Realised ecological forecast through interactive Ecological Platform for Assimilating Data into model (EcoPAD v1.0)

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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 (v1.0) is a web-based software system that automates data transfer and processing from sensor networks to ecological forecasting through data management, model simulation, data assimilation, forecasting 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 (v1.0) relies on data from observations, process-oriented models, DA techniques, and the web-based workflow.

We applied EcoPAD (v1.0) 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). Forecasting with EcoPAD-SPRUCE has revealed that 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 and accurate external forcing. Moreover, EcoPAD-SPRUCE stimulated active feedbacks between experimenters and modellers to identify model components to be improved and additional measurements to be made. It becomes the interactive model-experiment (ModEx) system and opens a novel avenue for interactive dialogue between modellers and experimenters. Altogether, EcoPAD (v1.0) acts to integrate multiple sources of information and knowledge to best inform ecological forecasting.

Key words:

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

1. Introduction

One ambitious goal of ecology as a science discipline is to forecast states and services of ecological systems. Forecasting 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, e.g., 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 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 uncertainties. 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 combine models with data. But previous data-model integration activities 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) estimated 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 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 modellers [*Dietze et al.*, 2013; *Lebauer et al.*, 2013]; 3) It is usually unidirectional 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 facilitate 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] 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 assimilation systems automate model parameterization and provided an avenue to systematically improve models through combining as much data as possible. Data-informed model improvements normally happen after the ending of a field experiment and the interactive data-model integration is limited as feedbacks from models to ongoing experimental studies are not adequately realised. In addition, 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 experimenters who have limited training in modelling.

The web-based technology facilitates interactions. Web-based modelling, which provides user-friendly interfaces to run models in the background, is usually supported by the scientific workflow, the sequence of processes through which a piece of work passes from initiation to completion. 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 the purpose of visualization, it largely broadens the application of data-model integration and strengthens the interaction between modelling researches and 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 simulations. Such a workflow has advantages, for example, making ecological modelling 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 uncertainties, i.e., the prior information for process-based models. Parameter uncertainties are propagated to model uncertainties and displayed as outputs. It is still not fully interactive in the way that states are not updated iteratively according to observations and the web-based data assimilation and then ecological forecasting have not yet been fully realised.

The iterative model-data integration provides an approach to constantly improve ecological forecasting and is an important step especially for realizing near real-time ecological forecasting. Instead of projecting into future through assimilating observations only once, the iterative forecasting constantly updates forecasting along with ongoing new data streams or/and improved models. Forecasting is likely to be improved unidirectionally in which either only models are updated through observations, or only data collections/field experimentations are improved according to theoretical/model information, but not both. Ecological forecasting can also be bidirectionally improved so that both models and field experimentations are optimized hand in hand over time. Although the bidirectional 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 traditionally 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, v1.0), to best inform ecological forecasting. The interactive feature of EcoPAD (v1.0) is reflected in the iterative model updating and forecasting through dynamically integrating models with new observations, bidirectional feedbacks between experimenters and modellers, 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, modellers and experimenters, scientists and the general public, to improve scientific understanding of ecological processes, to boost ecological forecasting practice and transform ecology towards quantitative forecasting.

In the following sections, we first describe the system design, major components and functionality of EcoPAD (v1.0). 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 (v1.0) for better ecological forecasting.

2 EcoPAD: system design, components, and functionality

2.1 General description: web-based data assimilation and forecast

EcoPAD (v1.0, 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 (v1.0) enables the automated near time ecological forecasting which works hand-in-hand between modellers and experimenters and updates periodically in a manner similar to the weather forecasting. The system is designed to streamline web request-response, data management, modelling, 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 (v1.0) include experiments/data, process-based models, data assimilation techniques and the scientific workflow (Figures 1-3). The scientific workflow of EcoPAD (v1.0) that wraps around ecological models and data assimilation algorithms acts to move datasets in and out of structured and catalogued 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 (v1.0) and EcoPAD (v1.0) offers systematic data management to digest diverse data streams. The 'big data' ecology generates a large volume 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 [*Baldocchi et al.*, 2001; *Johnson et al.*, 2010; *Robertson et al.*, 2012] . Such data contain information related to environmental forcing (e.g., precipitation, temperature and radiative forcing), site characteristics (e.g., soil texture and species composition) and biogeochemical information. Datasets in EcoPAD (v1.0) 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. Each project has a separate folder where data are stored. Data are generally separated into two categories. One is used as boundary conditions for modelling and the other category is related to observations that are used for data assimilation. Scheduled sensor data are appended to existing data files with prescribed frequency. 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 purposes since the workflow and data assimilation system of EcoPAD (v1.0) are relatively independent on the specific ecological model. Linkages among the workflow, data assimilation system and ecological model are based on messaging. For example, the data assimilation system generates parameters that are passed to ecological models. The state variables simulated from ecological models are passed back to the data assimilation system. Models may have different formulations. As long as they take in the same parameters and generate the same state variables, they are functionally identical from the "eye" of the data assimilation system.

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 modelling follows the general form of the Century model [*Parton et al.*, 1988] as in most Earth system models. 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 systematic 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. These ecological issues 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], derive emergent ecological relationships [*Bloom et al.*, 2016], 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 modelling (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 (v1.0) is open to different data assimilation techniques depending on the ecological questions under study since the scientific workflow of EcoPAD (v1.0) is relatively 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. The Bayesian based MCMC method 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 (v1.0) 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 operationally 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 (v1.0) relies on its scientific workflow to interface ecological models and data assimilation algorithms, managing diverse data streams, automates iterative ecological 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 detail below. The essential components of a scientific workflow of EcoPAD (v1.0) 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 (v1.0) also provides structured result access and visualization.

2.2.4.1 Metadata catalog and data management

Datasets can be placed and queried in EcoPAD (v1.0) 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 endeavour to provide efficient data management through storage of metadata including clear documentation of data provenance.

Similarly to these systems, EcoPAD (v1.0) takes advantage of modern information technology, especially the metadata catalog, to manage diverse data streams. The EcoPAD (v1.0) metadata schema includes description of the data product, security, access pattern, and timestamp of last metadata update *etc*. We use MongoDB (https://www.mongodb.com/), a NoSQL database technology, to manage heterogeneous datasets to make the documentation, query and storage fast and convenient. Through MongoDB, 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 (v1.0) is set to automatically fetch new data streams with adjustable frequency depending on research needs.

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 (v1.0) 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 (v1.0) through the use of simple HTTP headers and verbs (e.g., GET, PUT, POST, *etc*.). Hence, a user can incorporate summary data from EcoPAD (v1.0) 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 modelling.

Celery (https://github.com/celery/celery) is an asynchronous task/job queue that runs in 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 (v1.0) takes advantage of the RabbitMQ (https://www.rabbitmq.com/) to manage messaging. After the user submits 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 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 information technology (IT) infrastructures, which makes EcoPAD (v1.0) workflow 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 (v1.0) workflow enables parallelization and distributed computation of actual modelling tasks across various IT infrastructures, and is flexible in implementing additional computational resources by connecting additional workers.

Another key feature that makes EcoPAD (v1.0) easily portable and scalable among different operation systems is the utilization of the container-based virtualization platform, the docker (https://www.docker.com/). 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 lightweight and portable encapsulations through docker containers. Therefore, the entire EcoPAD (v1.0) is readily portable and applicable in different environments.

2.2.4.3 Structured result access and visualization

EcoPAD (v1.0) enables structured result storage, access and visualization to track and analyse data-model fusion practice. Upon the completion of the model task, the model wrapper code calls a post processing call-back function. This call-back 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 store and query of model results are realised 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 (v1.0) 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 (v1.0) 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 modelling studies instant and clear.

2.3 Scientific functionality

Scientific functionality of EcoPAD (v1.0) 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 and conducting ecological forecasting. These functions can be organized to answer various scientific questions. In addition to the general description in this section, the scientific functionality of EcoPAD (v1.0) is also illustrated through a few case studies in the following sections.

EcoPAD (v1.0) 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 modellers, experimenters and the general public. Model simulation and result analysis are automatically triggered after a click on the web-embedded button (Appendices Figures A2, A3 A6). Users are freed from repeatedly compiling code, running code and writing programs to analyse and display model results. Such ease of use has great potential to popularize complex modelling 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. Non-ecologists, such as 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 (v1.0) 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 modelling or data assimilation as large volumes of ecological measurements become available. To satisfy the growing need of model parameterization through observations, EcoPAD (v1.0) streamlines parameter estimations and updates. Researchers can review and download files that record parameter values from EcoPAD (v1.0) result repository. Since these parameters may have different biological, physical or chemical meanings, the functionality of EcoPAD (v1.0) 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 (v1.0). The threshold parameter beyond which further harvesting of fish might cause a crash of fish stocks can be extracted through fish stock assessment models and observations if mounted to EcoPAD (v1.0).

EcoPAD (v1.0) 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 [*Ellison*, 2004; *Bloom et al.*, 2016; *Jiang et al.*, 2018]. 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 (v1.0) platform to provide critical information for well informed decisions in face of pressing global change challenges. In addition, the archive capacity of EcoPAD (v1.0) facilitates future 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 (v1.0). Forecasting capability of EcoPAD (v1.0) 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 (v1.0) 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 (v1.0) 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 (v1.0) 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 (v1.0) promotes quantitatively evaluations while previous studies remain mostly qualitative [*Wallenstein and Hall*, 2012; *Shi et al.*, 2015]. We will further illustrate how EcoPAD (v1.0) 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 (v1.0) 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 long-term 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 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 difference between ambient and +0 treatment plots is the open-topped and controlled-environment enclosure.

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 modelling 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 (v1.0) 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 analyse/visualize model results. Detailed information about the interactive web portal is provided in the Appendices.

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 4). 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 modellers and experimenters

EcoPAD-SPRUCE provides a platform to stimulate interactive communications between modellers 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 hypothesis testing, and provide thorough or advanced information to improve field experiments. Through recursively exchanging information between modellers and experimenters, both models and field experiments can be improved. As illustrated in Figure 4, through extensive communication between modellers and experimenters, modellers 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 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 modeller-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 modellers 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 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 5). The mean CH_4:CO_2 ratio decreased from 0.675 (+0 ˚C treatment) to 0.505 (+9 ˚C), while the temperature sensitivity (Q_{10}) for CH_4 production decreased from 3.33 (+0 ˚C) 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 (v1.0) 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 (v1.0) 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 (v1.0) to systematically quantify acclimations in carbon cycling through time in the future.

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 (v1.0) 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 (v1.0) will rely on an ensemble of ecosystem models, the data assimilation system and climate forcing with quantified uncertainty. *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. Despite *Jiang et al.* [2018] does not quantify model structure uncertainty, the project of incorporating multiple models inside EcoPAD (v1.0) is in progress, and future uncertainty assessment will benefit from EcoPAD (v1.0) 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 (v1.0) through improvements in biophysical estimation. 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 (v1.0), *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 (v1.0) 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. realised simulations. For example, Figure 6 illustrates how updated 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 6 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 6a,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 6a,b red). Similarly, the stochastically generated forcing in Series 3 (S3) starts from January 2017 (Figure 6a,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.

GPP is highly sensitive to climate forcing. The differences between the updated (S2, 3) and initial forecasts (S1) reach almost 800 gC m^{-2} $year^{-1}$ (Figure 6c). The discrepancy is strongly dampened in the following 1-2 years. The impact of updated 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 updated 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 updated 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, realised ecological forecasting that integrates available resources is relative rare due to lack of relevant infrastructures.

EcoPAD (v1.0) provides such effective infrastructure with its interactive platform that rigorously integrates merits from models, observations, statistical advance, information technology and human resources from experimenters and modellers 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 predictions. Going beyond common practice of model-data assimilation from which model updating lags far behind observations, EcoPAD (v1.0) enables iterative model updating and forecasting through dynamically integrating models with new observations in near real-time. This near real-time interactive capacity relies on its scientific workflow that automates data management, model simulation, data simulation and result visualization. The system design encourages thorough interactions between experimenters and modellers. 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 incorporated into forecasting efficiently, making the forecasting system fully interactive and dynamical.

We also benefit from the interactive EcoPAD (v1.0) 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 modelling techniques because of their complexity and long learning curve. Because EcoPAD (v1.0) 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-modeller 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 more essence part of the system. The simplicity in use of EcoPAD (v1.0) 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.

4.2 Implications for better ecological forecasting

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. Not well constrained parameters, for example, caused by lack of information from observational data, contribute to high forecasting uncertainty and low reliability of forecasting results. 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]. Parameter values derived under the ambient condition was not applicable to the warming treatment in our methane case due to acclimation. 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. realised 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 modelled 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. realised 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, updated 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 (v1.0) 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 forecasting uncertainty changes with time, what are the dominate contributor of forecasting uncertainty (e.g., parameter, initial condition, model structure, observation errors, forcing *etc.*), how uncertainty sources interact among different components, or to what extent unconstrained parameters affect forecasting uncertainty are all valuable questions that can be explored through EcoPAD (v1.0).

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 (v1.0) 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 modelling 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 (v1.0) creates a smart interactive model-experiment (ModEx) system. ModEx has the capacity to form a feedback loop in which field experiment guides modelling and modelling influences experimental focus [*Luo et al.*, 2011a]. We demonstrated how EcoPAD (v1.0) works hand-in-hand between modellers 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 ecosystem modelling 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 modellers 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 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 (v1.0) 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 (v1.0) at FLUXNET, NEON or LTER sites includes three steps in general. First, build the climate forcing in the suitable formats of EcoPAD (v1.0) 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 (v1.0), and then run the EcoPAD (v1.0) with the dynamic data assimilation system. Furthermore, facing the proposed continental scale ecology study [*Schimel*, 2011], EcoPAD (v1.0) 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 (v1.0) benefits from observation and modelling and at the same time advances both observation and modelling of ecological studies.

4.4 Future developments

As we indicated, EcoPAD (v1.0) will expand as time goes on. The system is designed to incorporate multiple process-based models, diverse data assimilation techniques and various ecological state variables for different ecosystems. Case studies presented in earlier sections are based primarily on one model. 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 (v1.0). 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 studies. We focus mostly on carbon related state variables in the SPRUCE example, and the data assimilation system in EcoPAD (v1.0) 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 EcoPAD (v1.0) is to enable the research community to understand and reduce forecasting uncertainties from different sources and forecast various aspects of future biogeochemical and ecological changes as data become available. The example of *Jiang et al.* [2018] partitioned forecasting uncertainty from forcings and parameters. An exhaustive understanding of forecasting uncertainty in ecology need to also consider model structures, data assimilation schemes as well as different ecological state variables. Researchers interested in creating their own multiple model and/or multiple assimilation scheme version of EcoPAD (v1.0) can start from the GitHub repository (https://github.com/ou-ecolab) where the source code of the EcoPAD (v1.0) workflow is archived. To add a new variable that is not forecasted in the EcoPAD-SPRUCE example, it requires modellers and experimenters to work together to understand their process-based model, their observations and how messaging works in the workflow of EcoPAD (v1.0) following the example of EcoPAD-SPRUCE. To add a new model or a new data assimilation scheme for variables that are forecasted in EcoPAD-SPRUCE, researchers need to create additional dockers and mount them to the existing workflow with the knowledge of how information are passed within the workflow.

The power of EcoPAD (v1.0) 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 (v1.0) makes modelling 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 (v1.0) 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 accessible to different audience. It is supported by meta-databases of biogeochemical variables, libraries of modules of process models, toolbox of inversion techniques and the 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 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:

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.

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Tables

Table 1. Discussion stimulated by EcoPAD-SPRUCE forecasting among modellers 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 modelling 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 modelling 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.

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 (green arrows or lines). 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 modelling. Images from the SPRUCE field experiments (https://mnspruce.ornl.gov/) are used to represent data collection and the flowchart of TECO model is used to delegate ecological models.

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.

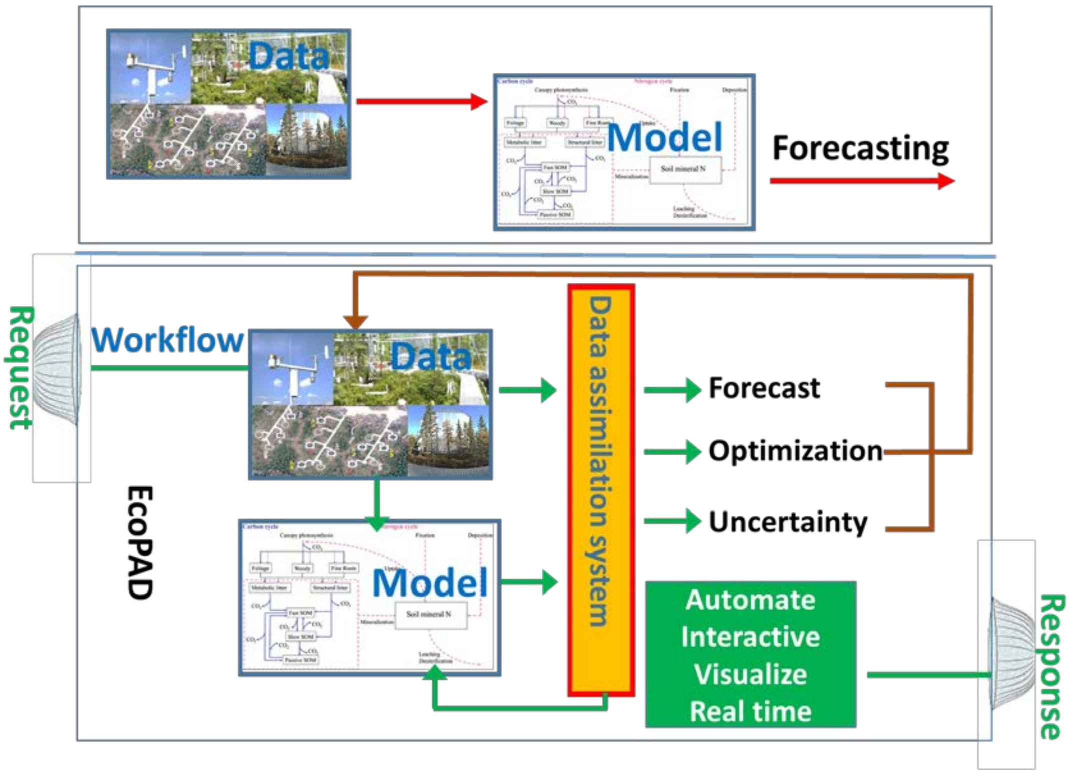
Figure 4. Schema of interactive communication between modellers and experimenters through the prediction-question-discussion-adjustment-prediction cycle to improve ecological forecasting. The schema is inspired by an episode of experimenter-modeller communication stimulated by the EcoPAD-SPRUCE platform. 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 modellers and experimenters with detailed information listed in Table 1. After extensive discussion, the model structure was adjusted and field observations were re-evaluated. And a second round of forecasting yielded more reliable predictions.

Figure 5. 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 6. Updated vs. un-updated forecasting of gross primary production (GPP, panels a,c) and soil organic C content (SoilC, panels b,d). The upper panels show 3 series of forecasting with updated vs. stochastically generated weather forcing. Cyan indicates forecasting with 100 stochastically generated weather forcing from January 2015 to December 2024 (S1); red corresponds to updated forecasting with two stages, that is, updating with measured weather forcing from January 2015 to July 2016 followed by forecasting with 100 stochastically

generated weather forcing from August 2016 to December 2024 (S2); and blue shows updated forecasting with measured weather forcing from January 2015 to December 2016 followed by forecasting with 100 stochastically generated weather forcing from January 2017 to December 2024 (S3). The bottom panels display mismatches between updated forecasting (S2,3) and the original un-updated 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 indicate 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
Model
Forecasting
Request
Workflow
Data
Data assimilation system
Forecast
Optimization
Uncertainty
EcoPAD
Model
Automate
Interactive
Visualize
Real time
Response

Figure 2

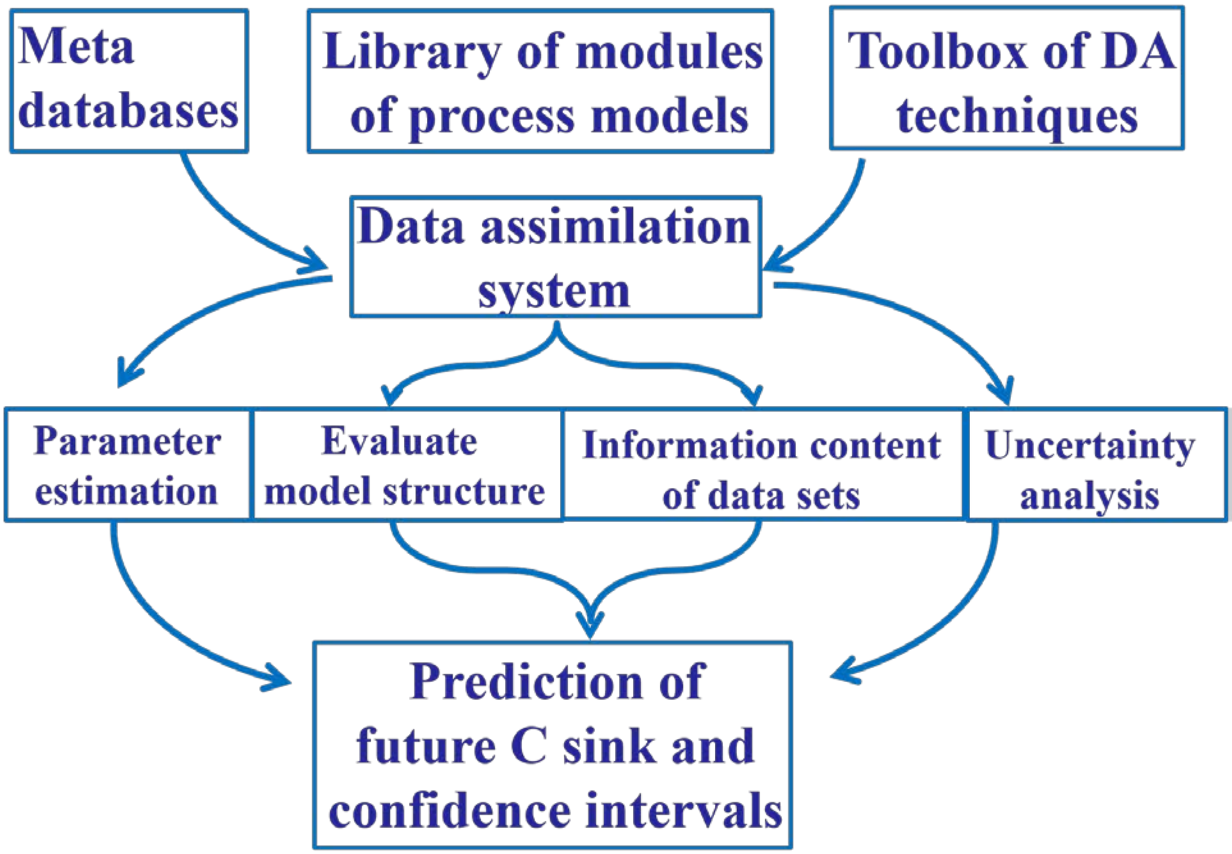

Meta databases
Library of modules of process models
Toolbox of DA techniques
Data assimilation system
Parameter estimation
Evaluate model structure
Information content of data sets
Uncertainty analysis
Prediction of future C sink and confidence intervals

Figure 3

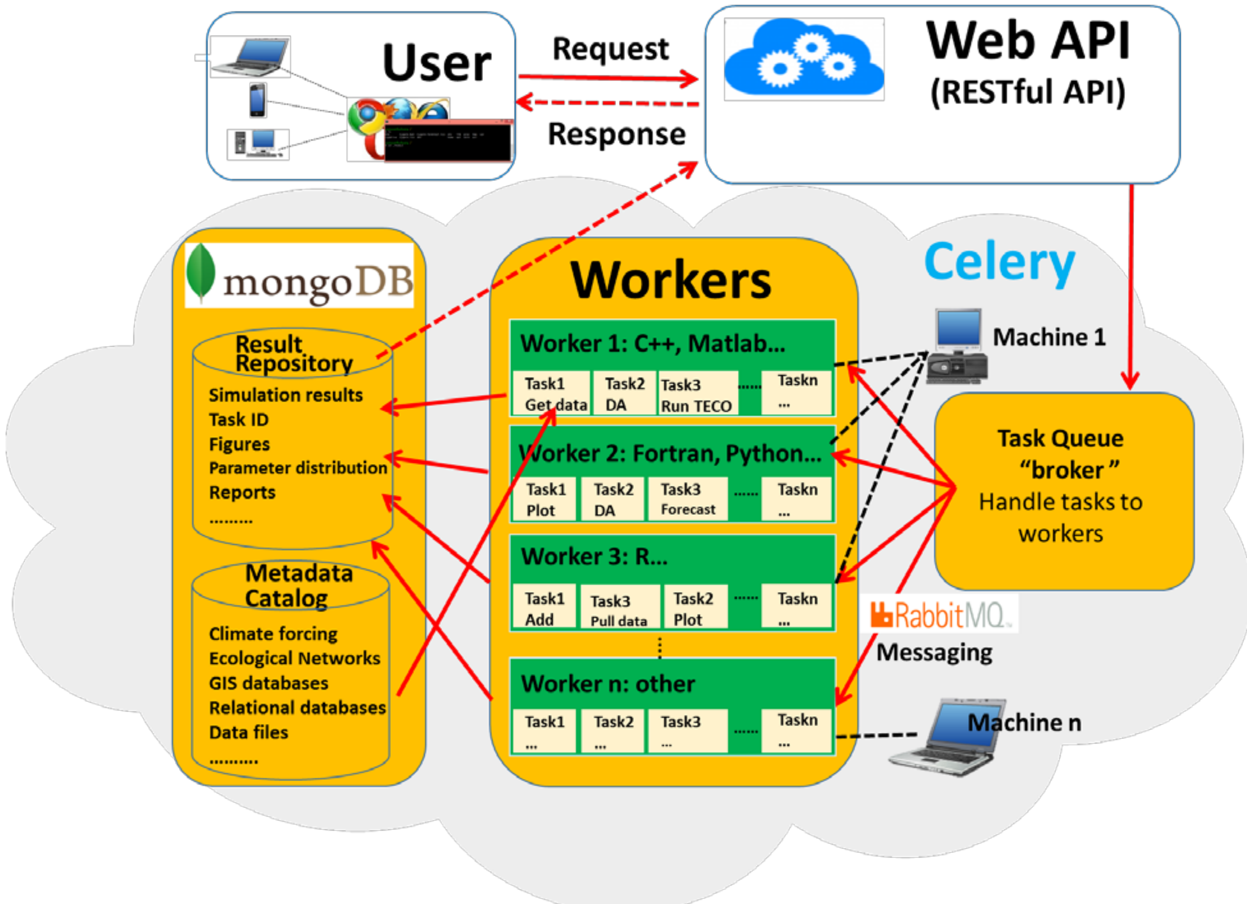
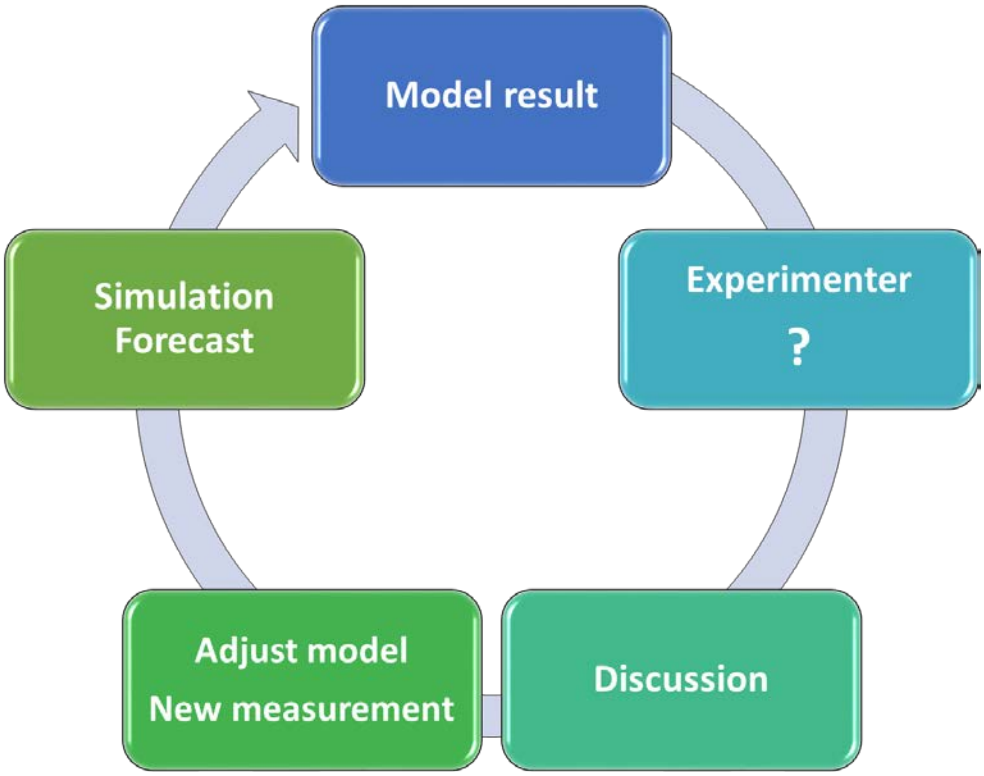

User
Request
Response
Web API
(RESTful API)
mongoDB
Result Repository
Simulation results
Task ID
Figures
Parameter distribution
Reports
....
Metadata Catalog
Climate forcing
Ecological Networks
GIS databases
Relational databases
Data files
....
Workers
Worker 1: C++, Matlab...
Task1 Get data
Task2 DA
Task3 Run TECO
Taskn ...
Worker 2: Fortran, Python...
Task1 Plot
Task2 DA
Task3 Forecast
Taskn ...
Worker 3: R...
Task1 Add
Task3 Pull data
Task2 Plot
Taskn ...
Worker n: other
Task1 ...
Task2 ...
Task3 ...
Taskn ...
Celery
Machine 1
Task Queue
"broker"
Handle tasks to workers
RabbitMQ
Messaging
Machine n

Figure 4



Model result
Experimenter
?
Discussion
Adjust model
New measurement
Simulation
Forecast

Figure 5

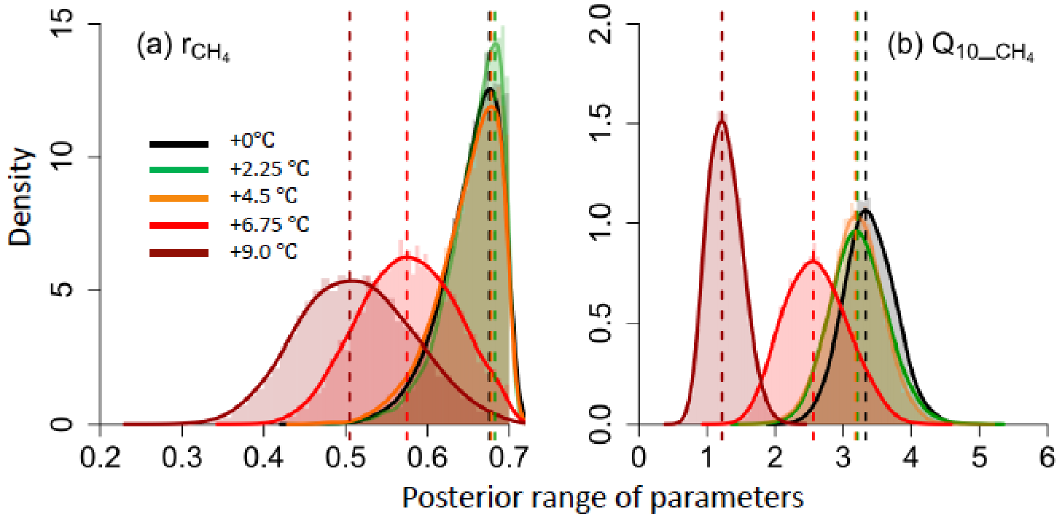
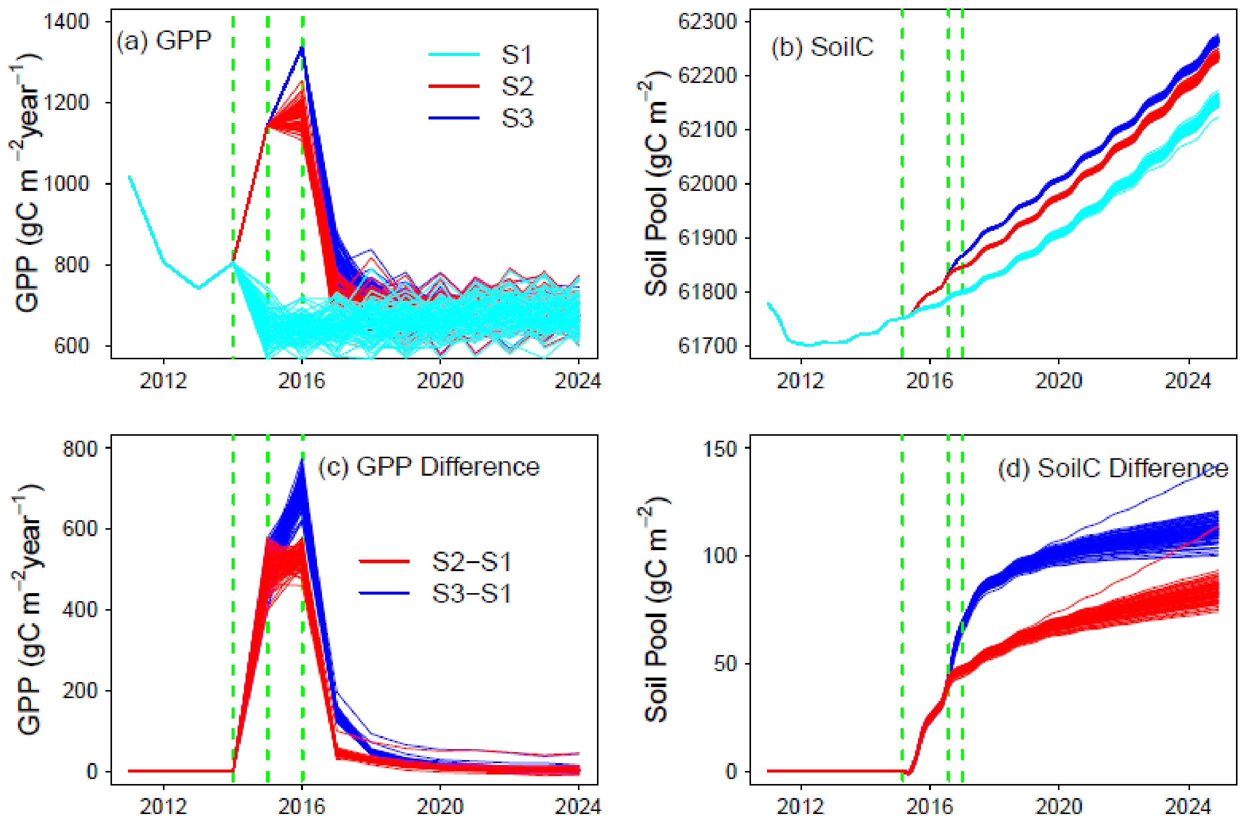

(a) r_{CH_4}
(b) $Q_{10\_CH_4}$
+0°C
+2.25 °C
+4.5 °C
+6.75 °C
+9.0 °C
Density
Posterior range of parameters
0
5
10
15
0.0
0.5
1.0
1.5
2.0
0.2
0.3
0.4
0.5
0.6
0.7
0
1
2
3
4
5
6

Figure 6



(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