AutoMATES: Automated Model Assembly from Text, Equations, and Software

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ml4ai.github.io/automates

Abstract

Models of complicated systems can be represented in different ways - in scientific papers, they are represented using natural language text as well as equations. But to be of real use, they must also be implemented as software, thus making code a third form of representing models. We introduce the AutoMATES project, which aims to build semantically-rich unified representations of models from scientific code and publications to facilitate the integration of computational models from different domains and allow for modeling large, complicated systems that span multiple domains and levels of abstraction.

1 Introduction

There exist today state-of-the-art computational models that can provide highly accurate predictions about complex phenomena such as crop growth and weather patterns. However, certain phenomena, such as food insecurity, involve a host of factors that cannot be modeled by any single one of these models, but which instead require the integration of multiple models.

To truly integrate these computational models, it is necessary to 'lift' them to a common representation that is (i) agnostic to the software implementation, (ii) semantically rich enough to represent the implicit domain knowledge in the models, and (iii) connected to the domain literature. The AutoMATES project aims to build technology to construct and curate semantically-rich representations of scientific models by integrating three different sources of information:

- natural language descriptions of models in publications and other technical documentation,
- the equations contained in these documents, and
- the software the implements these models.

An example of a model being represented in these three forms (text, equations, and software) is shown in Figure 1. This model is a differential equation describing the biophysical variable, leaf area index (LAI). The network on the right half of the figure is an aspirational representation of the model as a Bayesian network. Although this example is hand-crafted, our end goal is to be able to automatically assemble models with this level of semantic richness. In this paper, we describe our high-level approach[1] and present our latest results.

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[1]For more technical details, please visit ml4ai.github.io/automates/documentation/deliverable_reports.

Text

Subroutine LAIS is called for both phases to compute the change in leaf area index (dLAI). During vegetative period, LAI increases as a function of the rate of leaf number increase. The potential rate is limited by soil water stress (both deficit and saturation), through SWFAC, and temperature, through PT. Its value is given by:

Where PD is the plant density (plants/m²), EMP1 is the maximum leaf area expansion per leaf, (0.104 m /leaf) and a is given by:

Where EMP2 and nb are coefficients in the expolinear equation and N is the development age of the plant (leaf number).

Equations

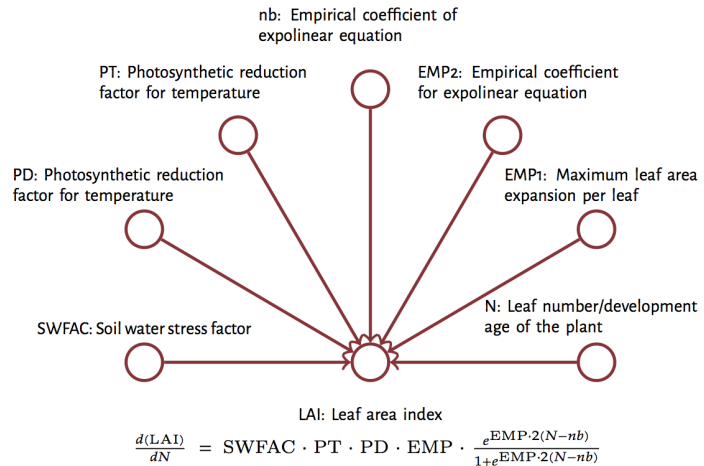$$dLAI = SWFAC \cdot PT \cdot PD \cdot EMP1 \cdot \frac{a}{1+a}$$
$$a = e^{EMP2 \cdot (N-nb)}$$

Software

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* dLAI = daily increase in leaf area index
(m2/m2/d)
* PD = plant density m−2
* EMP1 = empirical coef. for expoilinear eq.
* EMP2 = empirical coef. for expoilinear eq.
* nb = empirical coef. for expoilinear eq.
* dN = incremental leaf number
* N = leaf number
* PT = photosynthesis reduction factor for
temp.

a = exp(EMP2 * (N−nb))
dLAI = SWFAC * PD * EMP1 * PT * (a/(1+a)) * dN
```

nb: Empirical coefficient of expolinear equation

PT: Photosynthetic reduction factor for temperature

EMP2: Empirical coefficient for expolinear equation

PD: Photosynthetic reduction factor for temperature

EMP1: Maximum leaf area expansion per leaf

SWFAC: Soil water stress factor

N: Leaf number/development age of the plant

LAI: Leaf area index

$$\frac{d(\text{LAI})}{dN} = \text{SWFAC} \cdot \text{PT} \cdot \text{PD} \cdot \text{EMP} \cdot \frac{e^{\text{EMP}\cdot 2(N-nb)}}{1+e^{\text{EMP}\cdot 2(N-nb)}}$$

Semantically-Enriched Bayes Network

Figure 1: Integration of text, equations, and code into a semantically-enriched Bayesian network.

Significance: This work will dramatically advance the state-of-the-art in automated model curation and integration, enabling scientists and analysts to understand complex mechanisms that span multiple domains. By exposing the implicit domain knowledge baked into computational models, this effort will enable semantically rich automated model composition and reasoning in context, at scale.

2 Architecture Overview

The AutoMATES system is designed to extract information from several knowledge sources, link the extracted concepts into a unified model representation, compare models based on different features, and augment the models with supplementary information. Each of these components is implemented independently, but designed to interoperate with each other. A high-level view of the system's architecture is shown in Figure 2. This modular architecture provides AutoMATES with the extensibility required to support different knowledge sources in the future as it is extended to handle other domains. Briefly, the four main components of AutoMATES are:

1. *Extracting* model information from different aspects of source code and corresponding scientific publications and technical documents. From source code, we extract the model from the code implementation itself (3) as well as any supplementary information such as descriptions expressed in comments. From scientific publications and documentation, AutoMATES reads model information from text (5) and equations (4).
2. *Grounding* the extracted information by identifying when the same concept is expressed in different knowledge sources, and linking them together to form a unified, programming
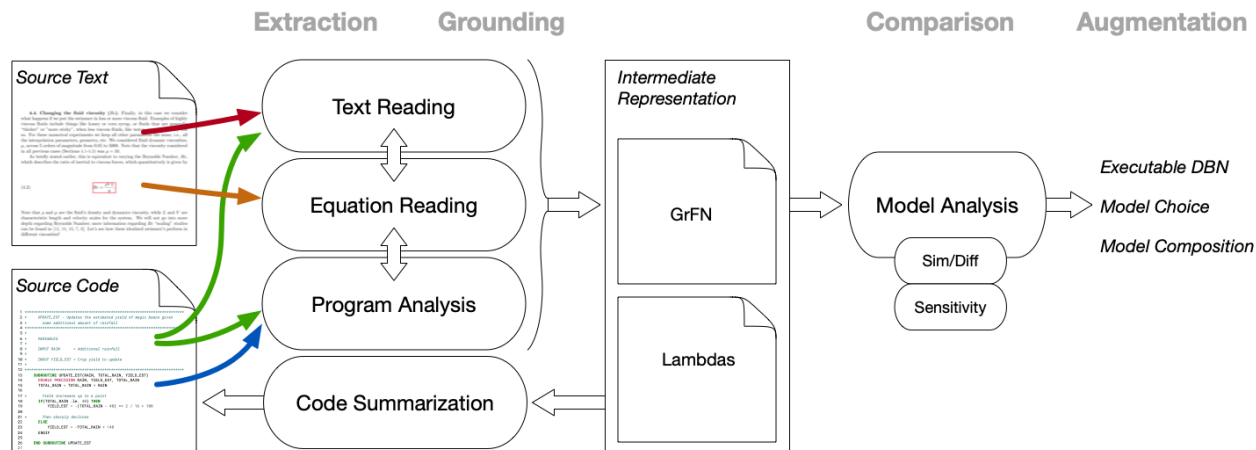
Figure 2: Architecture overview

language-agnostic intermediary model representation: a *Grounded Function Network (GrFN)*.

3. *Comparing* models, using the GrFN representation, by analyzing structural and functional (via sensitivity analysis) similarities and differences (6).

4. *Augmenting* models through selection of model components appropriate for a task, composing model components, generating model descriptions in context to augment existing documentation, and model execution.

3   Scalable Program Analysis

Our program analysis approach to extracting model information from the source code implementation begins with `for2py`, a front-end translator that maps Fortran source programs to a language-independent program analysis intermediate representation (PAIR) that is then used to generate files used as input to subsequent analysis. This design decouples input processing from output generation, and is motivated by the following:

1. *Performance and scalability.* Modules that are referenced by multiple program components do not have to be reanalyzed separately for each referencing component. Independent source-language modules can in principle, be analyzed concurrently.

2. *Support for source-language heterogeneity.* This design makes it possible, in principle, to support programs with different components written in different languages. It also allows us to reason about models implemented in different source languages.

3. *Independence of back-end tasks.* Different back-end analysis tasks, e.g., sensitivity analysis and comment analysis, can be carried out independently (and, if necessary, concurrently) on the PAIR.

`for2py` currently handles a significant subset of Fortran, including: data types such as scalars and arrays; control constructs such as conditionals, loops, functions, and subroutines; and input/output (I/O) primitives including formatted and list-directed I/O. We expect to soon complete the handling of modules and derived types.

A fundamental challenge we have to address is that of scalability, since software implementing sophisticated scientific models can encompass thousands of source files and hundreds of thousands of lines of code. We do this by performing analysis at the module level of granularity. Given

the source code for a scientific model, we analyze its modules to identify define-use relationships between them and construct a *module dependency graph* that identifies these dependencies between different modules. We use a topological sort of this graph to guide the subsequent analysis of the modules. The module dependency graph imposes a partial order on the modules of the analyzed system, indicating which modules are independent of each other and can therefore be analyzed in parallel. This ordering has three significant implications for scaling. First, it allows modern computer systems such as multi-core processors and cloud-based systems to be utilized effectively. Second, it provides the user a straightforward tunable tradeoff between computational resources and analysis efficiency. Finally, it means that the cost of analyzing a software system is proportional to the depth of its module dependency graph rather than its total size (number of nodes), resulting in sublinear asymptotic complexity.

4   Contextualized Equation Parsing

Models are often represented concisely as equations, at a level of abstraction that can supplement both the natural language description as well as the source code implementation. For humans to compare the equations and source code for several models, as is done in [2], is time consuming and expensive. Accordingly, we are developing an automated approach that identifies the relevant equations in text and rendered images of documents (PDFs treated as images) associated with scientific models, parse them into an intermediate symbolic mathematical representation, and ground the variables in the equations to text descriptions and source code variables.

Non-textual elements in PDFs have previously been identified using heuristics based on document structure [4] or statistical learning [3, 1]. Here, taking advantage of advances in deep learning [8], we identify the location of the bounding box surrounding the equations using machine vision techniques. After identifying the location of the equations in the PDF, the next step in the pipeline is to parse the rendered equation into an intermediate representation. We choose to use LaTeX because we have the LaTeX source code for each of the training examples, and also because LaTeX preserves all of the typographic information (e.g., boldface, subscript, etc.), which conveys variable semantics. We decompile the image using an encoder-decoder system that encodes the image of the equation through a series of convolutions and produces LaTeX commands that generate the image [6, 5]. We are currently evaluating this process on a held-out subset of the data from ArXiv.

This decoded LaTeX representation will then be parsed into Python code (by extending coverage of an open source rule-based system, `latex2sympy`[2], to equation elements frequently found in the domain) and then converted to a equation elements frequently found in the domain) and then converted to a GrFN representation. To ground the GrFN representation extracted from the equations, we locate text that references the equation, using the equation identifier when available and the lexical content when it is not.

5   Machine Reading for Scientific Models

We are developing a framework for reading and extracting model information from the scientific papers that directly describe the computational models (e.g., DSSAT, SWAP) whose source code we analyze (3).

Scientific papers are typically available as PDFs, which need to be preprocessed into a format that

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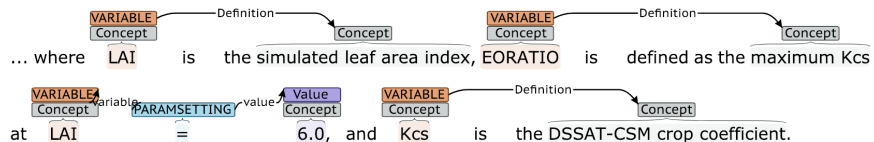
[2]https://github.com/augustt198/latex2sympy

Figure 3: Example of variables (represented as concepts, definitions and value assignments) extracted from scientific text as a result of the machine reading pipeline.
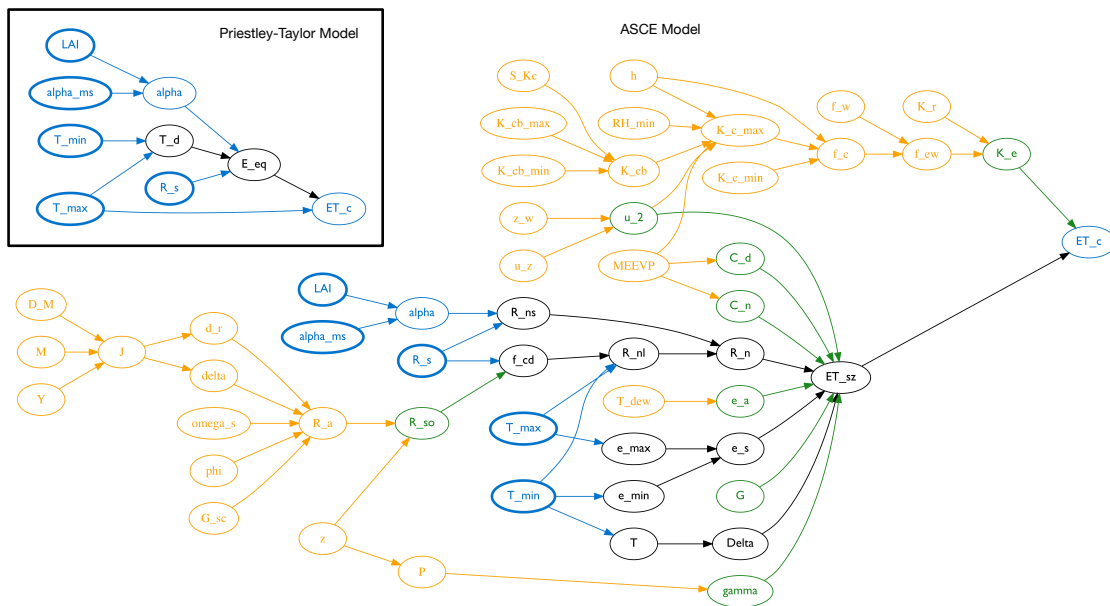

Figure 4: Results of comparing Priestly-Taylor (PT) and ASCE models. Blue nodes represent variables shared between PT and ASCE. Black nodes represent variables not shared but along directed paths between shared variables. Green nodes in the ASCE model represent variables whose states directly affect shared directed paths – if controlled, this isolates the portions of ASCE that overlap with PT. Finally, orange nodes represent variables in the ASCE model that can be isolated from the overlap in the comparison.

a machine reader can use. We make use of Science Parse[3], an open source tool that segments the sections based on the paper layout and typography.

Our framework then implements an open-domain information extraction system based on Eidos[4], a machine reading system designed to extract causal relations. At its core, Eidos has a grammar of rules [10, 9] that model linguistic patterns commonly used by authors to express causality in text. Here, where we are interested in gathering context about the models implemented in source code, causal relations are useful, but not sufficient. We have modified Eidos to extract mentions of model variables and their descriptions. Additionally, it will be critical to read for background assumptions (e.g., model preconditions) and additional contextual information which could inform the setting of parameters (using quantities and units identified by grobid-quantities[5]).
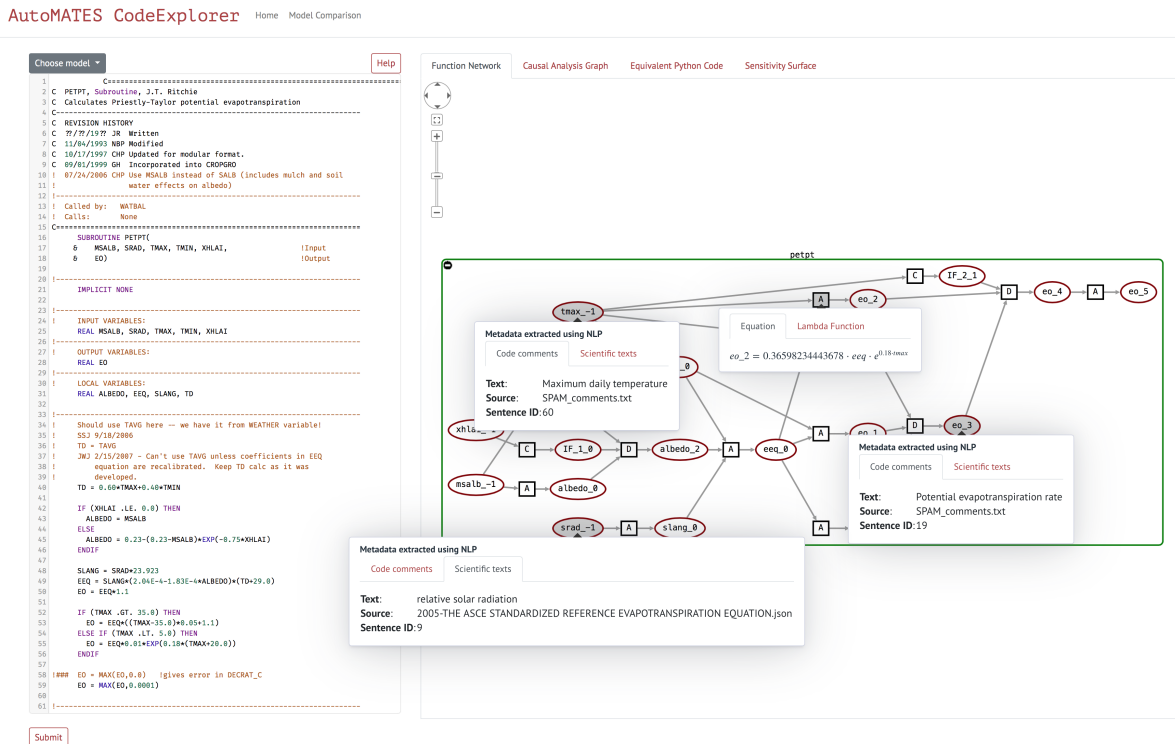
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[3] https://github.com/allenai/science-parse
[4] https://github.com/clulab/eidos
[5] https://github.com/kermitt2/grobid-quantities

Figure 5: Screenshot of the AutoMATES CodeExplorer (available at http://vanga.sista.arizona.edu/automates), showing the translation of a the Priestley-Taylor method for calculating potential evapotranspiration (a submodule in DSSAT [7]) into a computation graph. The __assign__ nodes are annotated with the automatically extracted LaTeX-typeset representation of the equation extracted from the code, which will facilitate linking with scientific publications. Additionally, the variable nodes are automatically aligned with descriptions extracted from code comments and scientific texts.

The extracted variables and their mentions will necessarily be aligned with the variables read from source code (3) and equations (4) to find and resolve commonalities and discrepancies in different representations of the same model. In Figure 3, we show a screenshot showing results of the current text reading pipeline.

6   Model Analysis

Model comparison and eventual augmentation is then enabled by our model analysis pipeline, which identifies which portions of two or more models share the same or similar computations about similar variables, and which components are different.

This analysis is enabled by the unified grounded function network (GrFN) representation, such that we first identify shared variables and then analyze the GrFN topology to identify differences in setting variables states. Figure 4 shows an example of comparing the PT and ASCE evapotranspiration models from the DSSAT crop modeling system [7]. Sensitivity analysis is then used to analyze the functional relationships between the variables. Because sensitivity analysis can be computationally expensive, we are developing methods that use automatic code differentiation to efficiently compute the derivatives of variables with respect to each other, and Bayesian optimiza-
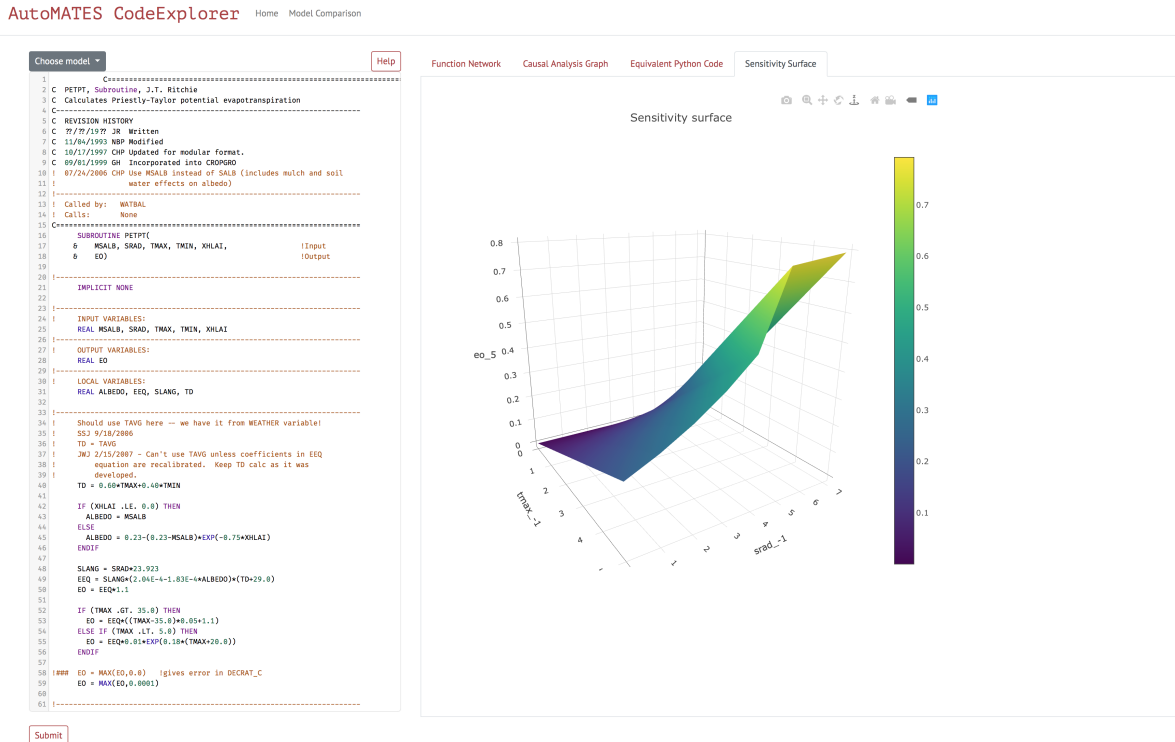
Figure 6: Initial results of automated sensitivity analysis. The pair of variables that the Priestley-Taylor model of evapotranspiration is most sensitive to has been automatically identified given bounds information for the input variables, and a surface plot has been generated that shows the effect of varying that pair of variables (maximum temperature and solar radiation) on the output variable (potential evapotranspiration).

tion techniques to estimate sensitivity functions with as few samples as possible. The final product of this analysis (a) includes modular executable representations of grounded models (as dynamic Bayesian networks), (b) provides results of model comparison to enable model choice in tasks, and (c) based on grounded model similarity and differences, enables model composition.

In Figure 6, we show some initial results from automated sensitivity analysis.

7   Conclusions

Systems of interest for scientific, humanitarian, and security reasons often require the integration of computational models from multiple domains - for example, modeling food security in a region requires the use of computational crop, weather, and hydrology models, to name but a few. However, this integration currently requires significant manual effort in the form of exposing and curating interfaces to the computational models. The framework we are developing will greatly speed up this curation and integration process, making it possible to effectively model large, complicated systems and reason about them at multiple levels of abstraction.

8   Resources, web sites, etc.

The system described here is open-source and publicly available at github.com/ml4ai/automates and github.com/ml4ai/delphi. We have also set up a public webapp, CodeExplorer (see screenshot in Figure 5), which shows off a subset of the functionality of the AutoMATES system, and is live at vanga.sista.arizona.edu/automates.

9   Acknowledgments

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