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A scientific workflow tool for biosphere modelling: Carbon Sink Archives

G.A. Alexandrov and T. Matsunaga
National Institute for Environmental Studies, Onogawa 16-2, Ibaraki 305-8506, Japan
g.alexandrov@nies.go.jp

Abstract: Scientific workflows in the field of biosphere modelling include assessment of the state of the art in modelling global biogeochemical cycles. The process of assessment consists of the following steps: collecting model outputs, performing model inter-comparison study, writing summary for policymakers, formulating an agenda for further research. Here, we present a web-based service that automates the entire process.

Keywords: web-based service, Carbon Sink Archives, biosphere modelling, NPP

1. INTRODUCTION

Carbon Sink Archives (CSA), a web-based service for storing, retrieving and analyzing 2-dimensional data as related to the problem of terrestrial carbon sink, provides a collection of model outputs that can be used for benchmarking newly developed models of the terrestrial carbon sink and its components, and a collection of web-based tools for performing relevant tests [Alexandrov and Matsunaga, 2009]. The current version focuses on the annual productivity of global vegetation, that is, terrestrial Net Primary Production (NPP). Terrestrial NPP is a starting point of carbon sink studies [Alexandrov and Matsunaga, 2008]. It shows limits to further growth of human appropriation of naturally produced organic matter and limits to the usage of human-induced carbon sinks for controlling the atmospheric concentration of CO_2.

2. CONCEPTUAL FRAMEWORK

CSA employs the Web 2.0 conceptual framework [O'Reilly, 2005]. This concept reflects and stimulates changes in the ways software developers and end-users use the Web. A Web 2.0 site allows users to change website content, not only to view the information that is provided to them. Moreover, the content of the website is produced and maintained through collaborative efforts that use peer-production method [Benkler and Nissenbaum, 2006] and are based on the self-correction principle [Suber, 2008].

The CSA data collection and software tools are intended to facilitate development of model independent knowledge on the terrestrial carbon sink that in its turn may serve as the basis for policies on stabilizing carbon dioxide concentration in the atmosphere. (For example, the current version of CSA facilitates development of the model independent knowledge on the biosphere potential to supply primary energy source for all non-autotrophic species including humans.) The knowledge developed to address the needs of policy making is referred to as policy relevant knowledge, and therefore, software tools are considered as services for deriving policy relevant knowledge from the model outputs, which are considered as knowledge components.

The tools for deriving policy relevant knowledge are based on the premises of evolutionary epistemology [Hull, 1988]. Scientific advances are assumed to be unpredictable (like genetic mutations). Their vitality, however, depends on whether they fit-for-purpose. In other words, the evolution of scientific theories is considered as a

Darwinian process of natural selection that determines which theory survives and drifts them toward consensus [Bradie, 1994].

The natural evolution of a particular field of science leads to distinction between frontier and core knowledge [Cole, 1992]. The latter is commonly accepted knowledge that has stood the test of time and is confirmed in a number of independent studies. The core knowledge serves as a normative knowledge -- that is, as the basis for judgement about what ought to be.

Once core knowledge is formed, natural selection prevents acceptance of contradicting concepts, theories, and even facts. This entails risk of coming to an evolutionary deadlock. New collaboration tools presented below are designed to avoid this risk and to accelerate internalization of contradicting facts. The contradicting facts are used to form an alternative knowledge, which in contrast to the normative knowledge serves as the basis for judgement about what might be.

3. DESIGN

The current version of CSA is to facilitate evolution of the normative knowledge on the terrestrial NPP, which is defined as an array of model independent estimates of NPP over a geographic grid of half-degree resolution. CSA consists of four major components: collection of models outputs, tools for benchmarking outputs of a new model, a tool for updating the normative knowledge proceeding from the outputs of a new model, a tool for reporting the updated normative knowledge in a policy relevant form.

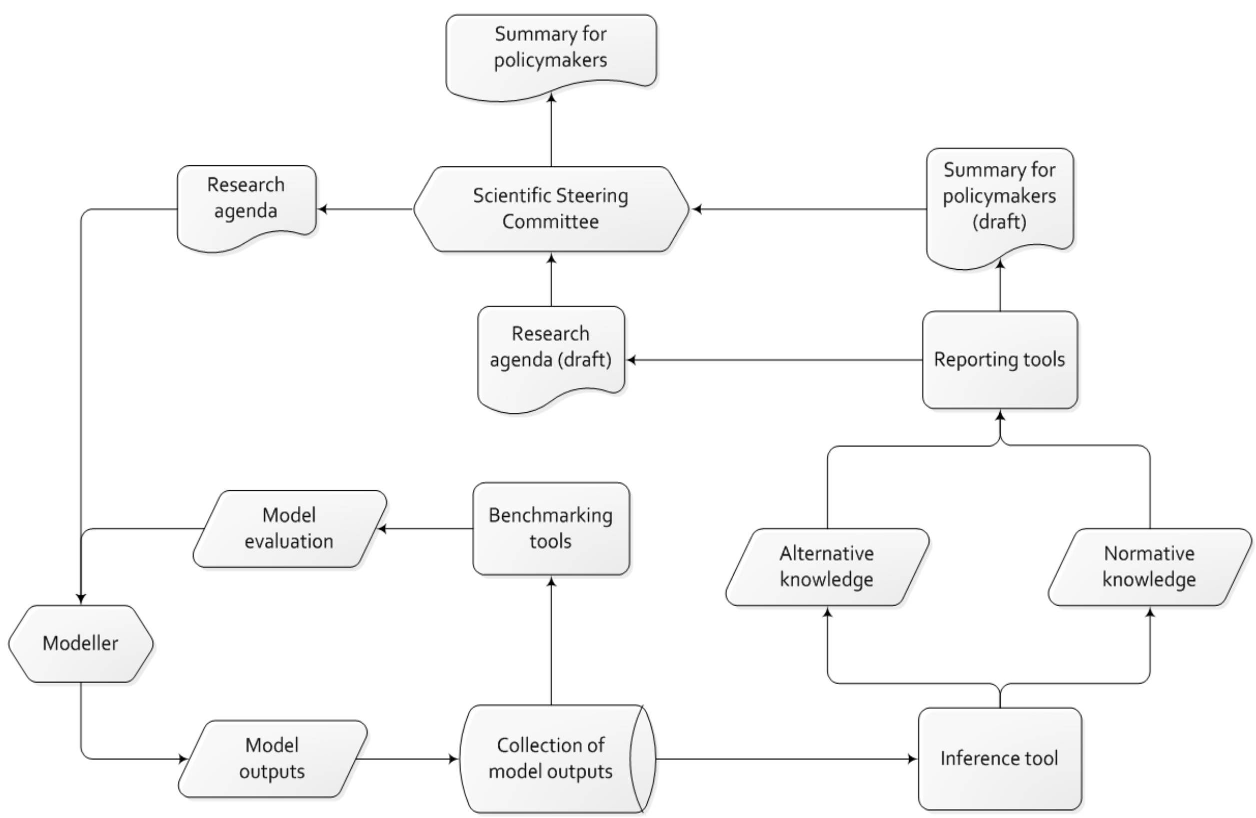

Figure 1. Scientific workflows that Carbon Sink Archives is designed to automate.

3.1 Collection of Models Outputs

The collection of model outputs contains, in present, the outputs of 12 models of terrestrial NPP and the outputs of model inter-comparison studies. The output data make an array of NPP estimates over a geographic grid with half-degree resolution.

3.2 Benchmarking Tools

Every new model of terrestrial NPP is purported to make a visible progress in the state-of-the-art by improving either a conceptual scheme or parameterization of a prior model. CSA includes a toolkit of web applications for comparison of global patterns of NPP produced by different models and for performing benchmark tests.

Perhaps the most fascinating of these tools is the tool for performing "progressivity test". The purpose of progressivity test is to visualize the progress in our knowledge of the global pattern of NPP. Proceeding from the premises of evolutionary epistemology, we assume that the progress can be measured by the decrease in uncertainty that stems from discrepancies in modelled estimates.

Modelled estimates of NPP for a given biome differ from one another, and so the state of the knowledge is conveyed by the mean value of the modelled estimates. The uncertainty in the mean value is quantified through the width of its confidence interval, which depends on the number of models and the standard deviation of the estimates. Since the width of the interval decreases with the number of the models, every new model is expected to improve the certainty of our knowledge. Hence, the metric of model progressivity may be defined as follows:

$$z = 100\frac{x-y}{x}$$

where x is the width of the confidence interval for the mean value of the modelled estimates, excluding the estimate produced by the new model, y is the width of the confidence interval for the mean value of modelled estimates including the estimate produced by the new model.

This metric penalizes the models that produce estimates that deviate largely from the normative mean value. The score depends also on the number of models: the more models, the lower a new model score. It is worth mentioning here that the test measures progressivity with respect to the normative knowledge. A really novel model may have a low score, if it opens new horizons in our vision of the global pattern of NPP.

3.3 Inference Tool

The collection of model outputs is viewed as a knowledge base for deriving normative knowledge on terrestrial productivity -- that is, a consensual estimate of this important characteristic of the Earth system. Every addition to data collection launches a computer program that updates normative knowledge. This program also updates the alternative (or frontier) knowledge.

The normative knowledge on NPP is expressed in the form of an array of numbers. Each number represents normative NPP at a given cell of the geographic grid of half-degree resolution, which is equal to the mean value of the normative estimates for this cell (so called, normative ensemble of estimates). The estimate produced by a new model is included into the normative ensemble if it falls within the boundaries implied by this ensemble and reduces the width of the confidence interval for the mean value. Otherwise, it is included into the alternative ensemble of estimates for this cell.

The details of the algorithm are explained elsewhere [Alexandrov and Matsunaga, 2008; Alexandrov and Matsunaga, 2009]. Here, we emphasize that the inference tool does not categorize models into normative and alternative. A model may give a quite usual estimate for one cell and an unusual estimate for another cell. Therefore, the inference tool categorizes the model estimate for a given cell instead of the whole array of model estimates.

3.4 Reporting Tool

The latest version of CSA has a reporting tool for continual updating of 'summaries for policy makers'. Every addition to the collection of model outputs results in automatic updating of the normative knowledge and generates updated versions of the 'summaries for policymakers' (Figure 1).

The normative NPP, expressed in the form of an array of numbers, needs a valid interpretation to be used in policy making. A "summary for policymakers" is to report the numbers in a policy relevant way. The reporting tool summarizes the current version of normative NPP according to given rules and updates corresponding fields (and figures) in the "summary for policymakers" template.

The current template is focused at the human share of terrestrial NPP. Human appropriation of NPP is assumed to be 1-2 tC/person/y. Hence, in the regions where NPP per capita is less than 2.5 tC/person/y, one may strive only for a survivable development, because nothing or little remains for other non-autotrophic species. The "summary for policymakers" reports

- the percentage of land that falls within the regions of high-productive, mid-productive, low-productive and non-productive climate, and the percentage of human population living there;
- the percentage of land that falls within the regions of survivable, barely sustainable, sustainable, and conservable development (defined in terms of NPP per capita), and the percentage of human population living there;
- the percentage of land that falls within the regions where sources of energy are highly technogenic, technoginic, biogenic, and highly biogenic (defined in terms of the ratio of industrial carbon dioxide emissions to NPP), and the percentage of human population living there.

4. DISCUSSION

The CSA software tools can be run under *Mathematica* [Wolfram, 1999] in an offline mode. The online access to these tools is provided through web*Mathematica* [Wickham-Jones, 2006] that integrates *Mathematica* with the web server technology. The obvious advantage of moving to software-as-a-service paradigm [Mell and Grance, 2009] is that the users need not have *Mathematica* to run the tools. The disadvantage is that the burden of maintaining computational infrastructure falls on the developers.

This burden is mainly of an institutional nature: the developers need to find an institution that will endorse and support the developed web-based service. In the case of CSA, this is not a trivial task. Research institutions (as well as funding agencies) are preoccupied with the impact. To be endorsed a research project should promise a research breakthrough. Although model assessment, benchmarking and inter-comparison are essential for understanding what is a real breakthrough and what is not, they cannot bring something that can be named as a research breakthrough by in and of itself.

The lack of a proper institutional framework does not serve, however, as an excuse for postponing community-based efforts to form consensual estimates of biosphere characteristics such as NPP and to form consensual understanding of the directions for further research. These efforts require new scientific workflow tools, because "our capacity to generate unprecedented quantities of new data means that the collaboration tools must enable researchers to quickly understand the information produced by their collaborators" [Frame et al., 2009]. *Carbon Sink Archives* provides the tools of this sort: for quick evaluation of a new model (or a new parameterization of an old model of terrestrial NPP), for quick updating of normative knowledge, and for quick formulation of an alternative hypothesis regarding the global pattern of NPP.

For example, terrestrial NPP is currently estimated at 60 GtC/yr. The consensus about this value was built in 1970s, although the estimates varied from 40 to 80 GtC/yr at that time, and re-analysis of the data [Alexandrov et al., 1999] revealed that estimates depend on how the data were classified with respect to the major regions of the world and that terrestrial NPP could be estimated at 50 or at 70 GtC/yr from the same set of observations.

Modelled estimates vary widely [Cramer et al., 1999] and the retrospective analysis of modelling efforts [Alexandrov and Matsunaga, 2008] revealed no convergence in modelled estimates of terrestrial NPP. The range of discrepancy remained roughly the same as it was ten years ago reflecting the structural uncertainty [Manning et al., 2004] in our knowledge of this essential biosphere characteristic and inefficiency of traditional means (such as occasional model inter-comparison projects) for reducing the structural uncertainty. Perhaps the progress in the biosphere science would be spurred by new collaboration tools like those provided by *Carbon Sink Archives*.

5. CONCLUSION

The policy relevant knowledge (or related research agenda) is traditionally produced by groups of scientists appointed to do this work on behalf of a research community. This is essentially a literary work the purpose of which is to write a review and a summary of the views presented in research articles. The widely known example is Intergovernmental Panel on Climate Change, which is considered as an adequate model for a system for assessing the state of knowledge of all key natural cycles including the carbon cycle [Seitzinger, 2009]. Nevertheless, if we are to substantiate words with numbers, then scientific workflow tools, like *Carbon Sink Archives*, are crucial for boosting evolution of the policy relevant knowledge. Since current knowledge on biosphere characteristics is expressed in digital form, most of the routine work related to model evaluation, forming research hypotheses, and developing policy relevant knowledge may be transferred to machines.

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