

The current state of carbon-cycle data assimilation

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Model–data fusion (MDF), also called ‘data assimilation’, describes the approach of combining as much data as possible with explicit dynamical models to constrain the evolution of any system. The paradigm is weather prediction. MDF holds the promise of combining the plethora of data available on the terrestrial carbon cycle but to date there have been few successful applications using multiple streams of data. The two most likely reasons for this are a lack of statistical sophistication in the attempts and weaknesses in current terrestrial biosphere models; these failures do not represent a failure of the paradigm. Solutions lie in a more rigorous consideration of the statistics of the problem and the inclusion of more elements of the model within the MDF framework.

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Introduction

The behavior of the terrestrial biosphere, now and in the future, represents a critical uncertainty in the global carbon cycle [1,2]. The terrestrial biosphere is more sensitive to direct human influence than the ocean as demonstrated by the large but uncertain flux of carbon to the atmosphere caused by land-use change [3]. This makes it a tempting target for interventions aimed at limiting atmospheric CO₂ concentrations. Finally the terrestrial biosphere is highly sensitive to short term climate variability [4,5] and among models this sensitivity is mirrored by a widely varying response to future climate change [6,7]. For these reasons, quantification of the current and future state of the terrestrial biosphere has attained practical as well as scientific importance.

The importance of the problem is matched by its difficulty. One obvious problem is the heterogeneity of the

biosphere. One can regard the conditions of soil type, climate and land-use history as exogenous to the biosphere.¹ If one maps the overlay of these three factors one immediately sees variations on the scale of hectares. If we regard the biosphere as a simple deterministic system responding to all these inputs we see already that any local measurement represents one point in an immense space of potential drivers. Thus the sampling problem to characterize the response to all these drivers is serious indeed.

The intractability of the measurement problem allied with the need for prediction provides practical motivation to construct models. The intellectual motivation is also to construct coherent and comprehensible views of the system. We know that similar physical and chemical processes occur in many different situations so we do have some basis for building generalized models. The large-scale responses to climate anomalies [e.g. 8, 5] suggest that there are coherent responses to such drivers but we cannot guarantee *a priori* that the emergent properties of the biosphere are predictable from understanding simple processes. Ref. [9] noted the difficulty of building predictive models. Various processes are not included in terrestrial biosphere models. Thus they fail to match some observations, casting doubt on their predictions. The proposed solution was to urge the testing of such models against as wide a range of observations as possible. Here I advocate the same solution but note that the traditional approach of running the model and comparing with observations does not account for the uncertainty of parameters in the model and is not necessarily an aid to model development.

Commensurate with the complexity of biospheric behavior and range of scales on which it responds, there are a wide range of measurements probing different aspects and covering different levels of spatial and temporal integration. These were summarized in [10^{*}]. The question of how to combine these measurements with models is the subject of this paper. Of course the problem of inferring underlying causes from their effects is widespread in science. The algorithms to do this are often termed inverse approaches since they reverse the direction of causality. The new field of carbon-cycle data assimilation inherits much of the apparatus and

¹ This is obviously a simplification since the evolution of soil is a result of biospheric function and even climate is influenced by changes in land cover.

intellectual background from other fields but the analogy is nowhere exact. It probably shares most with the assimilation used in modern numerical weather prediction with common points like a dynamical rather than static model, multiple types of measurements and an interest in forecasting. Numerical weather prediction does not usually concern itself with improving the underlying process understanding and work in the carbon cycle lacks the day-to-day testing of forecast evaluation but this is the paradigm I use.

After introducing the abstract framework I will briefly summarize the state of the art at the time of writing. This will highlight two significant problems, namely the statistical treatment of the observations and the elucidation of flaws in the models themselves. The last section of the paper will suggest approaches for addressing these.

A simple theory of model–data fusion

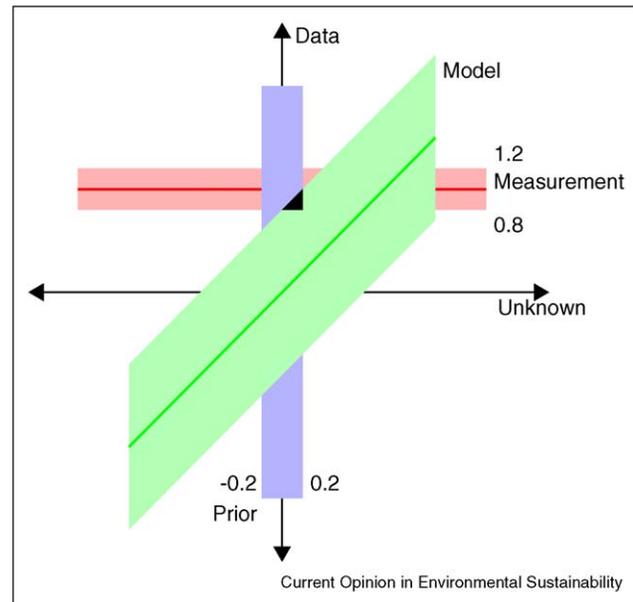
The usual description of the task of MDF is to constrain the behavior of a model by requiring it to match certain observations. I will show later that it is equally important to quantify the consistency between the model and the observations. This problem has been routinely treated differently within Applied Mathematics and Statistics. Ref. [11] showed the equivalence of these different descriptions. The statistical description [e.g. 12**] has come to dominate the field and we follow this approach.

Although it is possible to develop the theory using the most general description of a model I will simplify the definition here to illustrate the approach. I define a model as a numerical calculation which takes a series of inputs and calculates a series of outputs. The inputs can be divided into external forcing, initial conditions (both boundary conditions in the language of differential equations) and a series of parameters. We group these as the “unknowns” of the problem.² The usual case is a model which starts from an initial state (e.g. the current state of the atmosphere) and marches forward in time. At each timestep the model calculates a new state described by a set of state variables. The outputs from the model comprise both things we observe or things we would like to know. Often some of the intermediate state variables are observed but just as often the observables are themselves the product of complex calculation from state variables.

The MDF problem consists of using the observables to improve our knowledge of the unknowns and hence of the desired outputs. The problem is complicated by imperfections in both the model and the data while it

² In numerical weather prediction the unknowns are usually the initial state of the atmosphere.

Figure 1



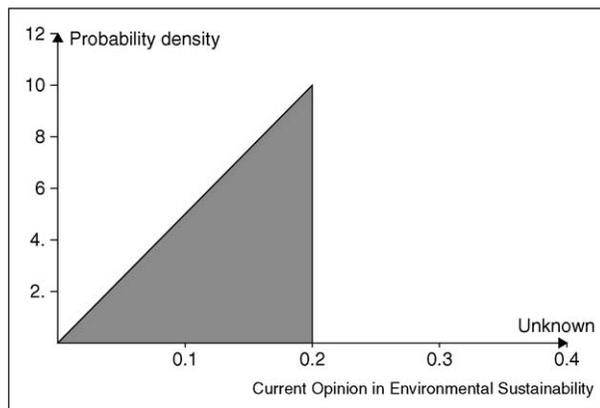
Schematic describing MDF with one unknown and one observable. The meaning of the colored regions is described in the text.

is usually ameliorated by the existence of prior knowledge (also imperfect) of the unknowns. Mathematically the task is to express then combine these three sources of information. We achieve this by expressing the information in the form of probability density functions (PDFs) then combining them by the laws of probability [see 12**, for a full development].

Figure 1 illustrates the approach for the simplest case of one unknown and one observable. The unknown is plotted on the X-axis and the observable on the Y-axis. The prior PDF of the unknown is represented by the vertically aligned, light blue rectangle between $x = -0.2$ and $x = 0.2$.³ The horizontally aligned, light red rectangle between $y = 0.8$ and $y = 1.2$ represents the PDF of the true value of the observable. This is likely to be based on a measurement indicated by the heavy red line. In this case the measurement corresponds to the expectation of the true value, that is, the measurement is unbiased. This is often not the case. Although we usually regard such measurement bias as an experimental problem it can equally be regarded (and often treated) as a statistical problem of the measurement PDF. The deterministic model is shown by the heavy green line. It describes what value the observable should have for a given value of the unknown. The model is imperfect however so the true

³ We do not show a heavy blue line indicating the central estimate to emphasize that the prior PDF can be a range from a literature survey or a range of physically meaningful values.

Figure 2



Solution of the inverse problem by projecting the solution shown in Figure 1 onto the unknown axis and normalizing it.

value of the observable lies within the green region. The solution is the region of the unknown-observable space consistent with all three inputs, the black triangle.

The ‘solution’ of the inverse problem is generated by projecting the black triangle shown in Figure 1 onto the unknown axis and normalizing it to give a total probability of 1. This is shown in Figure 2.

Many interesting features of data assimilation are evident in Figures 1 and 2. Figure 2 shows that only values of the unknown between 0.0 and 0.2 are possible after the measurement, that is, we have added information. The most likely value of the unknown is 0.2 while its mean is ≈ 0.13333 . Figure 1 shows that the perfect model (green line) is nowhere consistent with the prior unknown and measurement PDFs. Had the light green region been much narrower there would have been no overlap. This would constitute a falsification of the assumptions since the probability that our three pieces of information (prior knowledge, measurement and model) were simultaneously true would be zero. This would cast serious doubt on the model.

Real-world data assimilation problems are vastly larger than the one shown in Figure 1 but this is a computational not intellectual matter. More important is the usual form chosen to represent probabilities. We usually choose a Gaussian of the form

$$P(x) = K \exp - \frac{(x - \mu)^2}{2\sigma^2} \quad (1)$$

where μ is the mean, σ the standard deviation and K a normalization constant. σ describes the width of the distribution while μ describes its position. One important consequence of forms like Eqn (1) is that probabilities

never equal 0 but it remains true that some combinations of model, prior information and measurement are highly unlikely. Secondly the parameters μ and σ are sufficient to describe the PDF completely. Thirdly if the model is linear we can show that if the three input PDFs are Gaussian the combined PDF will also be Gaussian [12^{••}, Chapter 1]. In this case it suffices to find the mean and standard deviation of the posterior PDF to describe it completely.

Various other approximations and simplifications are necessary to turn the above theory into a practical assimilation system and there is a vast literature on the computational machinery for describing the posterior PDF or maximizing it but that is not critical to this discussion. Readers are referred to texts such as [12^{••},13] for the general theory, [14] for its application to biogeochemistry and [15] for aspects of numerical optimization.

Applying assimilation to the carbon cycle

The theory illustrated in ‘A simple theory of model-data fusion’ is exceedingly general. Within carbon-cycle research it has been applied in two forms. In flux inversions [e.g. 4,5,16–21] it is used to estimate surface carbon fluxes without the use of an explicit dynamical model.⁴

In assimilation studies we add an underlying dynamical constraint such as a carbon-cycle model.⁵ This imposes relationships among model outputs. Consequently observations can carry more weight since their influence is propagated by model dynamics. We see immediately that the quality of the inferences made depends critically on that of the dynamical model. It also depends on the quality of the mapping between quantities simulated by the model and those observed. This mapping is achieved by a submodel usually termed an observation operator. These can be as simple as an identity if the simulated quantity is directly observed and as complex as a radiative transfer model or atmospheric transport model.

A discussion of the relative value of inversion and assimilation is beyond my scope and is discussed in [22[•],23]. We can summarize some of the important points as:

- Only assimilation allows prediction.
- Inversion does not filter atmospheric data through imperfect carbon-cycle models.

⁴ However the outputs of dynamical models often inform the prior PDFs of fluxes.

⁵ Since assimilation as described here is technically more difficult it is often regarded as a desirable word in a title. The value judgment is incorrect and the field would be well served if the distinction was respected.

- Assimilation greatly reduces the underdeterminacy of the inverse problem [24].
- Assimilation can ingest a much wider variety of data.

For our purposes the last point is key. The ability of data assimilation systems to integrate the range of observations made of the carbon cycle makes them an attractive tool and an impressive intellectual structure for large measurement programs. This ability, however, imposes its own demands. For example, we never have just one measurement and the measurements are usually not of the same quantity. As we add new measurements the posterior PDF of the unknowns becomes more tightly focused, that is, their uncertainty is reduced. It is possible that the PDF will be reduced to zero, that is we cannot find a solution consistent with our prior information, model and measurements. We cannot know without considering simultaneously the uncertainties in all three components.

The question then is whether we can generate a quantitative description of the carbon cycle consistent with all available observations. In the next section I shall detail some recent steps toward this and draw some lessons from their common difficulties. I will break the problem down into some technical aspects, then describe some more fundamental problems.

The technical challenge

Before starting we need to know whether we could identify our target model even if we know it exists. Concretely this means describing the PDF of the unknowns consistent with the PDFs of model dynamics and measurements. [25•] showed that many of the techniques currently used for such calculations worked well for a simple biosphere model at one site. Despite the simplicity of the model it demonstrated sufficiently complex dynamics [26] to be a reasonable test of assimilation methods. [25•] found that the choice of cost function was much more important in the success of an assimilation than the choice of assimilation methods. A similar finding was noted by [27], who found that the experience of the practitioners was more important than the method chosen. Most of the methods trialed in [25•] were successful where success could be reasonably expected. Thus it seems the barriers to a carbon-cycle data assimilation system are not technical.

Experience to date

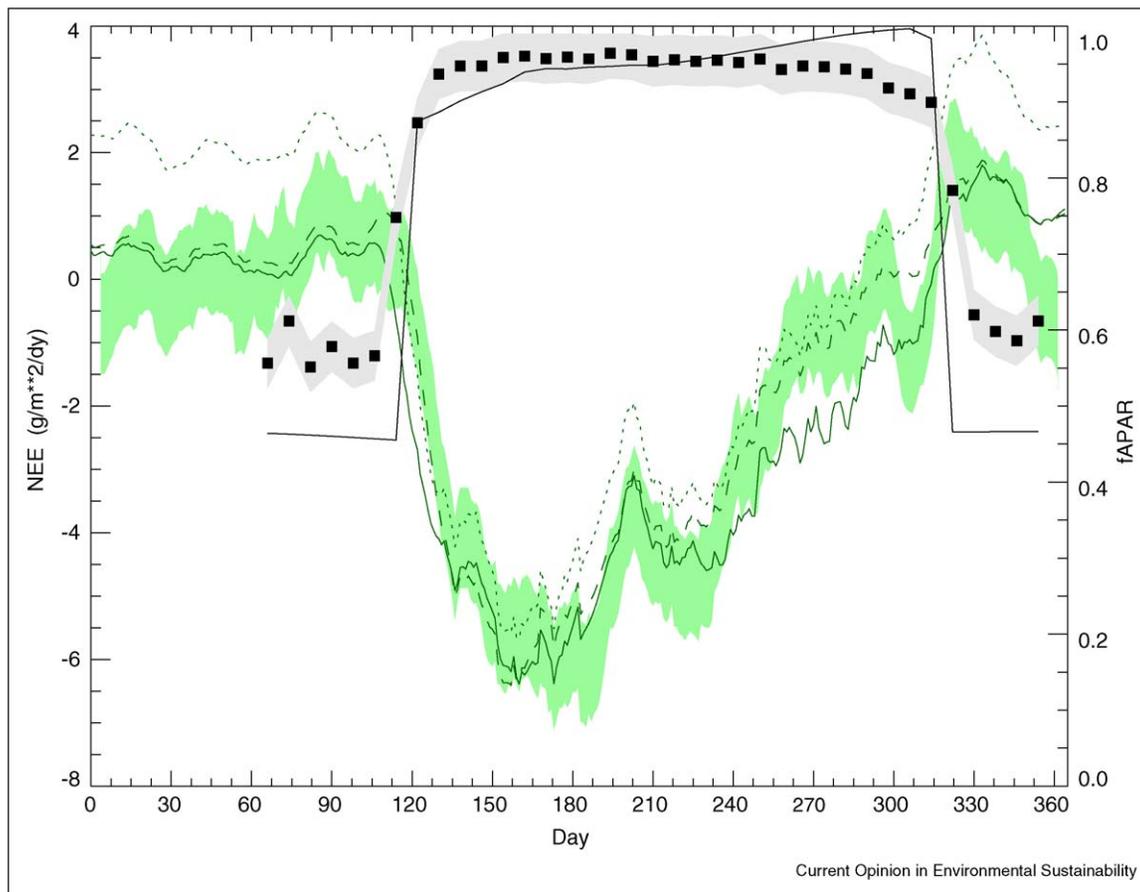
There have been a considerable number of studies using formal parameter estimation methods to constrain carbon-cycle models, for example [22•,23,28–37,38•]. Rather than give a comment on each of these here I have annotated them in the bibliography. Most of these studies have taken a similar form: perform an assimilation, check the quality of fit to the observations then make inferences on the carbon cycle using the constrained model.

There are two other important commonalities. Few of these studies use more than one type of data, for example, vegetation indices, eddy covariance measurements, and soil carbon measurements. One reason for this is structural. Experience from numerical weather prediction and the experience from CCDAS suggest that the ingestion of a new data type into a CCDAS requires two experts, one who understands the vagaries of the data (biases, levels of dependence among different measurements, etc.) and another capable of making the inevitable changes in the model needed to interface to the new data. The large consortia necessary to handle multiple streams of data generally do not exist within the carbon-cycle community.

The other reason is more profound and is demonstrated in Figure 3 taken from (Bacour, personal communication, Joint assimilation of eddy-covariance flux measurements and satellite observations within a process-oriented biosphere model, Glob Biogeochem Cycle 24, unpublished data) [39]. Here we attempt to fit simultaneously *in situ* measurements of the fraction of absorbed photosynthetically active radiation (FAPAR) and fluxes of CO₂ and water vapor. We optimize a series of parameters including those that control the timing of leaf onset and senescence and relationships between CO₂ and latent heat fluxes. We assimilate the observations either separately by type or together. The figure shows observations of FAPAR and CO₂ flux surrounded by their 1 σ uncertainties. We show the prior simulation of CO₂ flux plus the simulation assimilating either FAPAR or FAPAR and flux. Comparing the dashed and dotted green lines we see that assimilating FAPAR slightly degrades the fit to the CO₂ flux. Assimilating both quantities (solid green line) significantly improves the fit to the CO₂ flux data. Comparing the FAPAR simulation (solid black line) to its observations however shows that we cannot simultaneously fit both sets of observations. This suggests the model does not find the CO₂ and FAPAR observations consistent. So rather than optimize parameters of the model we have falsified some element of its structure. Far from seeing this as a disappointment I would argue it is an exemplary application of data assimilation. Note that if we had not carried out the parameter optimization we could never have distinguished between parametric and structural errors in the model.

The second common feature is rather a common lack. Only one of the cited studies [38•] attempts to test their parameter set against truly independent data. Even that study imposed the phenology both at the site for the assimilation and at the validation site. My comment is not a critique of these studies since it was not their aim to produce a general model of the terrestrial carbon cycle. However it is only a test against independent data which can give confidence in the generality and predictive power of an optimized model.

Figure 3



Comparison between flux and FAPAR observation data and the corresponding ORCHIDEE model simulations before assimilation (dotted), after assimilating FAPAR data (dashed) and after assimilating both FAPAR and *in situ* flux data (solid) at Fontainebleau France. Green lines represent NEE while the black line represents FAPAR. The light green band shows the measured $\pm 1\sigma$ confidence interval for the observed NEE while the gray region shows that for the FAPAR. Black squares represent FAPAR observations used in the assimilation.

It appears then that current terrestrial carbon-cycle models fail the test of generality, that is it is difficult to transfer understanding gained at one site or from one type of measurement to other places and other quantities. This is only to be expected. Conditions differ from site to site and we should not expect our models to function in the absence of complete knowledge. The methodology of data assimilation accounts for this since site-specific unknowns can be optimized at each site while still testing whether parameters optimized at one site are consistent with measurements at a second. Returning to Figure 1 we can ask where the prior information on the unknown came from. In reality it came from other measurements or experiments and the width of the distribution reflects the uncertainty in the unknown *after* these previous measurements. The uncertainty in the model simulation based on this prior PDF is a proper reflection of how much we expect to be able to transfer our knowledge. It is the compatibility of this distribution with the PDF of the

measurement which tells us whether our model has succeeded; a simple simulation of the mean model with the mean value of the prior would tell us almost nothing.

Some reasons for failure

If we accept that data assimilation has not delivered a general model of the terrestrial carbon cycle we can suggest some reasons for the problem.

Scaling. The different measurements of the terrestrial carbon-cycle appertain to different temporal and spatial scales. Ref. [40] pointed out that parameters that hold at one scale may not be valid for another. Thus if we infer the maximum photosynthetic rate (M_{MAX}) from a global assimilation using a model run at $2^\circ \times 2^\circ$ we should not expect it to apply to measurements from a point source like a flux tower. This is a computational not fundamental problem. Ref. [9] proposed the use of structural ecosystem models as one solution.

Information content of measurements. When assimilating any set of measurements we must assess the information which can be extracted from them. This is entirely model dependent as can be seen from Figure 1 where the model uncertainty and measurement uncertainty appear in the same dimension. The simplest measure of information content is the uncertainty we attach to the measurement. Statistical consistency requires that this uncertainty describes the distribution of the difference between the simulation of the optimized model and the measurements. For Gaussian distributions there are algorithms [41*] which adjust these uncertainties to achieve this. This, however, is the easy part of the problem. Much more difficult is the correlation between simulations of different measurements. In a periodic timeseries, such as hourly measurements of flux, a model is very likely to make the same mistake each day. This may well be true even after optimization. Thus there are consistent signals in the data which cannot be extracted by the model. Treating these measurements as independent pieces of data will both overestimate the failure of the model and overestimate the information content available from the measurements.

Approaches to this problem have usually involved either “thinning” the data or compositing it in some way. Ref. [31] chose a series of snapshots from their timeseries and optimized only these. Ref. [35] composited their timeseries into mean diurnal cycles and daily means. This is approximately subsetting the data by frequency rather than by time. More generally, in the context of their flux inversion, [16] projected measurements and model into frequency space. This took advantage of the fact that for stationary timeseries with multivariate Gaussian statistics, the errors in frequency space are independent.

Observation operators. Most terrestrial models exist as part of climate models and so their major focus is climate simulation. As noted in ‘Applying assimilation to the carbon cycle’, they must be coupled to observations via observation operators before use in assimilation mode. These introduce their own errors and often need extra variables in the assimilation that describe the observation process. Thus a detailed understanding of the process of making and simulating each observation is required for a meaningful assimilation.

Model deficiencies. The problems mentioned so far concern the conduct of MDF. Once these are addressed we will still see that our models do not meet the test of generality. Developers must then pay close attention to the core model. This process will be iterative, each time the model improves we will be able to extract more information from the measurements and our uncertainty specification must be revised.

Recommendations and conclusions

At the close of a rather negative appraisal of the status of carbon-cycle data assimilation, I will make some recommendations on improving the situation.

- MDF remains an essential tool for carbon-cycle research.
- The algorithmic details of MDF are not critical to its success.
- The task of data assimilation should move from the province of applications of a model into the development phase. As we have seen a common outcome of assimilation is a falsification of the model structure. This seems important information for model developers. The choice of parameterizations in a model is also amenable to assimilation via the addition of a discreet variable representing the choices. Applications to probabilistic climate forecasting are described in [42**] and references therein.
- Assimilation needs to respect the inherent scale in each measurement. This is computationally infeasible globally but it was shown in [43*] that flux and concentration measurements were mutually consistent with a high-resolution transport model. Thus this problem can be investigated in a regional assimilation.
- Much more attention should be paid to the information content retrievable from measurements. In particular assessments of the independence of residuals should form part of the assessment of quality of fit.
- More effort should be paid to the development of observation operators and their associated errors.

Acknowledgement

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