Sources of uncertainty in predicting land surface fluxes using diverse data and models

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***Abstract*— In the domain of predicting land surface fluxes, models are used to bring data from large observation networks and satellite remote sensing together to make predictions about present and future states of the Earth. Characterizing the uncertainty about such predictions is a complex process and one that is not yet fully understood. Uncertainty exists about initialization, measurement and interpolation of input variables; model parameters; model structure; and mixed spatial and temporal supports. Multiple models or structures often exist to describe the same processes. Uncertainty about structure is currently addressed by running an ensemble of different models and examining the distribution of model outputs. To illustrate structural uncertainty, a multi-model ensemble experiment we have been conducting using the Terrestrial Observation and Prediction System (TOPS) will be discussed. TOPS uses public versions of process-based ecosystem models that use satellite-derived inputs along with surface climate data and land surface characterization to produce predictions of ecosystem fluxes including gross and net primary production and net ecosystem exchange. Using the TOPS framework, we have explored the uncertainty arising from the application of models with different assumptions, structures, parameters, and variable definitions. With a small number of models, this only begins to capture the range of possible spatial fields of ecosystem fluxes. Few attempts have been made to systematically address the components of uncertainty in such a framework. We discuss the characterization of uncertainty for this approach including both quantifiable and poorly known aspects.**

Keywords: structural uncertainty, ensemble modeling, carbon flux, North America

I. INTRODUCTION

A. Predicting Land Surface Fluxes Spatially

The rising concentration of CO_2 (and other greenhouse gases) in the atmosphere, largely created by anthropogenic carbon emissions, represents a major threat to the Earth's climate. Yet the growth of atmospheric CO_2 does not equal emissions, as half of the emitted CO_2 is sequestered by natural reservoirs in the ocean and on land (IPCC, 2007). Between 2000 and 2006, for instance, global anthropogenic carbon emissions were about 9.1 PgC yr^{-1} (petagram of carbon per year), while carbon uptake by the ocean and land is 2.2 PgC yr^{-1} and 2.8 PgC yr^{-1}, respectively (Canadell et al., 2007). In North America, terrestrial ecosystems alone have sequestered 0.65 PgC yr^{-1} during the same period, offsetting one-third of carbon emissions of fossil fuel burning and cement manufacturing from the continent (Peters et al., 2007). However, these natural carbon sinks are limited and may diminish in the future (Canadell et al., 2007). Knowledge about their properties and how they are going to change over time remain challenges to the carbon cycling science community (NACP, 2002).

Ecosystem models provide the primary method for mapping regional to global terrestrial carbon fluxes from vegetation. They integrate the understanding of ecological processes obtained from local measurements and apply this knowledge to simulate ecosystem functions over broader regions. Since the 1980's, they have been applied on a spatial basis to create maps of predicted output variables. They are currently critical tools in the search for understanding the fate of carbon in the atmosphere.

B. Characterizing the Scientific Uncertainty of Predicted Surface Fluxes

Recognition is growing that results generated from ecosystem flux models must be accompanied by a quantification of scientific uncertainty. Uncertainty from models is unlike the case for measurements, where replicates can be obtained under constant conditions to quantify precision and comparisons made to a reference or standard to quantify bias. Models can be as precise as computational methods allow. References or standards are difficult to obtain, which is the reason that models are needed in the first place. Bias is therefore more difficult to quantify. A thorough understanding of the reasons that model results are uncertain lead to methods to express a more complete distribution of probable output values.

II. WHY PREDICTIONS ARE UNCERTAIN

A. Initialization, Measurement and Interpolation of Input Variables

Though the primary interest is in uncertainty about output variables, models require maps of input variables that are themselves uncertain. Several inputs to models that describe ecosystem processes (e.g. air temperature, precipitation, soil texture) are measured at quasi-point support. There is little or no sampling design involved in these measurements. Even meteorological networks, which provide some of the densest measurements across the domain of interest, represent a miniscule sampling fraction, have pervasive spatial clustering, and include an unknown bias. To supply a model with values at every grid cell for a simulation, values of these variables are interpolated across vast areas of unmeasured territory. These fields are then used in the models and resulting simulations therefore carry this interpolation uncertainty.

Before simulating for the time period of interest, initializing or "spinup" runs are usually required to bring state variables into equilibrium with climate and ancillary datasets. Different models may have different spinup algorithms (e.g., Sitch et al., 2003; Thornton and Rosenbloom, 2005), leading to another source of variation in simulation results.

B. *Model Parameters*

Parametric uncertainty has long been acknowledged in model exercises. Sensitivity analyses (Saltelli et al., 2004) address this aspect of uncertainty. Notable examples in the domain include Knorr and Heimann (2001).

C. *Model Structure*

Structural uncertainty arises from different representations of ecological processes in different models. Because the components of terrestrial ecosystems and the interactions among them are complicated or not well understood, simplifying assumptions must be made to describe them. Different modeling strategies adopt different simplifying assumptions, leading to different model complexity and behavior.

For a particular aspect of ecosystem function, structural differences of ecosystem models may be examined by directly comparing their mathematical formulation (e.g. Adams et al., 2004). However, characteristics of isolated model components do not fully reflect their functional behavior within the coupled system, where feedbacks and interactions between subsystems can play a critical role. Mathematical analysis of complicated systems can only go so far, so numerical experiments with multi-model ensemble (MMEs) have become the main means to tackle the problem. In general, an MME experiment runs a group of models with the same input data and under the same initial conditions; the multi-model means or medians are treated as the "best" simulation results, and the inter-model differences are used as a measure of the structural uncertainty (Tebaldi and Knutti, 2007). Following the successful example of the World Climate Research Programme's Coupled Model Intercomparison Project for the International Panel on Climate Change (IPCC), MME experiments are now broadly adopted in carbon-cycle studies, such as the Atmospheric Tracer Transport Model Intercomparison Project (Rayner and Law, 1995; Denning et al., 1999; Gurney, 2004). Despite the general agreement in the simulation results and the implied scientific significance (e.g., see Schimel et al., 2007), large differences among the models are also revealed, for instance, in estimates of contemporary global annual NPP (39.9~80.5 PgC yr-1; Cramer et al., 1999), or in the sensitivity of carbon storage to future climate change in the US (-39% ~ +40%; VEMAP, 1995).

D. *Spatial and Temporal Support*

Ecosystem models are not necessarily conceived with specific spatial or temporal supports in mind. That is, the notion of spatial unit size or duration often does not feature explicitly in model construction. Therefore, the only technical difference between running a model on a 1 km, 8 km, or 1 degree support may be the number of compute cycles needed – model structural elements may not be changed yet there is an implicit change in assumptions about what regions or periods have stationary parameters. For example, light use efficiency (LUE), a critical factor in many diagnostic models, may be assumed to be stationary across an ecoregion or across a small grid cell. These assumptions lead to problems in calibration and validation, as the spatial/temporal unit modeled may be much larger/longer or much smaller/shorter than the spatial/temporal unit measured. Raupach et al. (2005) refers to this as the "scale mismatch problem."

III. CREATING A MULTI-MODEL ENSEMBLE WITH THE TERRESTRIAL OBSERVATION AND PREDICTION SYSTEM

A. *TOPS*

We have been constructing a MME using the Terrestrial Observation and Prediction System (TOPS) to evaluate sources of uncertainty in carbon flux estimates resulting from structural differences among ecosystem models. TOPS is a data and modeling system to accomplish ecological monitoring, forecasting and related ecosystem analyses (Nemani et al., 2009). TOPS brings together meteorological records, satellite products, and various ancillary datasets from different sources. One of its key components is the Surface Observation and Gridding System (SOGS), which ingests daily observations of temperature, precipitation and other fields from meteorological stations and interpolates them to complete grids (Thornton et al., 1997; Jolly et al., 2005).

B. *Input Variable Datasets*

The spatial and temporal extent of our study covers the entire North American continent at 8km resolution for the time period 1982 to 2006. We used SOGS to generate daily meteorological fields. The source data on these variables were obtained from the Global Summary of the Day (GSOD) and the Cooperative Summary of the Day (TD3200) from the National Climatic Data Center (NCDC). GSOD is a global set based on data exchanged under the World Meteorological Organization World Weather Watch Program. GSOD has about 2000 reporting stations over North America, which is relatively sparse for interpolating climate variables such as daily precipitation over the whole continent. For this reason, we added the TD3200 network, which consists of about 8500 reporting stations in the US, primarily from the National Weather Service cooperative station network and principal climatological stations, significantly increasing the density of stations over the US.

For models requiring satellite-derived vegetation data, we used the leaf area index (LAI) dataset developed by Ganguly et al. (2008) The MODIS land cover product (Friedl et al., 2002) is used to describe the distribution of plant functional types (PFTs). A global dataset of land surface parameters, ECOCLIMAP (Masson et al., 2003), is used to specify soil properties (e.g., texture and depth) and other parameters (e.g., albedo).

C. *Ecosystem Models*

The architecture of TOPS provides a flexible interface for ecosystem models to be integrated. Public versions of four process-based ecosystem models, including Biome-BGC, LPJ, CASA, and TOPS-BGC comprised the ensemble (Table 1). Details of the application of these models are given in Wang et al. (unpublished).

TABLE I. SELECTED CHARACTERISTICS AND ATTRIBUTES OF MODELS USED IN THE MME.

	Biome-BGC	**LPJ**	**TOPS-BGC**	**CASA**
Type	prognostic	prognostic	diagnostic	diagnostic
Land Cover	prescribed	simulated	prescribed	prescribed
LAI	simulated	simulated	prescribed	prescribed
Carbon Pools	vegetation and soil	vegetation and soil	none	vegetation and soil
GPP[a] algorithm	Farquhar (1980)	Farquhar (1980)	LUE	2×NPP
NPP[b] algorithm	GPP – AR[c]	GPP – AR	0.5×GPP	LUE
NEE[d]/HR[e] algorithm	NPP – HR; HR estimated from soil pools	NPP – HR; HR estimated from soil pools	NPP-HR; HR estimated from base respiration rates	NPP – HR; HR estimated from soil pools
Dynamic N[f] Cycle	yes	no	no	no
Reference	Thornton et al., 2002	Sitch et al., 2003	Nemani et al., 2009	Potter et al., 1993

a Gross Primary Production b Net Primary Production c Autotrophic respiration d Net Ecosystem Exchange e Heterotrophic respiration f Nitrogen

IV. RESULTS AND DISCUSSION

Model outputs include monthly carbon fluxes (e.g., GPP, NPP, NEE, AR) and annual averaged carbon stocks (biomass and soil carbon pools). Global summaries as well as geographic patterns of all of these outputs show considerable ranges. For example, GPP from the four models (Figure 1) coincides in some regions of highs and lows, but significantly differs in other regions. Though four models are too few to accurately estimate ensemble summary statistics, some quantification of uncertainty is possible by examining the ranges spanned by model results.

A natural approach to allowing robust estimation of summary statistics of future MMEs is to boost the number of models represented. Given the multitude of sources of uncertainty (Section II), it might make more sense to address the range of unknowns in a more systematic fashion. For example, model hierarchies could provide increased understanding (Wang et al., 2009). Held (2005) suggests such an approach for climate models, which have similar challenges.

Flux tower measurements provide the most useful reference data (Baldocchi, 2003) for MME results, but the available sample of tower data is extremely sparse, not representative of the population of values, and their uncertainties are not fully characterized. Challenges to validation will persist for the foreseeable future.

V. CONCLUSIONS

MMEs are computationally expensive and time-consuming to construct and analyze. However, scientific knowledge is not fully captured by a single model. Our experiment with a high spatial resolution MME indicates there is large structural uncertainty in simulating carbon fluxes for North America, equal to or exceeding uncertainty due to input variable prediction or parameter estimation. Though it might be reasonable to suppose that a larger research effort should reduce scientific uncertainty, this study and other recent work (Chen et al., 2008; Mitchell et al., 2009) suggests the contrary. As the sources of uncertainty are increasingly acknowledged and quantified, the probability distribution of output values will become wider rather than narrower.

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