively according to observations and the web-based data assimilation and then ecoloical forecasting have not yet been fully realized.

The iterative model-data intergration is an important step to realize real or near real-time ecological forecasting. Instead of projecting into future only one time through assimulating available observations, interactive forecasting constantly updates forecasting as soon as new data stream arrives or/and model is modified. Forecasting is likely to be improved unidirectionally in which models are constantly updated through observations, or data collections/field experimentations are regularly improved according to theoretical/model information. Ecological forecasting can also be bidirectionally improved so that both models and field experimetations are optimized hand in hand over time. Although the bidirctional case is rare in ecological forecasting, the unidirectional iterative forecasting has been reported. One excellent example of forecasting through dynamically and repeatedly integrating data with models is from infectious disease studies [*Ong et al.*, 2010; *Niu et al.*, 2014]. Dynamics of infectious diseases are tranditionaly captured by Susceptible-Infected-Removed (SIR) models. In the forecasting of the Singapore H1N1-2009 infections, SIR model parameters and the number of individuals in each state were updated daily, combining data renewed from local clinical reports. The evolving of the epidemic related parameters and states were captured through iteratively assimilating observations to inform forecasting. As a result, the model correctly forecasted the timing of the peak and declining of the infection ahead of time. Iterative forecasting dynamically integrates data with model and makes best use of both data and theoretical understandings of ecological processes.

The aim of this paper is to present a fully interactive platform, a web-based Ecological Platform for Assimilating Data into models (EcoPAD), to best inform ecological forecasting. The interactive feature of EcoPAD is reflected in the iterative model updating and forecasting through dynamically integrating models with new observations, bidirectional feedbacks between experimenters and modelers, and flexible user-model communication through web-based simulation, data assimilation and forecasting. Such an interactive platform provides the infrastructure to effectively integrate available resources, from both models and data, modelers and experimenters, scientists and the general public, to improve scientific understanding of

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

ecological processes, to boost ecological forecasting practice and transform ecology towards qualitative forecasting.

In the following sections, we first describe the system design, major components and functionality of EcoPAD. We then use the Spruce and Peatland Responses Under Climatic and Environmental change (SPRUCE) experiment [*Hanson et al.*, 2017] as a testbed to elaborate new opportunities brought by the platform. We finally discuss implications of EcoPAD for better ecological forecasting.

2 EcoPAD: system design, components, and functionality

2.1 General description: web-based data assimilation and forecast

EcoPAD (https://ecolab.nau.edu/ecopad_portal/) focuses on linking ecological experiments/data with models and allows easily accessible and reproducible data-model integration with interactive web-based simulation, data assimilation and forecast capabilities. Specially, EcoPAD enables the automated near time ecological forecasting which works hand-in-hand between modelers and experimenters and updates periodically in a manner similar to the weather forecasting. The system is designed to streamline web request-response, data management, modeling, prediction and visualization to boost the overall throughput of observational data, promote data-model communication, inform ecological forecasting and improve scientific understanding of ecological processes.

To realize such data-informed ecological forecasting, the essential components of EcoPAD include experiments/data, process-based models, data assimilation techniques and the scientific workflow (Figures 1-3). The scientific workflow of EcoPAD that wraps around ecological models and data assimilation algorithms acts to move datasets in and out of structured and cataloged data collections (metadata catalog) while leaving the logic of the ecological models and data assimilation algorithms untouched (Figures 1, 3). Once a user makes a request through the web browser or command line utilities, the scientific workflow takes charge of triggering and executing corresponding tasks, be it pulling data from a remote server, running a particular ecological model, automating forecasting or making the result easily understandable to users (Figures 1, 3). With the workflow, the system is agnostic to operation system, environment and programming language and is built to horizontally scale to meet the demands of the model and the end user community.

2.2 Components

2.2.1 Data

Data is an important component of EcoPAD and EcoPAD offers systematic data management to digest diverse data streams. The 'big data' ecology generates plethora of very different datasets across various scales [*Hampton et al.*, 2013; *Mouquet et al.*, 2015]. These datasets might have high temporal resolutions, such as those from real time ecological sensors, or the display of spatial information from remote sensing sources and data stored in the geographic information system (GIS). These datasets may also include, but are not limited to, inventory data, laboratory measurements, FLUXNET databases or from long term ecological networks. Such data contain information related to environmental forcing (e.g., precipitation, temperature and radiative forcing), site characteristics (including soil texture, species composition) and biogeochemical information. Datasets in EcoPAD are derived from other research projects in comma separated value files or other loosely structured data formats. These datasets are first described and stored with appropriate metadata via either manual operation or scheduled automation from sensors.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Attention is then spent on how the particular dataset varies over space (x, y) and time (t). When the spatiotemporal variability is understood, it is then placed in metadata records that allow for query through its scientific workflow.

2.2.2 Ecological models

Process-based ecological model is another essential component of EcoPAD (Figure 1). In this paper, the Terrestrial ECOsystem (TECO) model is applied as a general ecological model for demonstration purpose since the workflow and data assimilation system of EcoPAD are independent on the specific ecological model. TECO simulates ecosystem carbon, nitrogen, water and energy dynamics [*Weng and Luo*, 2008; *Shi et al.*, 2016]. The original TECO model has 4 major submodules (canopy, soil water, vegetation dynamics and soil carbon/nitrogen) and is further extended to incorporate methane biogeochemistry and snow dynamics [*Huang et al.*, 2017; *Ma et al.*, 2017]. As in the global land surface model CABLE [*Wang and Leuning*, 1998; *Wang et al.*, 2010], canopy photosynthesis that couples surface energy, water and carbon fluxes is based on a two-big-leaf model [*Wang and Leuning*, 1998]. Leaf photosynthesis and stomatal conductance are based on the common scheme from *Farquhar et al.* [1980] and *Ball et al.* [1987] respectively. Transpiration and associated latent heat losses are controlled by stomatal conductance, soil water content and the rooting profile. Evaporation losses of water are balanced between the soil water supply and the atmospheric demand which is based on the difference between saturation vapor pressure at the temperature of the soil and the actual atmospheric vapor pressure. Soil moisture in different soil layers is regulated by water influxes (e.g., precipitation and percolation) and effluxes (e.g., transpiration and runoff). Vegetation dynamic tracks processes such as growth, allocation and phenology. Soil carbon/nitrogen module tracks carbon and nitrogen through processes such as litterfall, soil organic matter (SOM) decomposition and mineralization. SOM decomposition modeling follows the general form of the Century model [*Parton et al.*, 1988] as in most earth system models in which SOM is divided into pools with different turnover times (the inverse of decomposition rates) which are modified by environmental factors such as the soil temperature and moisture.

2.2.3 Data assimilation

Data assimilation is a cutting-edge statistical approach that integrates data with model in a systematical way (Figure 2). Data assimilation is growing in importance as the process based ecological models, despite largely simplifying the real systems, are in great need to be complex enough to address sophisticate ecological issues that are composed of an enormous number of biotic and abiotic factors interacting with each other. Data assimilation techniques provide a framework to combine models with data to estimate model parameters [*Shi et al.*, 2016], test alternative ecological hypotheses through different model structures [*Liang et al.*, 2015], assess information content of datasets [*Weng and Luo*, 2011], quantify uncertainties [*Weng et al.*, 2011; *Keenan et al.*, 2012; *Zhou et al.*, 2012], identify model errors and improve ecological predictions [*Luo et al.*, 2011b]. Under the Bayesian paradigm, data assimilation techniques treat the model structure, initial and parameter values as priors that represent our current understanding of the system. As new information from observations or data becomes available, model parameters and state variables can be updated accordingly. The posterior distributions of estimated parameters or state variables are imprinted with information from both the model and the observation/data as the chosen parameters act to reduce mismatches between observations and model simulations. Future predictions benefit from such constrained posterior distributions through forward modeling (Figure A1). As a result, the probability density function of predicted future states through data assimilation normally has a narrower spread than that without data assimilation when everything else is equal [*Luo et al.*, 2011b; *Weng and Luo*, 2011; *Niu et al.*, 2014].

EcoPAD is open to different data assimilation techniques depending on the ecological questions under study since the scientific workflow of EcoPAD is independent on the specific data assimilation algorithm. For demonstration, the Markov chain Monte Carlo (MCMC) [*Xu et al.*, 2006] is described in this study.

MCMC is a class of sampling algorithms to draw samples from a probability distribution obtained through constructed Markov Chain to approximate the equilibrium distribution, which makes Bayesian inference, especially these with multi-dimensional integrals, workable. The Bayesian based MCMC method is advantageous for better ecological forecasting as it takes into account various uncertainty sources which are crucial in interpreting and delivering forecasting results [*Clark et al.*, 2001]. In the application of MCMC, the posterior distribution of parameters for given observations is proportional to the prior distribution of parameters and the likelihood function which is linked to the fit/match (or cost function) between model simulations and observations. EcoPAD currently adopts a batch mode, that is, the cost function is treated as a single function to be minimized and different observations are standardized by their corresponding standard deviations [*Xu et al.*, 2006]. For simplicity, we assume uniform distributions in priors, and Gaussian or multivariate Gaussian distributions in observational errors, which can be easily expanded to other specific distribution forms depending on the available information. Detailed description is available in *Xu et al.* [2006].

2.2.4 Scientific workflow

EcoPAD relies on its scientific workflow to interface ecological models and data assimilation algorithms, managing diverse data streams, automates iterative ecological

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

forecasting in response to various user requests. Workflow is a relatively new concept in the ecology literature but essential to realize real or near-real time forecasting. Thus, we describe it in details below. The essential components of a scientific workflow of EcoPAD include the metadata catalog, web application-programming interface (API), the asynchronous task/job queue (Celery) and the container-based virtualization platform (Docker). The workflow system of EcoPAD also provides structured result access and visualization.

2.2.4.1 Metadata catalog and data management

Datasets can be placed and queried in EcoPAD via a common metadata catalog which allows for effective management of diverse data streams. Calls are common for good management of current large and heterogeneous ecological datasets [*Ellison*, 2010; *Michener and Jones*, 2012; *Vitolo et al.*, 2015]. Kepler [*Ludascher et al.*, 2006] and the Analytic Web [*Osterweil et al.*, 2010] are two example systems that endeavor to provide efficient data management through storage of metadata including clear documentation of data provenance. Similarly to these systems, EcoPAD takes advantage of modern information technology, especially the metadata catalog, to manage diverse data streams. The EcoPAD metadata schema includes description of the data product, security, access pattern, and timestamp of last metadata update *etc*. We use MongDB (https://www.mongodb.com/), a NoSQL database technology, to manage heterogeneous datasets to make the documentation, query and storage fast and convenient. Through MongDB, measured datasets can be easily fed into ecological models for various purposes such as to initialize the model, calibrate model parameters, evaluate model structure and drive model forecast. For datasets from real time ecological sensors that are constantly updating, EcoPAD is set to automatically fetch new data streams with adjustable frequency depending on research needs.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

2.2.4.2 Web API, asynchronous task queue and docker

The RESTful application-programming interface (API) which can deliver data to a wide variety of applications is the gateway of EcoPAD and enables a wide array of user-interfaces and data-dissemination activities. Once a user makes a request, such as through clicking on relevant buttons from a web browser, the request is passed through the Representational State Transfer (i.e., RESTful) API to trigger specific tasks. The RESTful API bridges the talk between the client (e.g., a web browser or command line terminal) and the server (Figure 3). The API exploits the full functionality and flexibility of the HyperText Transfer Protocol (HTTP), such that data can be retrieved and ingested from the EcoPAD through the use of simple HTTP headers and verbs (e.g., GET, PUT, POST, *etc*.). Hence, a user can incorporate summary data from EcoPAD into a website with a single line of html code. Users will also be able to access data directly through programming environments like R, Python and Matlab. Simplicity, ease of use and interoperability are among the main advantages of this API which enables web-based modeling.

Celery (https://github.com/celery/celery) is an asynchronous task/job queue that run at the background (Figure 3). The task queue (i.e., Celery) is a mechanism used to distribute work across work units such as threads or machines. Celery communicates through messages, and EcoPAD takes advantage of the RabbitMQ (https://www.rabbitmq.com/) to manage messaging. After the user submit a command, the request or message is passed to Celery via the RESTful API. These messages may trigger different tasks, which include, but not limited to, pull data from a remote server where original measurements are located, access data through metadata catalog, run model simulation with user specified parameters, conduct data assimilation which recursively updates model parameters, forecast future ecosystem status and post-process of model results for visualization. The broker inside Celery receives task messages and handles out

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

tasks to available Celery workers which perform the actual tasks (Figure 3). Celery workers are in charge of receiving messages from the broker, executing tasks and returning task results. The worker can be a local or remote computation resource (e.g., the cloud) that has connectivity to the metadata catalog. Workers can be distributed into different IT infrastructures, which makes EcoPAD workflow easily expandable. Each worker can perform different tasks depending on tools installed in each worker. And one task can also be distributed into different workers. In such a way, EcoPAD workflow enables parallelization and distributed computation of actual modeling tasks across various IT infrastructures, and is flexible in implementing additional computational resources by connecting additional workers.

Another key feature that makes EcoPAD easily portable and scalable among different operation systems is the utilization of the container-based virtualization platform, the docker. Docker can run many applications which rely on different libraries and environments on a single kernel with its lightweight containerization. Tasks that execute TECO in different ways are wrapped inside different docker containers that can "talk" with each other. Each docker container embeds the ecosystem model into a complete filesystem that contains everything needed to run an ecosystem model: the source code, model input, run time, system tools and libraries. Docker containers are both hardware-agnostic and platform-agnostic, and they are not confined to a particular language, framework or packaging system. Docker containers can be run from a laptop, workstation, virtual machine, or any cloud compute instance. This is done to support the widely varied number of ecological models running in various languages (e.g., Matlab, Python, Fortran, C and C++) and environments. In addition to wrap the ecosystem model into a docker container, software applied in the workflow, such as the Celery, Rabbitmq and MongoDB, are all

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

lightweight and portable encapsulations through docker containers. Therefore, the entire EcoPAD is readily portable and applicable in different environments.

2.2.4.3 Structured result access and visualization

EcoPAD enables structured result storage, access and visualization to track and analyze data-model fusion practice. Upon model task completion, the model wrapper code calls a post processing callback function. This callback function allows for model specific data requirements to be added to the model result repository. Each task is associated with a unique task ID and model results are stored within the local repository that can be queried by the unique task ID. The easy store and query of model results are realized via the MongoDB and RESTful API (Figure 3). Researchers are authorized to review and download model results and parameters submitted for each model run through a web accessible URL (link). EcoPAD webpage also displays a list of historical tasks (with URL) performed by each user. All current and historical model inputs and outputs are available to download, including the aggregated results produced for the graphical web applications. In addition, EcoPAD also provides a task report that contains all-inclusive recap of parameters submitted, task status, and model outputs with links to all data and graphical results for each task. Such structured result storage and access make sharing, tracking and referring to modeling studies instant and clear.

2.3 Scientific functionality

Scientific functionality of EcoPAD includes web-based model simulation, estimating model parameters or state variables, quantifying uncertainty of estimated parameters and projected states of ecosystems, evaluating model structures, assessing sampling strategies, conducting ecological forecasting. Those functions can be organized to answer various scientific questions. In addition to the general description in this section, the scientific functionality of EcoPAD is also illustrated through a few case studies in the following sections.

EcoPAD is designed to perform web-based model simulation, which greatly reduces the workload of traditional model simulation through manual code compilation and execution. This functionality opens various new opportunities for modelers, experimenters and the general public. Model simulation and result analysis are automatically triggered after a simple click on the web-embedded button (Appendices Figures A2, A3 A6). Users are freed from repeatedly compiling code, running code and writing programs to analyze and display model results. Such ease of use has great potential to popularize complex modeling studies that are difficult or inaccessible for experimenters and the general public. As illustrated through the outreach activities from the TreeWatch.Net [*Steppe et al.*, 2016], the potential functionality of such web-based model simulation goes beyond its scientific value as its societal and educational impacts are critical in solving ecological issues. The web based model simulation also frees users from model running environment, platform and software. Users can conduct model simulation and do analysis as long as they have internet access. For example, ecologists can conduct model simulation and diagnose the underlying reasons for a sudden increase in methane fluxes while they are making measurements in the field. Youngsters can study ecological dynamics through their phones or tablets while they are waiting for the bus. Resource managers can make timely assessment of different resource utilization strategies on spot of a meeting.

EcoPAD is backed up by data assimilation techniques, which facilitate inference of model parameters and states based on observations. Ecology have witnessed a growing number of studies focusing on parameter estimation using inverse modeling or data assimilation as large volumes of ecological measurements become available. To satisfy the growing need of model

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

parameterization through observations, EcoPAD streamlines parameter estimations and updates. Researchers can easily review and download files that record parameter values from EcoPAD result repository. Since these parameters may have different scientific values, the functionality of EcoPAD related to parameter estimations can potentially embrace diverse subareas in ecology. For example, soil scientists can study the acclimation of soil respiration to manipulative warming through shifts in the distribution of the decomposition rate parameter from EcoPAD. The threshold parameter beyond which further harvesting of fish might cause a crash of fish stocks can be easily extracted through fish stock assessment models and observations if mounted to EcoPAD.

EcoPAD promotes uncertainty analysis, model structure evaluation and error identification. One of the advantages of the Bayesian statistics is its capacity in uncertainty analysis compared to other optimization techniques [*Xu et al.*, 2006; *Wang et al.*, 2009; *Zhou et al.*, 2012]. Bayesian data assimilation (e.g., MCMC) takes into account observation uncertainties (errors), generates distributions of model parameters and enables tracking of prediction uncertainties from different sources. Uncertainty analysis through data assimilation applied to areas such as ecosystem phenology, fish life cycle and species migration [*Clark et al.*, 2003; *Cook et al.*, 2005; *Crozier et al.*, 2008; *Luo et al.*, 2011b], can potentially take advantage of EcoPAD platform to provide critical information for well informed decisions in face of pressing global change challenges. In addition, the archive capacity of EcoPAD facilitates inter-comparisons among different models or different versions of the same model to evaluate model structures and to disentangle structure uncertainties and errors.

The realization of both the near time and long term ecological forecast is one of the key innovations of EcoPAD. Forecasting capability of EcoPAD is supported by process based ecological models, multiple observational or experimental data, inverse parameter estimation and uncertainty quantification through data assimilation, and forward simulation under future external conditions. The systematically constrained forecast from EcoPAD is accompanied by uncertainty/confidence estimates to quantify the amount of information that can actually be utilized from a study. The automated near time forecast, which is constantly adjusted once new observational data streams are available, provides experimenters advanced and timely information to assess and adjust experimental plans. For example, with forecasted and displayed biophysical and biochemical variables, experimenters could know in advance what the most likely biophysical conditions are. Knowing if the water table may suddenly go aboveground in response to a high rainfall forecast in the coming week, could allow researcher to emphasize measurements associated with methane flux. In such a way, experimenters can not only rely on historical ecosystem dynamics, but also refer to future predictions. Experimenters will benefit especially from variables that are difficult to track in field due to situations such as harsh environment, shortage in man power or on instrument limitation.

Equally important, EcoPAD creates new avenues to answer classic and novel ecological questions, for example, the frequently reported acclimation phenomena in ecology. While growing evidence points to altered ecological functions as organisms adjust to the rapidly changing world [*Medlyn et al.*, 1999; *Luo et al.*, 2001; *Wallenstein and Hall*, 2012], traditional ecological models treat ecological processes less dynamical, as the governing biological parameters or mechanisms fails to explain such biological shifts. EcoPAD facilitates the shift of research paradigm from a fixed process representation to a more dynamic description of ecological mechanisms with constantly updated and archived parameters constrained by observations under different conditions. Specifically to acclimation, EcoPAD promotes

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

quantitatively evaluations while previous studies remain mostly qualitative [*Wallenstein and Hall*, 2012; *Shi et al.*, 2015]. We will further illustrate how EcoPAD can be used to address different ecological questions in the case studies of the SPRUCE project.

3 EcoPAD performance at testbed - SPRUCE

3.1 SPRUCE project overview

EcoPAD is being applied to the Spruce and Peatland Responses Under Climatic and Environmental change (SPRUCE) experiment located at the USDA Forest Service Marcell Experimental Forest (MEF, 47°30.476' N, 93°27.162' W) in northern Minnesota [*Kolka et al.*, 2011]. SPRUCE is an ongoing project focuses on responses of northern peatland to climate warming and increased atmospheric CO_2 concentration [*Hanson et al.*, 2017]. At SPRUCE ecologists measure various aspects of responses of organisms (from microbes to trees) and ecological functions (carbon, nutrient and water cycles) to a warming climate. One of the key features of the SPRUCE experiments is the manipulative deep soil/peat heating (0-3 m) and whole ecosystem warming treatments (peat + air warmings) which include tall trees (> 4 m) [*Hanson et al.*, 2017]. Together with elevated atmospheric CO_2 treatments, SPRUCE provides a platform for exploring mechanisms controlling the vulnerability of organisms, biogeochemical processes and ecosystems in response to future novel climatic conditions. The SPRUCE peatland is especially sensitive to future climate change and also plays an important role in feeding back to future climate change through greenhouse gas emissions as it stores a large amount of soil organic carbon. Vegetation in the SPRUCE site is dominated by *Picea mariana* (black spruce) and *Sphagnum spp* (peat moss). The studied peatland also has an understory which include ericaceous and woody shrubs. There are also a limited number of herbaceous species. The whole

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

ecosystem warming treatments include a large range of both aboveground and belowground temperature manipulations (ambient, control plots of + 0 °C, +2.25 °C, +4.5 °C, +6.75 °C and +9 °C) in large 115 m^2 open-topped enclosures with elevated CO_2 manipulations (+0 or +500 ppm).

The SPRUCE project generates a large variety of observational datasets that reflect ecosystem dynamics from different scales and are available from the project webpage (https://mnspruce.ornl.gov/) and FTP site (ftp://sprucedata.ornl.gov/). These datasets come from multiple sources: half hourly automated sensor records, species surveys, laboratory measurements, laser scanning images *etc*. Involvements of both modeling and experimental studies in the SPRUCE project create the opportunity for data-model communication. Datasets are pulled from SPRUCE archives and stored in the EcoPAD metadata catalog for running the TECO model, conducting data-model fusion or forecasting. The TECO model has been applied to simulate and forecast carbon dynamics with productions of CO_2 and CH_4 from different carbon pools, soil temperature response, snow depth and freeze-thaw cycles at the SRPUCE site [*Huang et al.*, 2017; *Ma et al.*, 2017; *Jiang et al.*, 2018].

3.2 EcoPAD-SPRUCE web portal

We assimilate multiple streams of data from the SPRUCE experiment to the TECO model using the MCMC algorithm, and forecast ecosystem dynamics in both near time and for the next 10 years. Our forecasting system for SPRUCE is available at https://ecolab.nau.edu/ecopad_portal/. From the web portal, users can check our current near and long term forecasting results, conduct model simulation, data assimilation and forecasting runs, and analyze/visualize model results. Detailed information about the interactive web portal is provided in the Appendices.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

3.3 Near time ecosystem forecasting and feedback to experimenters

As part of the forecasting functionality, EcoPAD-SPRUCE automates the near time (weekly) forecasting with continuously updated observations from SPRUCE experiments (Figure 5). We set up the system to automatically pull new data streams every Sunday from the SPRUCE FTP site that holds observational data and update the forecasting results based on new data streams. Updated forecasting results for the next week are customized for the SPRUCE experiments with different manipulative treatments and displayed in the EcoPAD-SPRUCE portal. At the same time, these results are sent back to SPRUCE communities and displayed together with near term observations for experimenter's reference.

3.4 New approaches to ecological studies towards better forecasting

3.4.1 Case 1: Interactive communications among modelers and experimenters

EcoPAD-SPRUCE provides a platform to stimulate interactive communications between modelers and experimenters. Models require experimental data to constrain initial conditions and parameters, and to verify model performance. A reasonable model is built upon correct interpretation of information served by experimenters. Model simulations on the other hand can expand hypotheses testing, and provide thorough or advanced information to improve field experiments. Through recursively exchanging information between modelers and experimenters, both models and field experiments can be improved. As illustrated in Figure 5, through extensive communication between modelers and experimenters, modelers generate model predictions. Model predictions provide experimenters advanced information, help experimenters think, question and understand their experiments. Questions raised by experimenters stimulate further discussion and communication. Through communication, models or/and measurements are adjusted. With new measurements or/and strengthened models, a second round of prediction is

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access
EGU

highly likely to be improved. As the loop of prediction-question-discussion-adjustment-prediction goes on, forecasting is informed with best understandings from both data and model.

We illustrate how the prediction-question-discussion-adjustment-prediction cycle and stimulation of modeler-experimenter communication improves ecological predictions through one episode during the study of the relative contribution of different pathways to methane emissions. An initial methane model was built upon information (e.g., site characteristics and environmental conditions) provided by SPRUCE field scientists, taking into account important processes in methane dynamics, such as production, oxidation and emissions through three pathways (i.e., diffusion, ebullition and plant-mediated transportation). The model was used to predict relative contributions of different pathways to overall methane emissions under different warming treatments after being constrained by measured surface methane fluxes. Initial forecasting results which indicated a strong contribution from ebullition under high warming treatments were sent back to the SPRUCE group. Experimenters doubted about such a high contribution from the ebullition pathway and a discussion was stimulated. It is difficult to accurately distinguish the three pathways from field measurements. Field experimenters provided potential avenues to extract measurement information related to these pathways, while modelers examined model structure and parameters that may not be well constrained by available field information. Detailed discussion is provided in Table 1. After extensive discussion, several adjustments were adopted as a first step to move forward. For example, the three-porosity model that was used to simulate the diffusion process was replaced by the Millington-Quirk model to more realistically represent methane diffusions in peat soil; the measured static chamber methane fluxes were also questioned and scrutinized more carefully to clarify that they did not capture the episodic ebullition events. Measurements such as these

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access
EGU

related to pore water gas data may provide additional inference related to ebullition. The updated forecasting is more reasonable than the initial results although more studies are in need to ultimately quantify methane fluxes from different pathways.

3.4.2 Case 2: Acclimation of ecosystem carbon cycling to experimental manipulations

As a first step, CH_4 static chamber flux measurements were assimilated into TECO to assess potential acclimation phenomena during methane production under 5 warming treatments (+0, +2.25, +4.5, +6.75, +9 °C). Initial results indicated a reduction in both the CH_4:CO_2 ratio and the temperature sensitivity of methane production based on their posterior distributions (Figure 6). The mean CH_4:CO_2 ratio decreased from 0.675 (control) to 0.505 (+9 ˚C treatment), while the temperature sensitivity (Q_{10}) for CH_4 production decreased from 3.33 (control) to 1.22 (+9 ˚C treatment). Such shifts quantify potential acclimation of methane production to warming and future climate warming is likely to have a smaller impact on emission than most of current predictions that do not take into account of acclimation.

Despite these results are preliminary as more relevant datasets are under collection with current ongoing warming manipulation and measurements, assimilating observations through EcoPAD provides a quantitative approach to timely assess acclimation through time. *Melillo et al.* [2017] revealed that the thermal acclimation of the soil respiration in the Harvard Forest is likely to be phase (time) dependent during their 26-year soil warming experiment. EcoPAD provides the possibility in tracing the temporal path of acclimation with its streamlined structure and archive capacity. *Shi et al.* [2015] assimilated carbon related measurements in a tallgrass prairie into the TECO model to study acclimation after 9-years warming treatments. They revealed a reduction in the allocation of GPP to shoot, the turnover rates of the shoot and root carbon pools, and an increase in litter and fast carbon turnovers in response to warming treatments. Similarly, as time goes on, the SPRUCE experiment will generate more carbon cycling related datasets under different warming and CO_2 treatments, which can be mounted to EcoPAD to systematically quantify acclimations in carbon cycling.

3.4.3 Case 3: Partitioning of uncertainty sources

Uncertainties in ecological studies can come from observations (include forcing that drives the model), different model structures to represent the real world and the specified model parameters [*Luo et al.*, 2016]. Previous studies tended to focus on one aspect of the uncertainty sources instead of disentangling the contribution from different sources. For example, the model intercomparison projects (MIPs), such as TRENDY, focus on uncertainty caused by different model structures with prescribed external forcing [*Sitch et al.*, 2008]. *Keenan et al.* [2012] used data assimilation to constrain parameter uncertainties in projecting Harvard forest carbon dynamics. *Ahlstrom et al.* [2012] forced one particular vegetation model by 18 sets of forcings from climate models of the Coupled Model Intercomparison Project Phase 5 (CMIP5), while the parameter or model structure uncertainty is not taken into account.

EcoPAD is designed to provide a thorough picture of uncertainties from multiple sources especially in carbon cycling studies. Through focusing on multiple instead of one source of uncertainty, ecologists can allocate resources to areas that cause relative high uncertainty. Attribution of uncertainties in EcoPAD relies on an ensemble of ecosystem models, the data assimilation system and climate forcing with quantified uncertainty. For example, *Jiang et al.* [2018] focused specifically on the relative contribution of parameter uncertainty vs. climate forcing uncertainty in forecasting carbon dynamics at the SPRUCE site. Through assimilating the pre-treatment measurements (2011-2014) from the SPRUCE experiment, *Jiang et al.* [2018] estimated uncertainties of key parameters that regulate the peatland carbon dynamics. Combined with the stochastically generated climate forcing (e.g., precipitation and temperature), *Jiang et al.* [2018] found external forcing resulted in higher uncertainty than parameters in forecasting carbon fluxes, but caused lower uncertainty than parameters in forecasting carbon pools. Therefore, more efforts are required to improve forcing measurements for studies that focus on carbon fluxes (e.g., GPP), while reductions in parameter uncertainties are more important for studies in carbon pool dynamics. Such kind of uncertainty assessment benefits from EcoPAD with its systematically archived model simulation, data assimilation and forecasting.

3.4.4 Case 4: Improving biophysical estimation for better ecological prediction

Carbon cycling studies can also benefit from EcoPAD through improvements in external forcing. Soil environmental condition is an important regulator of belowground biological activities and also feeds back to aboveground vegetation growth. Biophysical variables such as soil temperature, soil moisture, ice content and snow depth, are key predictors of ecosystem dynamics. After constraining the biophysical module by detailed monitoring data from the SPRUCE experiment through the data assimilation component of EcoPAD, *Huang et al.* [2017] forecasted the soil thermal dynamics under future conditions and studied the responses of soil temperature to hypothetical air warming. This study emphasized the importance of accurate climate forcing in providing robust thermal forecast. In addition, *Huang et al.* [2017] revealed non-uniform responses of soil temperature to air warming. Soil temperature responded stronger to air warming during summer compared to winter. And soil temperature increased more in shallow soil layers compared to deep soils in summer in response to air warming. Therefore, extrapolating of manipulative experiments based on air warming alone may not reflect the real temperature sensitivity of SOM if soil temperature is not monitored. As robust quantification of environmental conditions is known to be a first step towards better understanding of ecological process, improvement in soil thermal predictions through EcoPAD data assimilation system is helpful in telling apart biogeochemical responses from environmental uncertainties and also in providing field ecologists beforehand key environmental conditions.

3.4.5 Case 5: How do updated model and data contribute to reliable forecasting?

Through constantly adjusted model and external forcing according to observations and weekly archived model parameter, model structure, external forcing and forecasting results, the contribution of model and data updates can therefore be tracked through comparing forecasted vs. realized simulations. For example, Figure 7 illustrates how realized external forcing (compared to stochastically generated forcing) and shifts in ecosystem state variables shape ecological predictions. Similarly as in other EcoPAD-SPURCE case studies, TECO is trained through data assimilation with observations from 2011-2014 and is used to forecast GPP and total soil organic carbon content at the beginning of 2015. For demonstrating purpose, Figure 7 only shows 3 series of forecasting results instead of updates from every week. Series 1 (S1) records forecasted GPP and soil carbon with stochastically generated weather forcing from January 2015-December 2024 (Figure 7a,b cyan). Series 2 (S2) records simulated GPP and soil carbon with observed climate forcing from January 2015 to July 2016 and forecasted GPP and soil carbon with stochastically generated forcing from August 2016 - December 2024 (Figure 7a,b red). Similarly, the stochastically generated forcing in Series 3 (S3) starts from January 2017 (Figure 7a,b blue). For each series, predictions were conducted with randomly sampled parameters from the posterior distributions and stochastically generated forcing. We displayed 100 mean values (across an ensemble of forecasts with different parameters) corresponding to 100 forecasts with stochastically generated forcing.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

GPP is highly sensitive to climate forcing. The differences between the realized (S2, 3) and initial forecasts (S1) reach almost 800 gC m^{-2} $year^{-1}$ (Figure 7c). The discrepancy is strongly dampened in the following 1-2 years. The impact of realized forecasts is close to 0 after approximately 5 years. However, soil carbon pool shows a different pattern. Soil carbon pool is increased by less than 150 gC m^{-2}, which is relative small compared to the carbon pool size of *ca.* 62000 gC m^{-2}. The impact of realized forecasts grows with time and reaches the highest at the end of the simulation year 2024. GPP is sensitive to the immediate change in climate forcing while the updated ecosystem status (or initial value) has minimum impact in the long term forecast of GPP. The impact of updated climate forcing is relatively small for soil carbon forecasts during our study period. Soil carbon is less sensitive to the immediate change of climate compared to GPP. However, the alteration of system status affects soil carbon forecast especially in a longer time scale.

Since we are archiving realized forecasts every week, we can track the relative contribution of ecosystem status, forcing uncertainty and parameter distributions to the overall forecasting patterns of different ecological variables and how these patterns evolve in time. In addition, as growing observations of ecological variables (e.g., carbon fluxes and pool sizes) become available, it is feasible to diagnose key factors that promote robust ecological forecasting through comparing the archived forecasts vs. observation and analysing archives of model parameters, initial values and climate forcing *etc*.

4 Discussion

4.1 The necessity of interactive infrastructure to realize ecological forecasting

Substantial increases in data availability from observational and experimental networks, surges in computational capability, advancements in ecological models and sophisticated statistical methodologies and pressing societal need for best management of natural resources have shifted ecology to emphasis more on quantitative forecasts. However, quantitative ecological forecast is still young and our knowledge about ecological forecasting is relatively sparse, inconsistent and disconnected [*Luo et al.*, 2011b; *Petchey et al.*, 2015]. Therefore, both optimistic and pessimistic viewpoints exist on the predictability of ecology [*Clark et al.*, 2001; *Beckage et al.*, 2011; *Purves et al.*, 2013; *Petchey et al.*, 2015; *Schindler and Hilborn*, 2015]. Ecological forecasting is complex and advantages in one single direction, for example, observations alone or statistical methodology alone, is less likely to lead to successful forecasting compared to approaches that effectively integrate improvements from multiple sectors. Unfortunately, realized ecological forecasting that integrates available resources is relative rare due to lack of relevant infrastructures.

EcoPAD provides such effective infrastructure with its interactive platform that rigorously integrates merits from models, observations, statistical advance, information technology and human resources from experimenter, modeler as well as the general public to best inform ecological forecasting, boost forecasting practice and delivery of forecasting results. Interactions enable exchanging and extending of information so as to benefit from collective knowledge. For example, manipulative studies will have a much broader impact if the implications of their results can be extended from the regression between environmental variable and ecosystem response, such as be integrated into an ecosystem model through model-data communication. Such an approach will allow gaining information about the processes responsible for ecosystem's response, constraining models, and making more reliable

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access
EGU

predictions. Going beyond common practice of model-data assimilation from which model updating lags far behind observations, EcoPAD enables iterative model updating and forecasting through dynamically integrating models with new observations in near real time. This real-time interactive capacity relies on its scientific workflow that automates data management, model simulation, data simulation and result visualization. The open, timely, convenient, transparent, flexible, reproducible and traceable characteristics of this platform, also thanks to its scientific workflow, encouraged thorough interactions between experimenters and modelers. Forecasting results from SPRUCE were timely shared among research groups with different background through the web interface. Expertise from different research groups was integrated to improve a second round of forecasting. Again, thanks to the workflow, new information or adjustment is relatively easy to incorporate into future forecasting, making the forecasting system fully interactive and dynamical.

We also benefit from the interactive EcoPAD platform to broaden user-model interactions and to broadcast forecasting results. Learning about the ecosystem models and data-model fusion techniques may lag one's productivity and even discourage learning the modeling techniques because of their complexity and long learning curve. Because EcoPAD can be accessed from a web browser and does not require any coding from the user's side, the time lag between learning the model structure and obtaining model-based results for one's study is minimal, which opens the door for non-modeler groups to "talk" with models. The online storage of one's results lowers the risk of data loss. The results of each model run can be easily tracked and shared with its unique ID and web address. In addition, the web-based workflow also saves time for experts with automated model running, data assimilation, forecasting, structured result access and instantaneous graphic outputs, bringing the possibility for thorough exploration of

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

more essence part of the system. The simplicity in use of EcoPAD at the same time may limit their access to the code and lowers the flexibility. Flexibility for users with higher demands, for example, those who wanted to test alternative data assimilation methods, use a different carbon cycle model, change the number of calibrated parameters, include the observations for other variables, is provided through the GitHub repository (https://github.com/ou-ecolab). This GitHub repository contains code and instruction for installing, configuring and controlling the whole system, users can easily adapt the workflow to wrap their own model based on his or her needs.

In addtion to benefit from its workflow, the advantage of EcoPAD is also reflected in its data assimilation capacity especially for land carbon studies. One focus of EcoPAD is to constrain parameters of terrestrial carbon models to predict long-term carbon dynamics (e.g., 100 years) which are determined more by parameters than initial values of state variables [*Weng and Luo*, 2011]. EcoPAD incorporates the Bayesian framework, especially the MCMC method, to constrain parameters. In comparison, DART uses the Ensemble Kalman Filter to adjust model state variables, instead of parameters, to match observations over time. In the past, complex models could not assimilate pool-related data to constrain their parameter estimation due to insurmountable computational demand in large scale studies. For example, CCDAS normally only assimilates flux-based data [*Peylin et al.*, 2016]. EcoPAD is flexible in assimilating both pool- and flux-based data into complex models so that both fluxes and turnover rates of pools can be constrained with its matrix representation [*Hararuk et al.*, 2014; *Luo*, 2017] and its capability to wrap different models.

4.2 Implications for better ecological forecasting

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Specifically to reliable forecasting of carbon dynamics, our initial exploration from EcoPAD-SPRUCE indicates that realistic model structure, correct parameterization and accurate external environmental conditions are essential. Model structure captures important known mechanisms that regulate ecosystem carbon dynamics. Adjustment in model structure is critical in our improvement in methane forecasting. Model parameters may vary between observation sites, change with time or environmental conditions [*Medlyn et al.*, 1999; *Luo et al.*, 2001]. A static or wrong parameterization misses important mechanisms (e.g., acclimation and adaptation) that regulate future carbon dynamics. Correct parameterization is especially important for long term carbon pool predictions as parameter uncertainty resulted in high forecasting uncertainty in our case study [*Jiang et al.*, 2018]. Although the picture about how neglecting of parameter shift affects carbon predictions has not yet been fully revealed from EcoPAD-SPRUCE as field measurements are still ongoing, our initial exploration indicates non-negligible acclimation of ecosystem methane production in response to warming. External environmental condition is another important factor in carbon predictions. External environmental condition includes both the external climatic forcing that is used to drive ecosystem models and also the environmental condition that is simulated by ecosystem models. As we showed that air warming may not proportionally transfer to soil warming, realistic soil environmental information needs to be appropriately represented to predict soil carbon dynamics [*Huang et al.*, 2017]. The impact of external forcing is especially obvious in short term carbon flux predictions. Forcing uncertainty resulted in higher forecasting uncertainty in carbon flux compared to that from parameter uncertainty [*Jiang et al.*, 2018]. Mismatches in forecasted vs. realized forcing greatly increased simulated GPP and the discrepancy diminished in the long run. Reliable external environmental condition, to some extent, reduces the complexity in diagnosing modeled carbon dynamics.

Pool-based vs. flux-based predictions are regulated differently by external forcing and initial states, which indicates that differentiated efforts are required to improve short vs. long term predictions. External forcing, which has not been well emphasized in previous carbon studies, has strong impact on short term forecasting. The large response of GPP to forecasted vs. realized forcing as well the stronger forcing-caused uncertainty in GPP predictions indicate correct forcing information is a key step in short term flux predictions. In this study, we stochastically generated the climate forcing based on local climatic conditions (1961-2014), which is not sufficient in capturing local short term climate variability. As a result, realized GPP went outside our ensemble forecasting. On the other hand, parameters and historical information about pool status are more important in long term pool predictions. Therefore, improvement in long term pool size predictions cannot be reached by accurate climatic information alone. Instead, it requires accumulation in knowledge related to site history and processes that regulate pool dynamics.

Furthermore, reliable forecasting needs understanding of uncertainty sources in addition to the future mean states. Uncertainty and complexity are major reasons that lead to the belief in "computationally irreducible" and low intrinsic predictability of ecological systems [*Coreau et al.*, 2010; *Beckage et al.*, 2011; *Schindler and Hilborn*, 2015]. Recent advance in computational statistical methods offers a way to formally accounting for various uncertainty sources in ecology [*Clark et al.*, 2001; *Cressie et al.*, 2009]. And the Bayesian approach embedded in EcoPAD brings the opportunity to understand and communicate forecasting uncertainty. Our case study revealed that forcing uncertainty is more important in flux-based predictions while parameter uncertainty is more critical in pool-based predictions. Actually, how uncertainty in carbon forecasting changes with time, what are the dominate sources of uncertainty (parameter, initial condition, model structure, observation errors, forcing *etc.*) under different conditions, how uncertainty sources interact among different components are all valuable questions that can be explored through EcoPAD.

4.3 Applications of EcoPAD to manipulative experiments and observation sites

Broadly speaking, data-model integration stands to increase the overall precision and accuracy of model-based experimentation [*Luo et al.*, 2011b; *Niu et al.*, 2014]. Systems for which data have been collected in the field and which are well represented by ecological models therefore have the capacity to receive the highest benefits from EcoPAD to improve forecasts. In a global change context, experimental manipulations including ecosystem responses to changes in precipitation regimes, carbon dioxide concentrations, temperatures, season lengths, and species compositional shifts can now be assimilated into ecosystem models [*Xu et al.*, 2006; *Gao et al.*, 2011; *Lebauer et al.*, 2013; *Shi et al.*, 2016]. Impacts of these global change factors on carbon cycling and ecosystem functioning can now be measured in a scientifically transparent and verifiable manner. This leads to ecosystem modeling of systems and processes that can obtain levels of confidence that lend credibility with the public to the science's forward progress toward forecasting and predicting [*Clark et al.*, 2001]. These are the strengths of a widely-available interface devoted to data-model integration towards better forecasting.

The data-model integration framework of EcoPAD creates a smart interactive model-experiment (ModEx) system. ModEx has the capacity to form a feedback loop in which field experiment guides modeling and modeling influences experimental focus [*Luo et al.*, 2011a]. We demonstrated how EcoPAD works hand-in-hand between modelers and experimenters in the life-cycle of the SPRUCE project. Field experiment from SPRUCE community provides basic data to set up the ecosystem model and update model parameters recursively, while the forecasting from

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development
Discussions
Open Access

ecosystem modeling informs experimenters the potential key mechanisms that regulate ecosystem dynamics and help experimenters to question and understand their measurements. The EcoPAD-SPRUCE system operates while experimenters are making measurements or planning for future researches. Information is constantly fed back between modelers and experimenters, and simultaneous efforts from both parties illustrate how communications between model and data advance and shape our understanding towards better forecasts during the lifecycle of a scientific project. ModEx can be easily extended to other experimental systems to: 1, predict what might be an ecosystem's response to treatments once experimenter selected a site and decided the experimental plan; 2, assimilate data experimenters are collecting along the experiment to constrain model predictions; 3, project what an ecosystem's responses may likely be in the rest of the experiment; 4, tell experimenters what are those important datasets experimenters may want to collect in order to understand the system; 5, periodically updates the projections; and 6, improve the models, the data assimilation system, and field experiments during the process.

In addition to the manipulative experimental, the data assimilation system of EcoPAD can be used for automated model calibration for FLUXNET sites or other observation networks, such as the NEON and LTER [*Johnson et al.*, 2010; *Robertson et al.*, 2012]. The application of EcoPAD at FLUXNET, NEON or LTER sites includes three steps in general. First, build the climate forcing in the suitable formats of EcoPAD from the database of each site; Second, collect the prior information (include observations of state variables) in the data assimilation system from FLUXNET, NEON or LTER sites; Third, incorporate the forcing and prior information into EcoPAD, and then run the EcoPAD with the dynamic data assimilation system. Furthermore, facing the proposed continental scale ecology study [*Schimel*, 2011], EcoPAD once properly applied could also help evaluate and optimize field deployment of environmental sensors and supporting cyberinfrastructure, that will be necessary for larger, more complex environmental observing systems being planned in the US and across different continents. Altogether, with its milestone concept, EcoPAD benefits from observation and modeling and at the same time advances both observation and modeling of ecological studies.

4.4 Future developments

As we indicated, EcoPAD will expand as time goes on. The system is designed to incorporate multiple biogeochemical models, diverse data assimilation techniques and various ecosystem state variables. A multiple (or ensemble) model approach is helpful in tracking uncertainty sources from our process understanding. With rapid evolving ecological knowledge, emerging models with different hypotheses, such as the microbial-enzyme model [*Wieder et al.*, 2013], enhance our capacity in ecological prediction but can also benefit from rapid tests against data if incorporated into EcoPAD. In addition to MCMC [*Braswell et al.*, 2005; *Xu et al.*, 2006], a variety of data assimilation techniques have been recently applied to improve models for ecological forecasting, such as the EnKF [*Gao et al.*, 2011], Genetic Algorithm [*Zhou and Luo*, 2008] and 4-d variational assimilation [*Peylin et al.*, 2016]. Future development will incorporate different optimization techniques to offer users the option to search for the best model parameters by selecting and comparing the possibly best method for their specific study. We focus mostly on carbon related state variables in the SPRUCE example, and the data assimilation system in EcoPAD needs to include more observed variables for constraining model parameters. For example, the NEON sites not only provide measured ecosystem CO_2 fluxes and soil carbon stocks, but also resources (e.g., GPP/Transpiration for water and GPP/intercepted PAR for light) use efficiency [*Johnson et al.*, 2010]. With these improvements, one goal of the EcoPAD is to

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

enable the research community to run models and forecast various aspects of future biogeochemical changes as data becomes available.

The power of EcoPAD not only lies in its scientific values, but also in the potential service it can bring to the society. Forecasting with carefully quantified uncertainty is helpful in providing support for natural resource manager and policy maker [*Clark et al.*, 2001]. It is always difficult to bring the complex mathematical ecosystem models to the general public, which creates a gap between current scientific advance and public awareness. The web-based interface from EcoPAD makes modeling as easy as possible without losing the connection to the mathematics behind the models. It will greatly transform environmental education and encourage citizen science [*Miller-Rushing et al.*, 2012; *Kobori et al.*, 2016] in ecology and climate change with future outreach activities to broadcast the EcoPAD platform.

5 Conclusion

The fully interactive web-based Ecological Platform for Assimilating Data (EcoPAD) into models aims to promote data-model integration towards predictive ecology through bringing the complex ecosystem model and data assimilation techniques easily accessible to different audience. It is supported by meta-databases of biogeochemical variables, libraries of modules of process models, toolbox of inversion techniques and easily scalable scientific workflow. Through these components, it automates data management, model simulation, data assimilation, ecological forecasting, and result visualization, providing an open, convenient, transparent, flexible, scalable, traceable and readily portable platform to systematically conduct data-model integration towards better ecological forecasting.

We illustrated several of its functionalities through the Spruce and Peatland Responses Under Climatic and Environmental change (SPRUCE) experiment. The iterative forecasting

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access
EGU

approach from EcoPAD-SPRUCE through the prediction-question-discussion-adjustment-prediction cycle and extensive communication between model and data creates a new paradigm to best inform forecasting. In addition to forecasting, EcoPAD enables interactive web-based approach to conduct model simulation, estimate model parameters or state variables, quantify uncertainty of estimated parameters and projected states of ecosystems, evaluate model structures, and assess sampling strategies. Altogether, EcoPAD-SPRUCE creates a smart interactive model-experiment (ModEx) system from which experimenters can know what an ecosystem's response might be at the beginning of their experiments, constrain models through collected measurements, predict ecosystem's response in the rest of the experiments, adjust measurements to better understand their system, periodically update projections and improve models, the data assimilation system, and field experiments.

Specifically to forecasting carbon dynamics, EcoPAD-SPRUCE revealed that better forecasting relies on improvements in model structure, parameterization and accurate external forcing. Accurate external forcing is critical for short-term flux-based carbon predictions while right process understanding, parameterization and historical information are essential for long term pool based predictions. In addition, EcoPAD provides an avenue to disentangle different sources of uncertainties in carbon cycling studies and to provide reliable forecasts with accountable uncertainties.

Code availability:

EcoPAD portal is available at https://ecolab.nau.edu/ecopad_portal/ and code is provided at the GitHub repository (https://github.com/ou-ecolab).

Data availability:

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

Relevant data for this manuscript is available at the SPRUCE project webpage (https://mnspruce.ornl.gov/) and the EcoPAD web portal (https://ecolab.nau.edu/ecopad_portal/). Additional data can be requested from the corresponding author.

Competing interests:

The authors declare that they have no conflict of interest.

Acknowledgement:

SPRUCE components of this work (PJH, DMR) are based upon work supported by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research. Oak Ridge National Laboratory is managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

Literature Cited

Ahlstrom, A., G. Schurgers, A. Arneth, and B. Smith (2012), Robustness and uncertainty in terrestrial ecosystem carbon response to CMIP5 climate change projections,Environmental Research Letters,7(4), doi:10.1088/1748-9326/7/4/044008

Anderson, J., T. Hoar, K. Raeder, H. Liu, N. Collins, R. Torn, and A. Avellano (2009), The data assimilation research testbed A Community Facility,Bulletin of the American Meteorological Society,90(9), 1283-1296, doi:10.1175/2009bams2618.1

Ball, J. T., I. E. Woodrow, and J. A. Berry (1987), A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions, in *Progress in Photosynthesis Research*, edited by J. Biggens, pp. 221– 224, Martinus Nijhoff, Zoetermeer, Netherlands.

Bastiaanssen, W. G. M., and S. Ali (2003), A new crop yield forecasting model based on satellite measurements applied across the Indus Basin, Pakistan,Agriculture Ecosystems & Environment,94(3), 321-340, doi:10.1016/s0167-8809(02)00034-8

Beckage, B., L. J. Gross, and S. Kauffman (2011), The limits to prediction in ecological systems,Ecosphere,2(11), doi:10.1890/es11-00211.1

Botkin, D. B., H. Saxe, M. B. Araujo, R. Betts, R. H. W. Bradshaw, T. Cedhagen, P. Chesson, T. P. Dawson, J. R. Etterson, D. P. Faith, S. Ferrier, A. Guisan, A. S. Hansen, D. W. Hilbert, C. Loehle,

C. Margules, M. New, M. J. Sobel, and D. R. B. Stockwell (2007), Forecasting the effects of global warming on biodiversity,Bioscience,57(3), 227-236, doi:10.1641/b570306

Braswell, B. H., W. J. Sacks, E. Linder, and D. S. Schimel (2005), Estimating diurnal to annual ecosystem parameters by synthesis of a carbon flux model with eddy covariance net ecosystem exchange observations,Global Change Biology,11(2), 335-355, doi:10.1111/j.1365-2486.2005.00897.x

Clark, J. S., S. R. Carpenter, M. Barber, S. Collins, A. Dobson, J. A. Foley, D. M. Lodge, M. Pascual, R. Pielke, W. Pizer, C. Pringle, W. V. Reid, K. A. Rose, O. Sala, W. H. Schlesinger, D. H. Wall, and D. Wear (2001), Ecological forecasts: An emerging imperative,Science,293(5530), 657-660, doi:10.1126/science.293.5530.657

Clark, J. S., M. Lewis, J. S. McLachlan, and J. HilleRisLambers (2003), Estimating population spread: What can we forecast and how well?,Ecology,84(8), 1979-1988, doi:10.1890/01-0618

Cook, B. I., T. M. Smith, and M. E. Mann (2005), The North Atlantic Oscillation and regional phenology prediction over europe,Global Change Biology,11(6), 919-926, doi:10.1111/j.1365-2486.2005.00960.x

Corbet, S. A., N. M. Saville, M. Fussell, O. E. PrysJones, and D. M. Unwin (1995), The competition box: A graphical aid to forecasting pollinator performance,Journal of Applied Ecology,32(4), 707-719, doi:10.2307/2404810

Coreau, A., G. Pinay, J. D. Thompson, P. O. Cheptou, and L. Mermet (2009), The rise of research on futures in ecology: rebalancing scenarios and predictions,Ecology Letters, 12(12), 1277-1286, doi:10.1111/j.1461-0248.2009.01392.x

Coreau, A., S. Treyer, P. O. Cheptou, J. D. Thompson, and L. Mermet (2010), Exploring the difficulties of studying futures in ecology: what do ecological scientists think?,Oikos,119(8), 1364-1376, doi:10.1111/j.1600-0706.2010.18195.x

Craft, C., J. Clough, J. Ehman, S. Joye, R. Park, S. Pennings, H. Y. Guo, and M. Machmuller (2009), Forecasting the effects of accelerated sea-level rise on tidal marsh ecosystem services,Frontiers in Ecology and the Environment,7(2), 73-78, doi:10.1890/070219

Cressie, N., C. A. Calder, J. S. Clark, J. M. V. Hoef, and C. K. Wikle (2009), Accounting for uncertainty in ecological analysis: the strengths and limitations of hierarchical statistical modeling,Ecological Applications,19(3), 553-570, doi:10.1890/07-0744.1

Crozier, L. G., R. W. Zabel, and A. F. Hamlett (2008), Predicting differential effects of climate change at the population level with life-cycle models of spring Chinook salmon,Global Change Biology,14(2), 236-249, doi:10.1111/j.1365-2486.2007.01497.x

Dietze, M. C., D. S. Lebauer, and R. Kooper (2013), On improving the communication between models and data,Plant Cell and Environment,36(9), 1575-1585, doi:10.1111/pce.12043

Diez, J. M., I. Ibanez, A. J. Miller-Rushing, S. J. Mazer, T. M. Crimmins, M. A. Crimmins, C. D. Bertelsen, and D. W. Inouye (2012), Forecasting phenology: from species variability to community patterns,Ecology Letters,15(6), 545-553, doi:10.1111/j.1461-0248.2012.01765.x

Ellison, A. M. (2010), Repeatability and transparency in ecological research,Ecology,91(9), 2536-2539, doi:10.1890/09-0032.1

Farquhar, G. D., S. V. Caemmerer, and J. A. Berry (1980), A biochemical-model of photosynthetic CO2 assimilation in leaves of C3 species,Planta,149(1), 78-90, doi:10.1007/bf00386231

Fordham, D. A., H. R. Akcakaya, M. B. Araujo, J. Elith, D. A. Keith, R. Pearson, T. D. Auld, C. Mellin, J. W. Morgan, T. J. Regan, M. Tozer, M. J. Watts, M. White, B. A. Wintle, C. Yates, and B. W. Brook (2012), Plant extinction risk under climate change: are forecast range shifts alone a good indicator of species vulnerability to global warming?,Global Change Biology,18(4), 1357-1371, doi:10.1111/j.1365-2486.2011.02614.x

Gao, C., H. Wang, E. S. Weng, S. Lakshmivarahan, Y. F. Zhang, and Y. Q. Luo (2011), Assimilation of multiple data sets with the ensemble Kalman filter to improve forecasts of forest carbon dynamics,Ecological Applications,21(5), 1461-1473,

Hampton, S. E., C. A. Strasser, J. J. Tewksbury, W. K. Gram, A. E. Budden, A. L. Batcheller, C. S. Duke, and J. H. Porter (2013), Big data and the future of ecology,Frontiers in Ecology and the Environment,11(3), 156-162, doi:10.1890/120103

Hanson, P. J., J. S. Riggs, W. R. Nettles, J. R. Phillips, M. B. Krassovski, L. A. Hook, L. Gu, A. D. Richardson, D. M. Aubrecht, D. M. Ricciuto, J. M. Warren, and C. Barbier (2017), Attaining whole-ecosystem warming using air and deep-soil heating methods with an elevated CO2 atmosphere,Biogeosciences,14, 861-883, doi:10.5194/bg-14-861-2017

Hararuk, O., J. Y. Xia, and Y. Q. Luo (2014), Evaluation and improvement of a global land model against soil carbon data using a Bayesian Markov chain Monte Carlo method,Journal of Geophysical Research-Biogeosciences,119(3), 403-417, doi:10.1002/2013jg002535

Hare, J. A., M. A. Alexander, M. J. Fogarty, E. H. Williams, and J. D. Scott (2010), Forecasting the dynamics of a coastal fishery species using a coupled climate-population model, Ecological Applications,20(2), 452-464, doi:10.1890/08-1863.1

Huang, Y., J. Jiang, S. Ma, D. Ricciuto, P. J. Hanson, and Y. Luo (2017), Soil thermal dynamics, snow cover and frozen depth under five temperature treatments in an ombrotrophic bog: Constrained forecast with data assimilation,Journal of Geophysical Research: Biogeosciences, doi:10.1002/2016JG003725

Jiang, J., Y. Huang, S. Ma, M. Stacy, Z. Shi, D. M. Ricciuto, P. J. Hanson, and Y. Luo (2018), Forecasting responses of a northern peatland carbon cycle to elevated CO2 and a gradient of experimental warming,Journal of Geophysical Research: Biogeosciences, doi:10.1002/2017jg004040

Johnson, B. R., T. U. Kampe, and M. Kuester (2010), Development of airborne remote sensing instrumentations for NEON, paper presented at SPIE Optical Engineering+ Applications, International Society for Optics and Photonics.

Kearney, M. R., B. A. Wintle, and W. P. Porter (2010), Correlative and mechanistic models of species distribution provide congruent forecasts under climate change,Conservation Letters,3(3), 203-213, doi:10.1111/j.1755-263X.2010.00097.x

Keenan, T. F., E. Davidson, A. M. Moffat, W. Munger, and A. D. Richardson (2012), Using model-data fusion to interpret past trends, and quantify uncertainties in future projections, of terrestrial ecosystem carbon cycling,Global Change Biology,18(8), 2555-2569, doi:10.1111/j.1365-2486.2012.02684.x

Kobori, H., J. L. Dickinson, I. Washitani, R. Sakurai, T. Amano, N. Komatsu, W. Kitamura, S. Takagawa, K. Koyama, T. Ogawara, and A. J. Miller-Rushing (2016), Citizen science: a new approach to advance ecology, education, and conservation,Ecological Research,31(1), 1-19, doi:10.1007/s11284-015-1314-y

Kolka, R. K., S. D. Sebestyen, E. S. Verry, and K. N. Brooks (2011), *Peatland biogeochemistry and watershed hydrology at the Marcell Experimental Forest*, 488 pp., CRC Press Boca Raton

Lebauer, D. S., D. Wang, K. T. Richter, C. C. Davidson, and M. C. Dietze (2013), Facilitating feedbacks between field measurements and ecosystem models,Ecological Monographs, 83(2), 133-154, doi:10.1890/12-0137.1

Liang, J. Y., D. J. Li, Z. Shi, J. M. Tiedje, J. Z. Zhou, E. A. G. Schuur, K. T. Konstantinidis, and Y. Q. Luo (2015), Methods for estimating temperature sensitivity of soil organic matter based on incubation data: A comparative evaluation,Soil Biology & Biochemistry,80, 127-135, doi:10.1016/j.soilbio.2014.10.005

Ludascher, B., I. Altintas, C. Berkley, D. Higgins, E. Jaeger, M. Jones, E. A. Lee, J. Tao, and Y. Zhao (2006), Scientific workflow management and the Kepler system,Concurrency and Computation-Practice & Experience,18(10), 1039-1065, doi:10.1002/cpe.994

Luo, Y. Q., and J. F. Reynolds (1999), Validity of extrapolating field CO2 experiments to predict carbon sequestration in natural ecosystems,Ecology,80(5), 1568-1583, doi:10.1890/0012-9658(1999)080[1568:voefce]2.0.co;2

Luo, Y. Q., S. Q. Wan, D. F. Hui, and L. L. Wallace (2001), Acclimatization of soil respiration to warming in a tall grass prairie,Nature,413(6856), 622-625, doi:10.1038/35098065

Geoscientific Model Development Discussions

Luo, Y. Q., J. Melillo, S. L. Niu, C. Beier, J. S. Clark, A. T. Classen, E. Davidson, J. S. Dukes, R. D. Evans, C. B. Field, C. I. Czimczik, M. Keller, B. A. Kimball, L. M. Kueppers, R. J. Norby, S. L. Pelini, E. Pendall, E. Rastetter, J. Six, M. Smith, M. G. Tjoelker, and M. S. Torn (2011a), Coordinated approaches to quantify long-term ecosystem dynamics in response to global change,Global Change Biology,17(2), 843-854, doi:10.1111/j.1365-2486.2010.02265.x

Luo, Y. Q., K. Ogle, C. Tucker, S. F. Fei, C. Gao, S. LaDeau, J. S. Clark, and D. S. Schimel (2011b), Ecological forecasting and data assimilation in a data-rich era,Ecological Applications, 21(5), 1429-1442,

Luo, Y. Q., A. Ahlstrom, S. D. Allison, N. H. Batjes, V. Brovkin, N. Carvalhais, A. Chappell, P. Ciais, E. A. Davidson, A. C. Finzi, K. Georgiou, B. Guenet, O. Hararuk, J. W. Harden, Y. J. He, F. Hopkins, L. F. Jiang, C. Koven, R. B. Jackson, C. D. Jones, M. J. Lara, J. Y. Liang, A. D. McGuire, W. Parton, C. H. Peng, J. T. Randerson, A. Salazar, C. A. Sierra, M. J. Smith, H. Q. Tian, K. E. O. Todd-Brown, M. Torn, K. J. van Groenigen, Y. P. Wang, T. O. West, Y. X. Wei, W. R. Wieder, J. Y. Xia, X. Xu, X. F. Xu, and T. Zhou (2016), Toward more realistic projections of soil carbon dynamics by Earth system models,Global Biogeochemical Cycles,30(1), 40-56, doi:10.1002/2015gb005239

Luo, Y. Q. (2017), Transient dynamics of terrestrial carbon storage: mathematical foundation and its applications,

Ma, S., J. Jiang, Y. Huang, D. Ricciuto, P. J. Hanson, and Y. Luo (2017), Data-constrained projections of methane fluxes in a Northern Minnesota Peatland in response to elevated CO2 and warming (Accepted),Journal of Geophysical Research: Biogeosciences,

Medlyn, B. E., F. W. Badeck, D. G. G. De Pury, C. V. M. Barton, M. Broadmeadow, R. Ceulemans, P. De Angelis, M. Forstreuter, M. E. Jach, S. Kellomaki, E. Laitat, M. Marek, S. Philippot, A. Rey, J. Strassemeyer, K. Laitinen, R. Liozon, B. Portier, P. Roberntz, K. Wang, and P. G. Jarvis (1999), Effects of elevated CO2 on photosynthesis in European forest species: a meta-analysis of model parameters,Plant Cell and Environment,22(12), 1475-1495, doi:10.1046/j.1365-3040.1999.00523.x

Melillo, J. M., S. D. Frey, K. M. DeAngelis, W. J. Werner, M. J. Bernard, F. P. Bowles, G. Pold, M. A. Knorr, and A. S. Grandy (2017), Long-term pattern and magnitude of soil carbon feedback to the climate system in a warming world,Science,358(6359), 101-105, doi:10.1126/science.aan2874

Michener, W. K., and M. B. Jones (2012), Ecoinformatics: supporting ecology as a data-intensive science,Trends in Ecology & Evolution,27(2), 85-93, doi:10.1016/j.tree.2011.11.016

Miller-Rushing, A., R. Primack, and R. Bonney (2012), The history of public participation in ecological research,Frontiers in Ecology and the Environment,10(6), 285-290, doi:10.1890/110278

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Moorcroft, P. R. (2006), How close are we to a predictive science of the biosphere?,Trends in Ecology & Evolution,21(7), 400-407, doi:10.1016/j.tree.2006.04.009

Mouquet, N., Y. Lagadeuc, V. Devictor, L. Doyen, A. Duputie, D. Eveillard, D. Faure, E. Garnier, O. Gimenez, P. Huneman, F. Jabot, P. Jarne, D. Joly, R. Julliard, S. Kefi, G. J. Kergoat, S. Lavorel, L. Le Gall, L. Meslin, S. Morand, X. Morin, H. Morlon, G. Pinay, R. Pradel, F. M. Schurr, W. Thuiller, and M. Loreau (2015), REVIEW: Predictive ecology in a changing world,Journal of Applied Ecology,52(5), 1293-1310, doi:10.1111/1365-2664.12482

Niu, S. L., Y. Q. Luo, M. C. Dietze, T. F. Keenan, Z. Shi, J. W. Li, and F. S. Chapin (2014), The role of data assimilation in predictive ecology,Ecosphere,5(5), doi:10.1890/es13-00273.1

Ong, J. B. S., M. I. C. Chen, A. R. Cook, H. C. Lee, V. J. Lee, R. T. P. Lin, P. A. Tambyah, and L. G. Goh (2010), Real-Time Epidemic Monitoring and Forecasting of H1N1-2009 Using Influenza-Like Illness from General Practice and Family Doctor Clinics in Singapore,Plos One,5(4), doi:10.1371/journal.pone.0010036

Osterweil, L. J., L. A. Clarke, A. M. Ellison, E. Boose, R. Podorozhny, and A. Wise (2010), Clear and Precise Specification of Ecological Data Management Processes and Dataset Provenance,Ieee Transactions on Automation Science and Engineering,7(1), 189-195, doi:10.1109/tase.2009.2021774

Parton, W. J., J. W. B. Stewart, and C. V. Cole (1988), Dynamics of c, n, p and s in grassland soils - a model,Biogeochemistry,5(1), 109-131, doi:10.1007/bf02180320

Parton, W. J., J. A. Morgan, G. M. Wang, and S. Del Grosso (2007), Projected ecosystem impact of the Prairie Heating and CO2 Enrichment experiment,New Phytologist,174(4), 823-834, doi:10.1111/j.1469-8137.2007.02052.x

Perretti, C. T., S. B. Munch, and G. Sugihara (2013), Model-free forecasting outperforms the correct mechanistic model for simulated and experimental data,Proceedings of the National Academy of Sciences of the United States of America,110(13), 5253-5257, doi:10.1073/pnas.1216076110

Petchey, O. L., M. Pontarp, T. M. Massie, S. Kefi, A. Ozgul, M. Weilenmann, G. M. Palamara, F. Altermatt, B. Matthews, J. M. Levine, D. Z. Childs, B. J. McGill, M. E. Schaepman, B. Schmid, P. Spaak, A. P. Beckerman, F. Pennekamp, and I. S. Pearse (2015), The ecological forecast horizon, and examples of its uses and determinants,Ecology Letters,18(7), 597-611, doi:10.1111/ele.12443

Peylin, P., C. Bacour, N. MacBean, S. Leonard, P. Rayner, S. Kuppel, E. Koffi, A. Kane, F. Maignan, F. Chevallier, P. Ciais, and P. Prunet (2016), A new stepwise carbon cycle data assimilation system using multiple data streams to constrain the simulated land surface carbon cycle,Geoscientific Model Development,9(9), 3321-3346, doi:10.5194/gmd-9-3321-2016

Purves, D., J. Scharlemann, M. Harfoot, T. Newbold, D. P. Tittensor, J. Hutton, and S. Emmott (2013), Time to model all life on Earth,Nature,493(7432), 295-297,

Robertson, G. P., S. L. Collins, D. R. Foster, N. Brokaw, H. W. Ducklow, T. L. Gragson, C. Gries, S. K. Hamilton, A. D. McGuire, and J. C. Moore (2012), Long-term ecological research in a human-dominated world,BioScience,62(4), 342-353,

Schaefer, K., C. R. Schwalm, C. Williams, M. A. Arain, A. Barr, J. M. Chen, K. J. Davis, D. Dimitrov, T. W. Hilton, D. Y. Hollinger, E. Humphreys, B. Poulter, B. M. Raczka, A. D. Richardson, A. Sahoo, P. Thornton, R. Vargas, H. Verbeeck, R. Anderson, I. Baker, T. A. Black, P. Bolstad, J. Q. Chen, P. S. Curtis, A. R. Desai, M. Dietze, D. Dragoni, C. Gough, R. F. Grant, L. H. Gu, A. Jain, C. Kucharik, B. Law, S. G. Liu, E. Lokipitiya, H. A. Margolis, R. Matamala, J. H. McCaughey, R. Monson, J. W. Munger, W. Oechel, C. H. Peng, D. T. Price, D. Ricciuto, W. J. Riley, N. Roulet, H. Q. Tian, C. Tonitto, M. Torn, E. S. Weng, and X. L. Zhou (2012), A model-data comparison of gross primary productivity: Results from the North American Carbon Program site synthesis,Journal of Geophysical Research-Biogeosciences,117, doi:10.1029/2012jg001960

Schimel, D. (2011), The era of continental-scale ecology,Frontiers in Ecology and the Environment,9(6), 311-311,

Schindler, D. E., and R. Hilborn (2015), Prediction, precaution, and policy under global change,Science,347(6225), 953-954, doi:10.1126/science.1261824

Scholze, M., T. Kaminski, P. Rayner, W. Knorr, and R. Giering (2007), Propagating uncertainty through prognostic carbon cycle data assimilation system simulations,Journal of Geophysical Research-Atmospheres,112(D17), doi:10.1029/2007jd008642

Shi, Z., X. Xu, O. Hararuk, L. F. Jiang, J. Y. Xia, J. Y. Liang, D. J. Li, and Y. Q. Luo (2015), Experimental warming altered rates of carbon processes, allocation, and carbon storage in a tallgrass prairie,Ecosphere,6(11), doi:10.1890/es14-00335.1

Shi, Z., Y. H. Yang, X. H. Zhou, E. S. Weng, A. C. Finzi, and Y. Q. Luo (2016), Inverse analysis of coupled carbon-nitrogen cycles against multiple datasets at ambient and elevated CO2, Journal of Plant Ecology,9(3), 285-295, doi:10.1093/jpe/rtv059

Sitch, S., C. Huntingford, N. Gedney, P. E. Levy, M. Lomas, S. L. Piao, R. Betts, P. Ciais, P. Cox, P. Friedlingstein, C. D. Jones, I. C. Prentice, and F. I. Woodward (2008), Evaluation of the terrestrial carbon cycle, future plant geography and climate-carbon cycle feedbacks using five Dynamic Global Vegetation Models (DGVMs),Global Change Biology,14(9), 2015-2039, doi:10.1111/j.1365-2486.2008.01626.x

Steppe, K., J. S. von der Crone, and D. J. W. Pauw (2016), TreeWatch.net: A Water and Carbon Monitoring and Modeling Network to Assess Instant Tree Hydraulics and Carbon Status,Frontiers in Plant Science,7, doi:10.3389/fpls.2016.00993

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Stumpf, R. P., M. C. Tomlinson, J. A. Calkins, B. Kirkpatrick, K. Fisher, K. Nierenberg, R. Currier, and T. T. Wynne (2009), Skill assessment for an operational algal bloom forecast system,Journal of Marine Systems,76(1-2), 151-161, doi:10.1016/j.jmarsys.2008.05.016

Sugihara, G., R. May, H. Ye, C. H. Hsieh, E. Deyle, M. Fogarty, and S. Munch (2012), Detecting Causality in Complex Ecosystems,Science,338(6106), 496-500, doi:10.1126/science.1227079

Tan, Z. X., S. G. Liu, C. A. Johnston, T. R. Loveland, L. L. Tieszen, J. X. Liu, and R. Kurtz (2005), Soil organic carbon dynamics as related to land use history in the northwestern Great Plains,Global Biogeochemical Cycles,19(3), doi:10.1029/2005gb002536

Thomas, R. Q., E. B. Brooks, A. L. Jersild, E. Ward, R. H. Wynne, T. J. Albaugh, H. Dinon-Aldridge, H. E. Burkhart, J. Domec, T. R. Fox, C. A. Gonzalez-Benecke, T. A. Martin, A. Noormets, D. A. Sampson, and R. O. Teskey (2017), Leveraging 35 years of Pinus taeda research in the southeastern US to constrain forest carbon cycle predictions: regional data assimilation using ecosystem experiments,Biogeosciences,14, 3525-3547,

Vitolo, C., Y. Elkhatib, D. Reusser, C. J. A. Macleod, and W. Buytaert (2015), Web technologies for environmental Big Data,Environmental Modelling & Software,63, 185-198, doi:10.1016/j.envsoft.2014.10.007

Walker, A. P., P. J. Hanson, M. G. De Kauwe, B. E. Medlyn, S. Zaehle, S. Asao, M. Dietze, T. Hickler, C. Huntingford, C. M. Iversen, A. Jain, M. Lomas, Y. Q. Luo, H. McCarthy, W. J. Parton, I. C. Prentice, P. E. Thornton, S. S. Wang, Y. P. Wang, D. Warlind, E. S. Weng, J. M. Warren, F. I. Woodward, R. Oren, and R. J. Norby (2014), Comprehensive ecosystem model-data synthesis using multiple data sets at two temperate forest free-air CO2 enrichment experiments: Model performance at ambient CO2 concentration,Journal of Geophysical Research-Biogeosciences,119(5), 937-964, doi:10.1002/2013jg002553

Wallenstein, M. D., and E. K. Hall (2012), A trait-based framework for predicting when and where microbial adaptation to climate change will affect ecosystem functioning, Biogeochemistry,109(1-3), 35-47, doi:10.1007/s10533-011-9641-8

Wang, Y. P., and R. Leuning (1998), A two-leaf model for canopy conductance, photosynthesis and partitioning of available energy I: Model description and comparison with a multi-layered model,Agricultural and Forest Meteorology,91(1-2), 89-111, doi:10.1016/s0168-1923(98)00061-6

Wang, Y. P., C. M. Trudinger, and I. G. Enting (2009), A review of applications of model-data fusion to studies of terrestrial carbon fluxes at different scales,Agricultural and Forest Meteorology,149(11), 1829-1842, doi:10.1016/j.agrformet.2009.07.009

Wang, Y. P., R. M. Law, and B. Pak (2010), A global model of carbon, nitrogen and phosphorus cycles for the terrestrial biosphere,Biogeosciences,7(7), 2261-2282, doi:10.5194/bg-7-2261-2010

Ward, E. J., E. E. Holmes, J. T. Thorson, and B. Collen (2014), Complexity is costly: a meta-analysis of parametric and non-parametric methods for short-term population forecasting, Oikos,123(6), 652-661, doi:10.1111/j.1600-0706.2014.00916.x

Weng, E. S., and Y. Q. Luo (2008), Soil hydrological properties regulate grassland ecosystem responses to multifactor global change: A modeling analysis,Journal of Geophysical Research-Biogeosciences,113(G3), doi:10.1029/2007jg000539

Weng, E. S., and Y. Q. Luo (2011), Relative information contributions of model vs. data to short- and long-term forecasts of forest carbon dynamics,Ecological Applications,21(5), 1490-1505,

Weng, E. S., Y. Q. Luo, C. Gao, and R. Oren (2011), Uncertainty analysis of forest carbon sink forecast with varying measurement errors: a data assimilation approach,Journal of Plant Ecology,4(3), 178-191, doi:10.1093/jpe/rtr018

Wieder, W. R., G. B. Bonan, and S. D. Allison (2013), Global soil carbon projections are improved by modelling microbial processes,Nature Climate Change,3(10), 909-912, doi:10.1038/nclimate1951

Xu, T., L. White, D. F. Hui, and Y. Q. Luo (2006), Probabilistic inversion of a terrestrial ecosystem model: Analysis of uncertainty in parameter estimation and model prediction, Global Biogeochemical Cycles,20(2), doi:10.1029/2005gb002468

Zhou, T., and Y. Q. Luo (2008), Spatial patterns of ecosystem carbon residence time and NPP-driven carbon uptake in the conterminous United States,Global Biogeochemical Cycles,22(3), doi:10.1029/2007gb002939

Zhou, X. H., T. Zhou, and Y. Q. Luo (2012), Uncertainties in carbon residence time and NPP-driven carbon uptake in terrestrial ecosystems of the conterminous USA: a Bayesian approach,Tellus Series B-Chemical and Physical Meteorology,64, doi:10.3402/tellusb.v64i0.17223

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Tables

Table 1. Discussion stimulated by EcoPAD-SPRUCE forecasting among modelers and experimenters on how to improve predictions of the relative contribution of different pathways of methane emissions

	Discussion
1	No strong bubbles are noted at field and a non-observation constrained modeling study at a similar site from another project concluded minor ebullition contribution, which are at odds with TECO result.
2	CH_4:CO_2 ratio might explain the discrepancy. The other modeling study assumed that decomposed C is mainly turned into CO_2 and a smaller fraction is turned into CH_4. The large CH_4:CO_2 ratio at this site may result in higher CH4 flux. It seems that the most “flexible” term is ebullition because any "excess" (above saturation) CH4 is immediately released to ebullition, while the plant transport term is constrained by vegetation data.
3	Experimental researches on the relative contribution to methane emission from three different pathways are rare.
4	Current available observations include net surface flux of methane from the large collars, incubation data that should represent methane sources within the profile, and gas/DOC profile data that can indicate active zones within the peat profile. What are additional data needed to constrain relative contribution of different pathways?
5	I had always thought that peatlands don’t bubble much, but the super-sensitive GPS measurements found movements of the surface of the GLAP peatlands consistent with degassing events, and subsurface radar images did show layers that were interpreted as bubble-layers.
6	Pore water gas data, perhaps N_2 or Ar may shed some light on the relative importance of ebullition.
7	It is really hard to accurately distinguish the three pathways. It has to rely on multiple approaches. Particularly for the SPRUCE site, the vegetation cover varies, vegetation species varies. How many channels each species has affect the transport? Meanwhile, the presence of plant (even not vascular plant) will lead to more gas transport, but as bubbles, rather than plant-mediated transport.
8	It depends on model structure and algorithm to simulate diffusion, vascular, and ebullition. Most models assume a threshold to allow ebullition. Diffusion is treated in similar ways as ebullition in some models (most one layer or two layers models). For the multiple layers models, the diffusion occurs from bottom to top mm by mm, layer by layer, therefore, the gas diffusion from top layer to atmosphere is considered the diffusion flux. If that is the case, the time step and wind speed and pressure matter (most models do not consider wind and pressure impacts). Plant transport is really dependent on the parameter for plant species, aerenchyma, etc. The gas transportability of plant is associated with biomass, NPP, or root biomass, seasonality of plant growth, etc. in models. All these differences might cause biases in the final flux.
9	With only the CH_4 emission data cannot constrain the relative contribution of three pathways. Concentration data in different soil layers may help constrain.
10	Diffusion coefficient calculation in TECO adopts the "three-porosity-model" which is ideal for mineral soil, but may not fit the organic soil. "Millington-Quirk model" for should be a better choice for peat soil.
11	The boundary condition should be taken care of, but it brings in more uncertainties including the wind speed and piston velocity, etc.,
12	CH_4 emissions captured in static chambers does not include the episodic ebullition events. So (1) the static chambers underestimate the total methane emission and (2) might need to exclude the ebullition pathway when using the observation data to constrain the CH_4 emission. But this point seems haven't been paid attention to in other models.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

Figure Legends

Figure 1 Schema of approaches to forecast future ecological responses from common practice (the upper panel) and the Ecological Platform for Assimilation of Data (EcoPAD) (bottom panel). The common practice makes use of observations to develop or calibrate models to make predictions while the EcoPAD approach advances the common practice through its fully interactive platform. EcoPAD consists of four major components: experiment/data, model, data assimilation and the scientific workflow. Data and model are iteratively integrated through its data assimilation systems to improve forecasting. And its near-real time forecasting results are shared among research groups through its web interface to guide new data collections. The scientific workflow enables web-based data transfer from sensors, model simulation, data assimilation, forecasting, result analysis, visualization and reporting, encouraging broad user-model interactions especially for the experimenters and the general public with limited background in modeling.

Figure 2 The data assimilation system inside the Ecological Platform for Assimilation of Data (EcoPAD) towards better forecasting of terrestrial carbon dynamics

Figure 3 The scientific workflow of EcoPAD. The workflow wraps ecological models and data assimilation algorithms with the docker containerization platform. Users trigger different tasks through the Representational State Transfer (i.e., RESTful) application-programming interface (API). Tasks are managed through the asynchronous task queue, Celery. Tasks can be executed concurrently on a single or more worker servers across different scalable IT infrastructures. MongoDB is a database software that takes charge of data management in EcoPAD and RabbitMQ is a message broker.

Figure 4. Near time forecasting of EcoPAD-SPRUCE. EcoPAD automatically synchronizes real time observations from environmental sensors managed by the SPRUCE experimental communities. Data from observations are assimilated and used to update forecasting. Weekly forecasting results are displayed in the EcoPAD-SPRUCE web portal (http://ecolab.cybercommons.org/ecopad_portal/) as well as sent back to the experimental groups to guide future experimental design and sampling.

Figure 5. Schema of interactive communication between modelers and experimenters through the prediction-question-discussion-adjustment-prediction cycle to improve ecological forecasting. The schema is inspired by an episode of experimenter-modeler communication stimulated by the EcoPAD-SPRUCE platform. The initial methane model constrained by static chamber methane measurements was used to predict relative contributions of three methane emission pathways (i.e., ebullition, plant mediated transportation (PMT) and diffusion) to the overall methane fluxes under different warming treatments (+ 0 °C, +2.25 °C, +4.5 °C, +6.75 °C and +9 °C). The initial results indicated a dominant contribution from ebullition especially under +9 °C which was doubted by experimenters. The discrepancy stimulated communications between modelers and experimenters with detailed information listed in Table 1. After extensive discussion, the model structure was adjusted and field observations were reevaluated. And a second round of forecasting yielded more reliable predictions.

Figure 6. Posterior distribution of the ratio of CH_4:CO_2 (panel a) and the temperature sensitivity of methane production (Q_{10_CH4}, panel b) under 5 warming treatments.

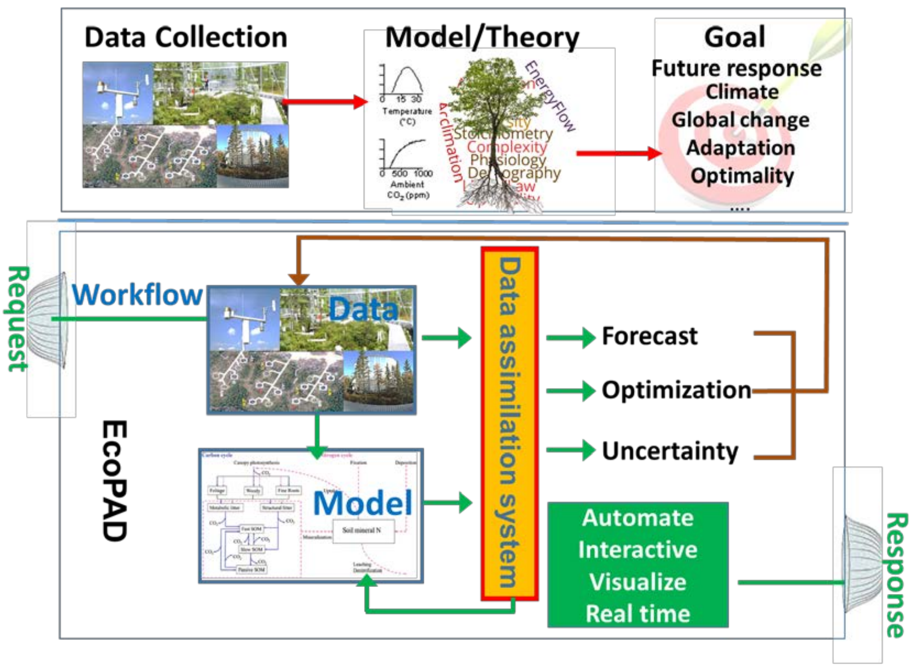
Figure 7. Realized vs. unrealized forecasting of gross primary production (panels a,c) and soil organic C content (panels b,d). The upper panels show 3 series of forecasting with different weather forcing. Cyan indicates forecasting with 100 stochastically generated weather forcing

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

from January 2015 to December 2024 (S1); red corresponds to realized forecasting with measured weather forcing from January 2015 to July 2016 followed by forecasting with 100 stochastically generated weather forcing (S2); and blue shows realized forecasting with measured weather forcing from January 2015 to December 2016 followed by forecasting with 100 stochastically generated weather forcing (S3). The bottom panels display mismatches between realized forecasting (S2,3) and the original unrealized forecasting (S1). Red displays the difference between S2 and S1 (S2-S1) and blue shows discrepancy between S3 and S1 (S3-S1). Dashed green lines indicates the start of forecasting with stochastically generated weather forcing. Note that the left 2 panels are plotted on yearly time-scale and the right 2 panels show results on monthly time-scale.

Figure 1


Data Collection
Model/Theory
Goal
Future response
Climate
Global change
Adaptation
Optimality
EnergyFlow
Acclimation
Stoichiometry
Complexity
Physiology
Demography
Request
Workflow
Data
Model
Data assimilation system
Forecast
Optimization
Uncertainty
EcoPAD
Automate
Interactive
Visualize
Real time
Response

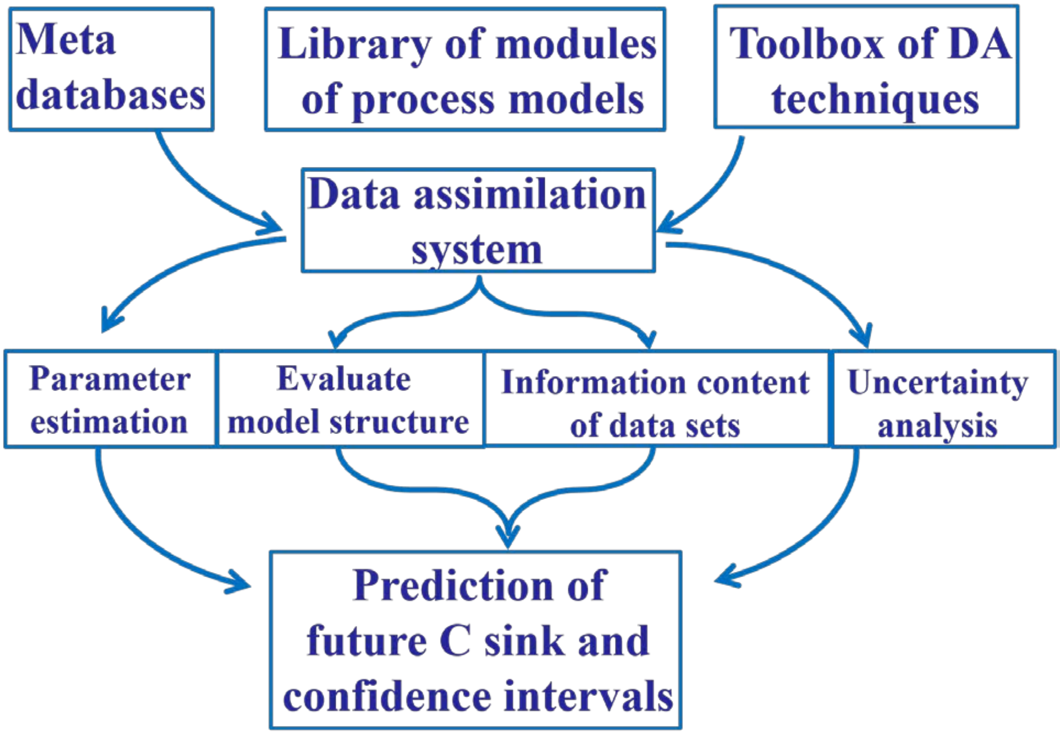
Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access

1256

1257 **Figure 2**

1258



1259

1260

1261

1262

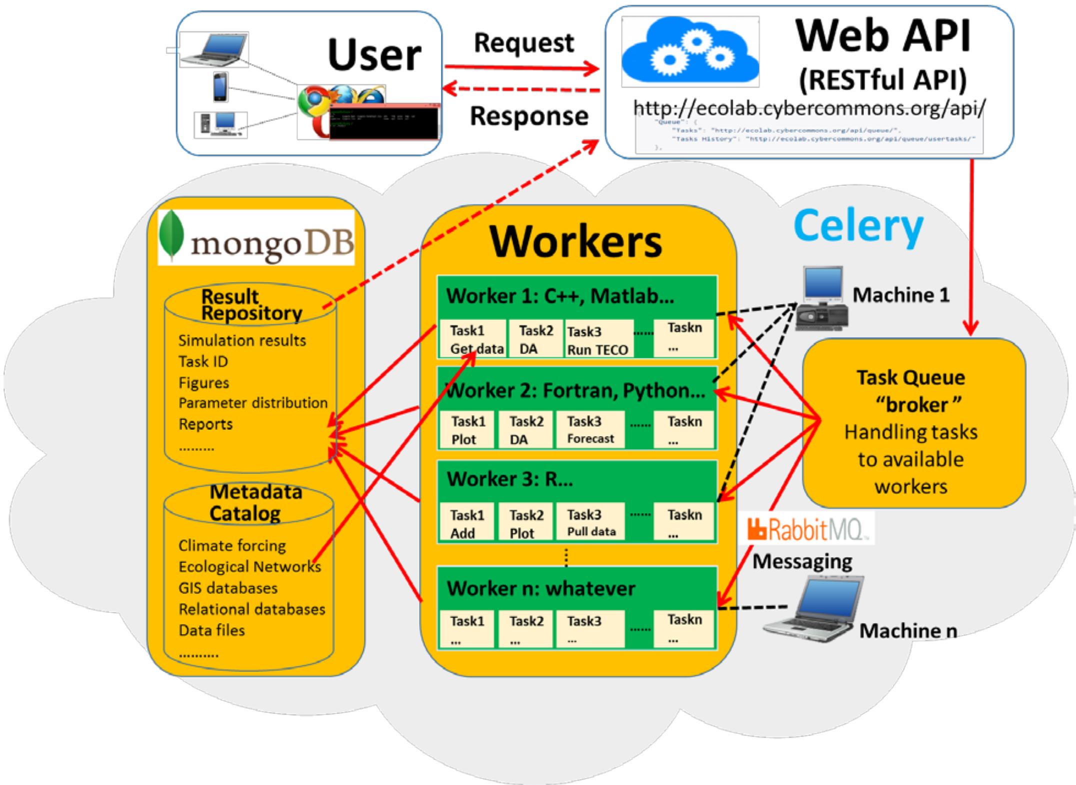
1263

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development
Discussions

1264 **Figure 3**

1265



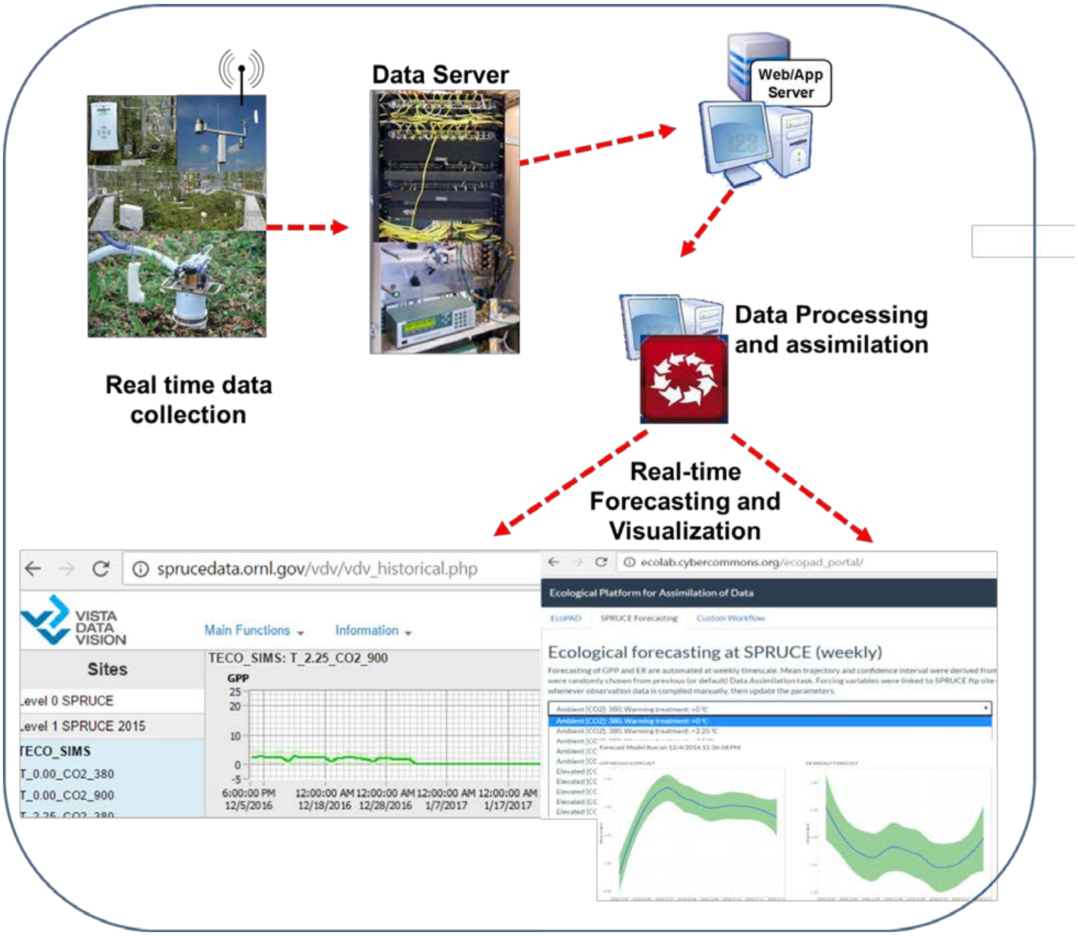
1266

1267

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

1268

1269 **Figure 4**



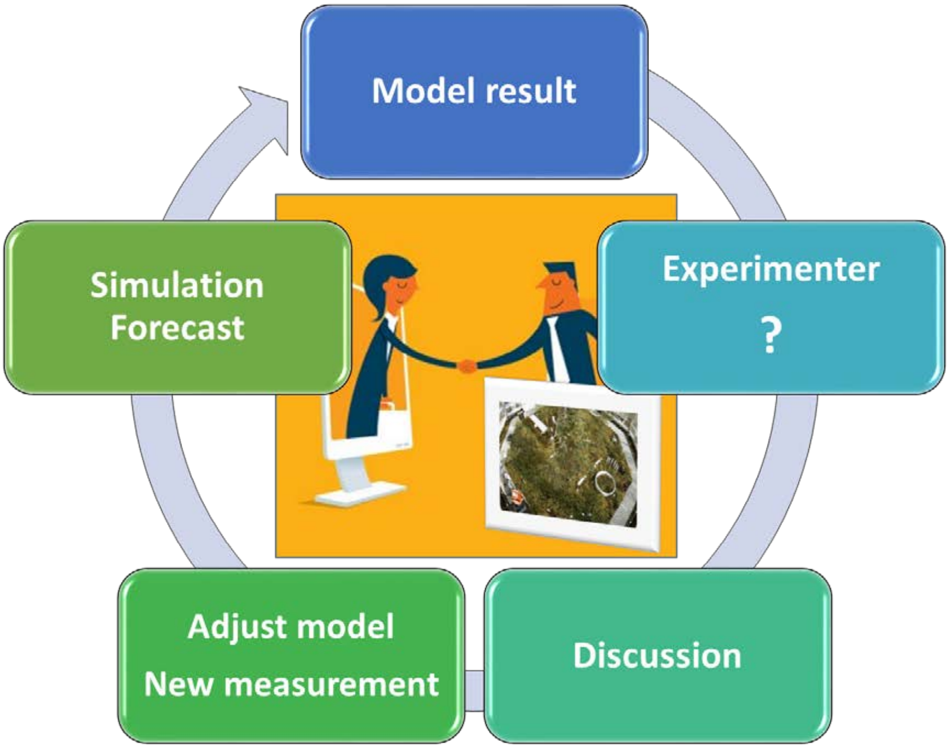
1270

1271

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access

1272 **Figure 5**



1273

1274

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access

Figure 6

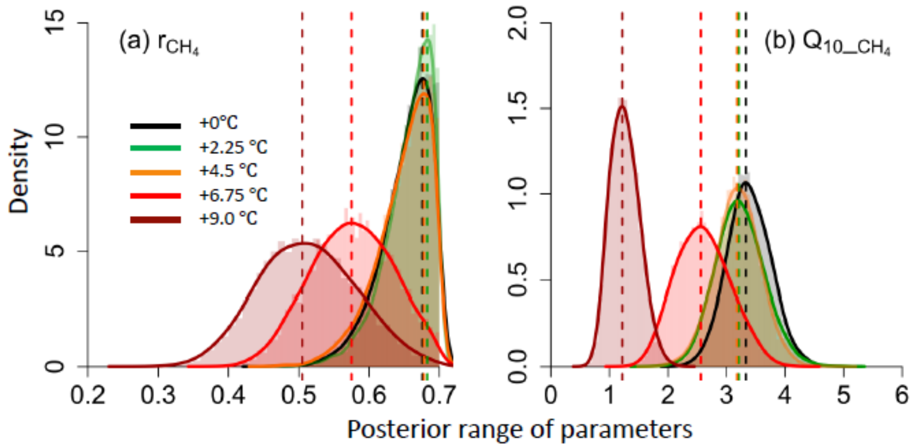
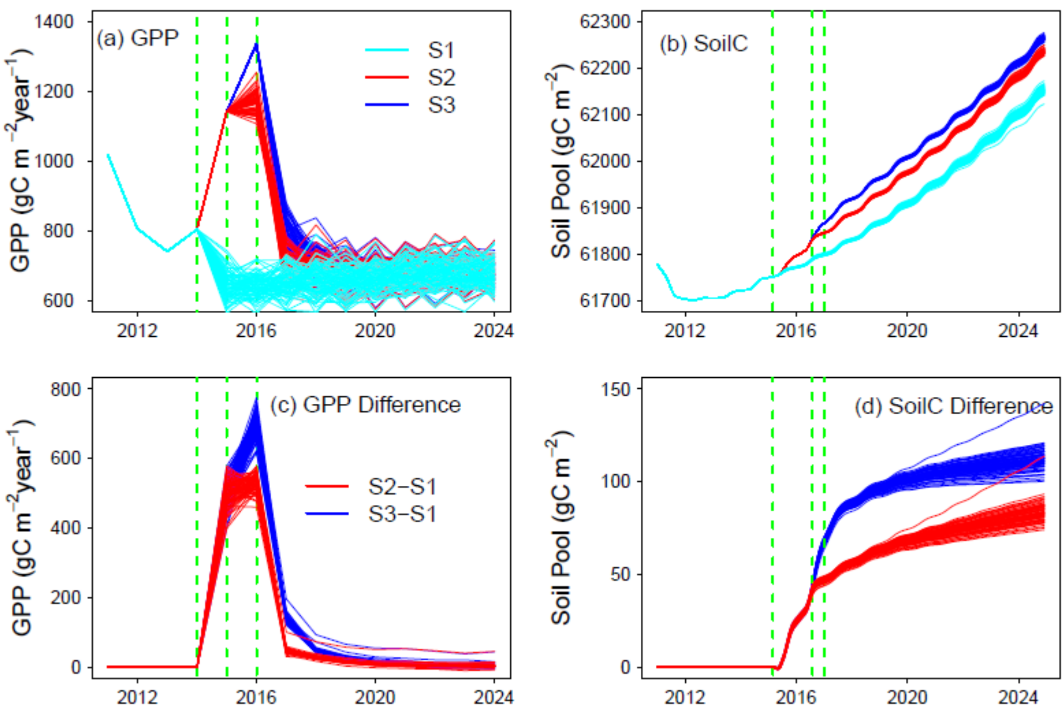


Figure 7


(a) GPP
S1
S2
S3
GPP (gC m^{-2}year^{-1})
1400
1200
1000
800
600
2012
2016
2020
2024
(b) SoilC
Soil Pool (gC m^{-2})
62300
62200
62100
62000
61900
61800
61700
(c) GPP Difference
S2−S1
S3−S1
800
600
400
200
0
(d) SoilC Difference
150
100
50

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access

Appendices

Appendix 1

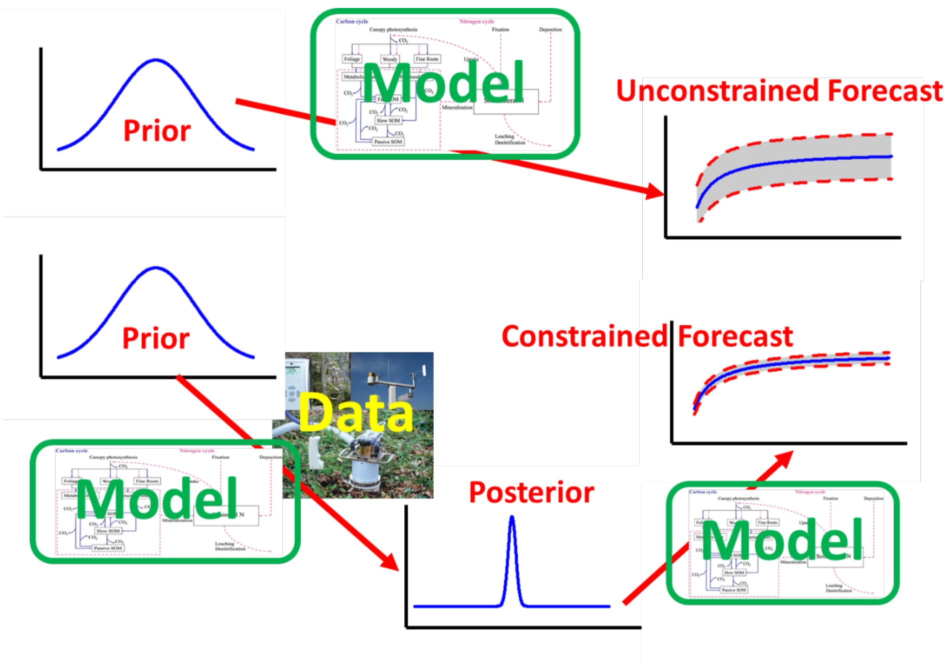


Figure A1. Conceptual demonstration of how data assimilation that updates models through observations constrains forecasting. The grey shading area corresponds to forecasting uncertainties.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Appendix 2 EcoPAD-SPRUCE web portal

We assimilate multiple streams of data from the SPRUCE experiment to the TECO model using the MCMC algorithm, and forecast ecosystem dynamics in both near time and for the next 10 years. Our forecasting system for SPRUCE is available at https://ecolab.nau.edu/ecopad_portal/ (the new portal) or http://ecolab.cybercommons.org/ecopad_portal_up/ (the older portal). From the web portal, users can check our current near and long term forecasting results, conduct model simulation, data assimilation and forecasting runs, and analyze/visualize model results (Username: test00 and password:test01 for the new portal; Username: chris and password:chris for the old portal if login information is required). The login account we created for the new portal is limited to Simulation only and registration is required for more functionalities.

The main page of the EcoPAD-SPRUCE portal includes animation demos and a brief description of the system. The animation demos display the dynamic change of gross primary productivity (GPP), ecosystem respiration (ER), foliage carbon (foliage C), wood carbon (wood C), root carbon (root C) and soil carbon (soil C) under 10 manipulative warming and elevated atmospheric CO_2 treatments. Each animation shows observations in data assimilation period during which parameters are constrained (2011-2014) as well as model results (with uncertainty) from data assimilation and 10 years forecasting from an ensemble of model runs. Warming generally increase GPP, ER and different carbon pools. Users can also get a sense on how uncertainties in forcing variables, such as light, temperature, and precipitation that drive carbon fluxes in terrestrial ecosystem, and limited observations affect uncertainty of GPP prediction.

Under the Custom Workflow menu, users can choose different modes to run TECO model from the task dropdown box: Simulation, Data Assimilation (DA) and Forecasting (Figure A2). In the Simulation mode, users are allowed change the initial parameters through “Set Initial

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Parameters" button. TECO-SPRUCE currently allows 33 key parameters to be adjustable by end-users. These 33 parameters include parameters that control soil water dynamics, plant growth, photosynthesis, carbon allocation among different plant organs, turnover rates of different pools, temperature sensitivity, and plant phenology. Researchers can choose other parameters according to their models and specific needs. The simulation runs TECO one time with user supplied initial parameters and the run normally takes several minutes in the background. Each requested task from the user is assigned a unique task ID. Users can check information such as task id, timestamp, parameters, result status, result URL from a web-enabled report once the task is submitted under the "Task History" tab. If the task status shows "SUCESS" (Figure A3), users can check datasets relevant to model simulation from the result URL (for example, http://ecolab.oscer.ou.edu/ecopad_tasks/8b4bcd9b-172c-4031-94b7-4b080e459025, where "8b4bcd9b-172c-4031-94b7-4b080e459025" is the unique task ID for this example). The URL directs users to the location (result repository) where information related to model simulation is stored. Result repository stores parameters supplied to the model run in .txt format. Yearly and daily simulation results for carbon fluxes and pools are also written in .txt file format. It also contains .png file format plots of simulated carbon fluxes and pools compared to observations (Figure A4). Users can check the results from the Task History any time with the right task ID. With several "Simulation" runs, users can easily get a sense on the sensitivity of the SPRUCE peatland carbon cycle to different parameters and what are the key processes regulate the northern peatland carbon dynamics.

Data Assimilation mode enables users to conduct data-model fusion research through a web portal. A unique feature of the data assimilation portal is that users can pick whatever parameters to be constrained among the pool of 18 parameters which are important in ecosystem carbon

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

cycling (Figure A5). Users can change the range of a parameter they are interested in and modify the initial values of parameters supplied to MCMC. Similarly as in Simulation mode, user can easily check data assimilation results through the result URL. Results from data assimilation contain parameter ranges and initial values supplied by users, parameter values accepted in MCMC, histograms of posterior distribution of parameters (Figure A5), and simulations of carbon fluxes and pools with 500 randomly chosen accepted parameters. Data assimilation results are also written into the universal .txt format which makes further utilization of the result convenient. For example, researchers interested in the pattern and uncertainty in GPP simulation can quickly get a handle on GPP with an ensemble of easily readable model results.

From the Forecasting mode, users are enabled to set up parameters, or choose posterior parameters from previous data assimilation results, specify forecast starting and ending dates, and select warming (0-9 degree Celsius) and CO_2 (380-900 ppm) treatments (Figure A6). If a specific data assimilation result was chosen as input for forecasting simulation, TECO-SPRUCE would read the constrained posterior parameter file, match the name of constrained parameters to the whole parameter pool, and then randomly choose 100 sets of constrained parameters to run forecast. Results from forecast store carbon fluxes and pools from simulations based on the 100 randomly chosen parameters and projected 10 years into the future at the daily time scale. Users can analyze forecasting dynamics and uncertainties based on stored results. EcoPAD-SPRUCE result repositories also provide figures that combine observation in data assimilation period, simulation results in data assimilation as well as forecasting periods, and simulation uncertainty (Figure A7) to speed up the post-processing of model results.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access
EGU

Figure A2. The Custom Workflow web portal of the EcoPAD applied for the SPRUCE project. Users can select among "Simulation", "Data Assimilation (DA)" and "Forecasting" modes from the task drop-down box to run ecological models in the background. In each mode, users are allowed to customize the model run, such as set the initial parameter values for "Simulation" and "Data Assimilation (DA)", choose the updated parameters from "Data Assimilation (DA)" to conduct "Forecasting" or change the "Forecasting" periods.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions

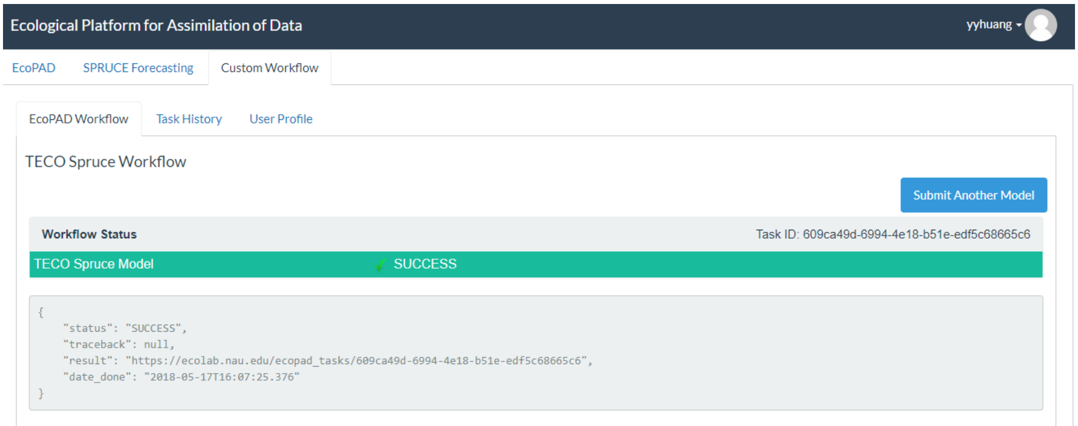


Figure A3. An example of a successful model simulations. In EcoPAD, each task is assigned a unique task ID. The input, output, report and plot relevant to a model task are archived and easy to tack through the unique web link based on the task ID.

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

Geoscientific Model Development Discussions
Open Access

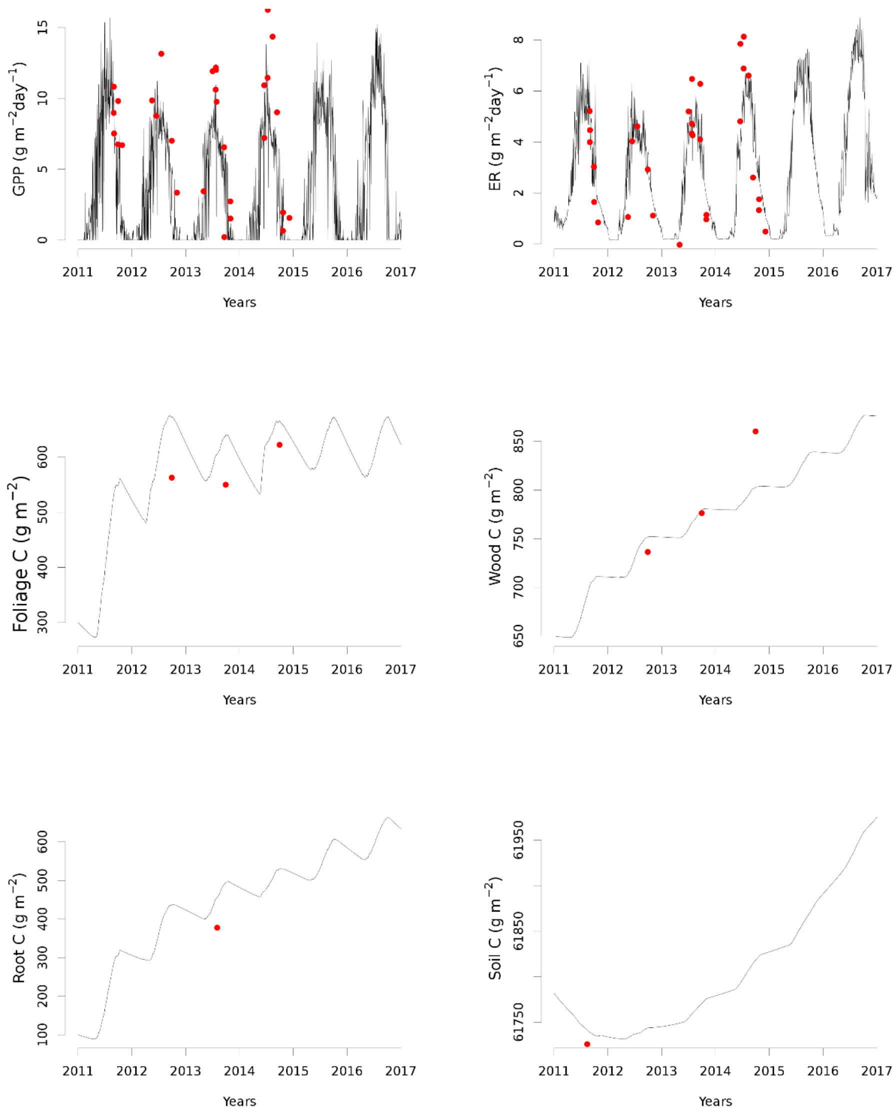


Figure A4. An example of the carbon flux and pool size produced from the "Simulation" mode in EcoPAD-SPRUCE. Red dots indicate available observations and gray lines correspond to model simulation results. The upper two panels display carbon fluxes: gross primary productivity (GPP, left panel) and ecosystem respiration (ER, right panel). The lower four panels show result for foliage carbon (foliage C), wood carbon (wood C), root carbon (root C) and soil carbon (soil C).

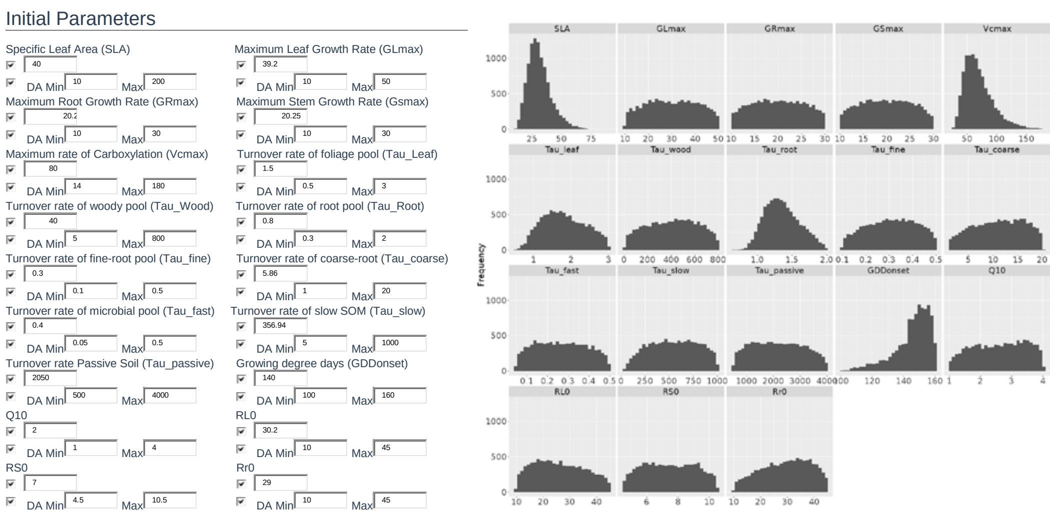


Figure A5 Parameters that are allowed to modify in EcoPAD-SPRUCE. The left panel shows the user interface where users can change the initial parameter value and its range supplied to "Data Assimilation (DA)". The right panel shows the histogram of the posterior distribution of each parameter that participated in the "Data Assimilation (DA)". The right panel is automatically generated and archived for each "Data Assimilation (DA)" task.

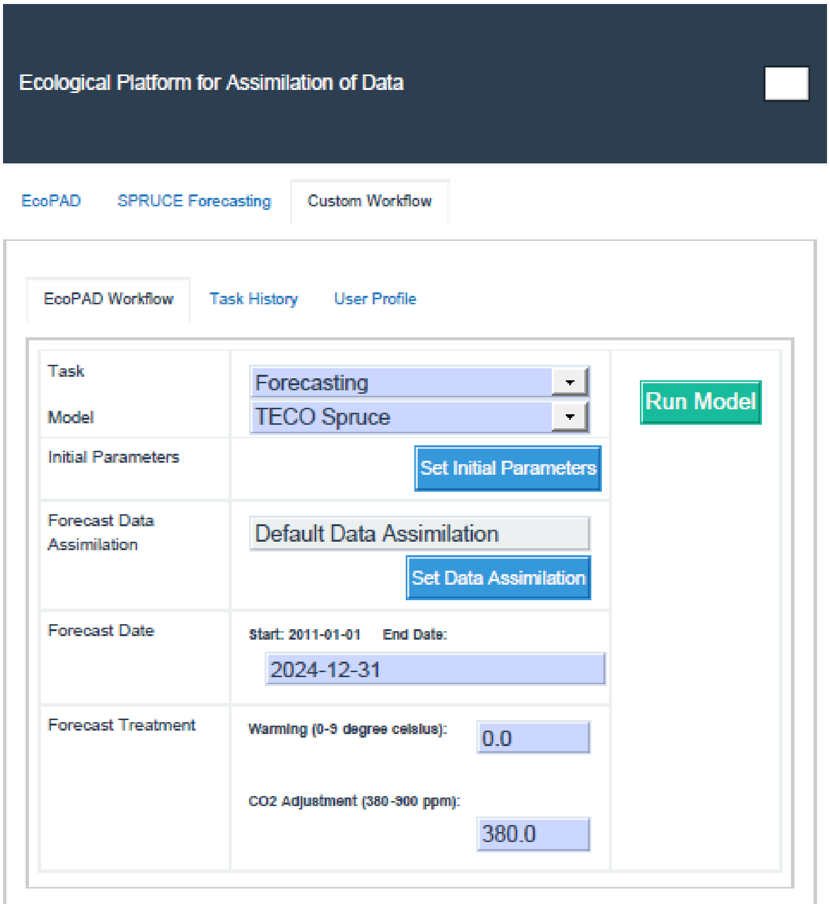
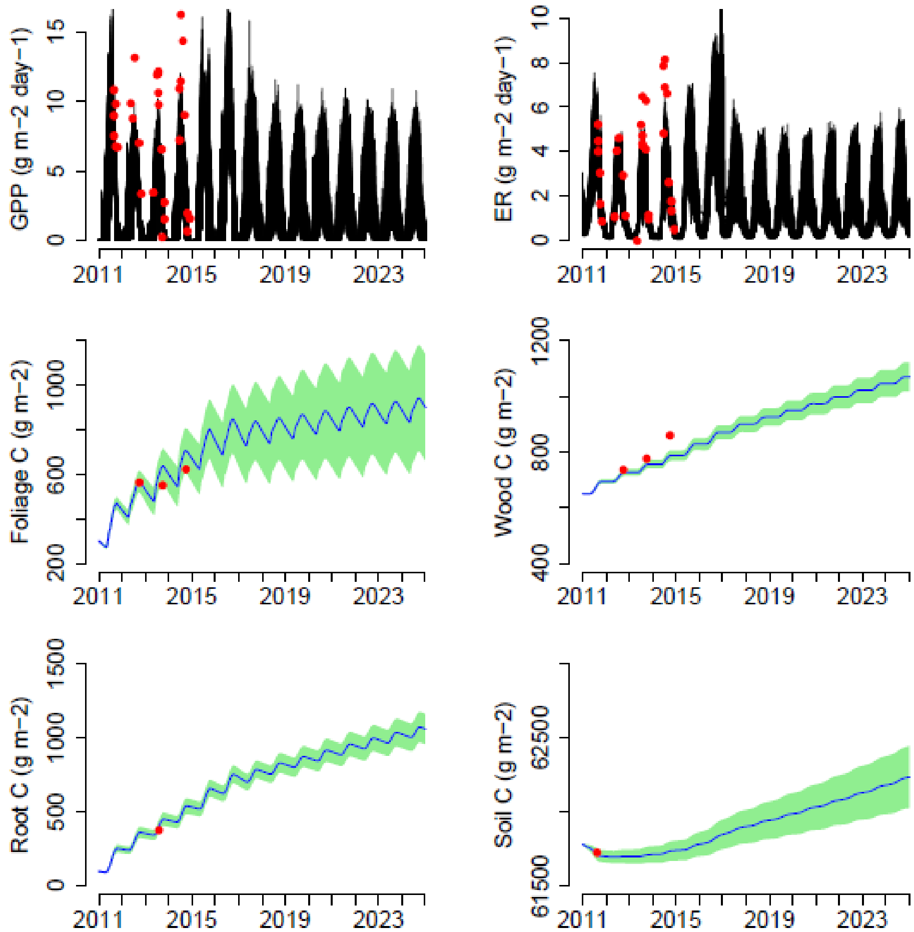


Figure A6 An example user interface of the "Forecasting" mode in EcoPAD-SPRUCE.

1432



1433

1434 **Figure A7.** An example figure produced from the "Forecasting" mode in EcoPAD-SPRUCE.
1435 Red dots indicate observations used in the data assimilation period (2011-2014). Forecasting
1436 runs from 2015-2024. The upper two panels display dynamic changes of carbon fluxes: gross
1437 primary productivity (GPP, left panel) and ecosystem respiration (ER, right panel). The lower
1438 four panels show result for foliage carbon (foliage C), wood carbon (wood C), root carbon (root
1439 C) and soil carbon (soil C). Blue lines indicate the mean and green shading areas corresponding

Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-76
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 25 May 2018

to simulation uncertainties for carbon pools generated from an ensemble of model simulations with randomly chosen parameters from their posterior distributions.