Towards Democratizing Modeling at Scale

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***Abstract*—We use AI techniques to create a modeling environment that makes sophisticated models accessible to non-experts. Our AI framework for Model INTegration (MINT) assists users to explore scenarios, which MINT can run in a local environment or at scale in a supercomputing facility. We are using MINT with hydrology, agriculture, and drought models for food security.**

Keywords—AI, semantic metadata, modeling

I. Introduction

Creating a model in a specific domain or area of expertise is very challenging because there are many models that can be adapted for specific areas or situations. Our focus has been on geoscience processes and their interaction with human processes. In this context, a model is an idealized representation of a physical system that can be used to characterize, understand, predict, and manage the system. The modeling approach can vary widely, from empirical (e.g., the likely return period of a weather event for a particular area based on prior events) to theoretical (e.g., biological or physical laws), from having 2D to 3D spatial extent, varying spatial and temporal granularities, and different simplifications and assumptions. Our work to date has been on food security, specifically developing models of how floods and droughts affect crop production and food availability. A major challenge is that modelers who are expert in hydrology are the only ones who can use their models, and instead we would like to allow decision makers and other non-expert users to use the models. We are developing a modeling approach that uses artificial intelligence (AI) techniques to reduce modeling effort while ensuring utility for decision making. These AI techniques target the following modeling challenges:

- *Delays in decision making*: Several months are typically needed to generate modeling products. This is because data must be located and transformed as needed by models. Workarounds have to be found when data is not available, and models have to be set up and refined to make accurate predictions. AI systems with the ability to understand data needs and data sources could guide users to find appropriate data.
- *Limited scenario exploration*: Decision makers are interested in exploring interventions that solve potential problems. In contrast, many models typically focus on prediction from static inputs and have limited representations of interventions, if any. AI systems could include knowledge of scenarios and interventions linked to models in order to guide users to explore possible futures on their own.
- *Restricted domain modeling*: While a decision maker has holistic questions, in practice models tend to have many parameters that are too disconnected from high-level decisions. Furthermore, model parameters are often not independent, and it requires substantial expertise to realize that altering one parameter means considering other parameters. When using several models, coordinating the settings of each increases the modeling complexity. It takes significant effort for a modeler to learn to use correctly new models outside their area of expertise. AI systems could capture expert knowledge about models in order to guide users to set up model parameters and validate model runs.

Our approach is implemented in the MINT (Model INTegration) framework [1], and currently includes data and models to analyze the interactions between natural and human systems involving climate, water availability, agricultural production, and markets.

II. Modeling with MINT

A. AI Techniques for Modeling

Our work to date on using AI techniques for modeling makes several innovative contributions: 1) An intelligent user interface that guides analysts to frame their modeling problem and assists them by suggesting relevant choices and automating steps along the way; 2) Semantic metadata for models, including their modeling variables and constraints, that ensures model relevance and proper use for a given decision making problem; and 3) Semantic representations of datasets in terms of modeling variables that enable automated data selection and data transformations.

B. Metadata about Models in MINT

The MINT Model Catalog takes a unique perspective on how to describe models [2]. While other model catalogs assign an entry to each model, in MINT we create a catalog entry for self-contained software components that correspond to a particular functionality and use of any given model. Therefore, a model can have many entries in the catalog, which we call model components. For each model component, we represent extensive metadata about the formats of the input and output data and the physical variables that each file represents. We also represent the constraints of use of the model, which are used to guide users to choose appropriate models for their scenarios. A particularly challenging aspect is exposing only the model parameters that non-expert users should adjust to their scenarios, so model components are more usable.

Figure 1 illustrates the main metadata categories of the MINT Model Catalog on the right. The semantic metadata and constraints are then used by MINT's AI reasoners to assist users to develop scenarios, select appropriate models, explore possible interventions, and consider diverse options and tradeoffs.

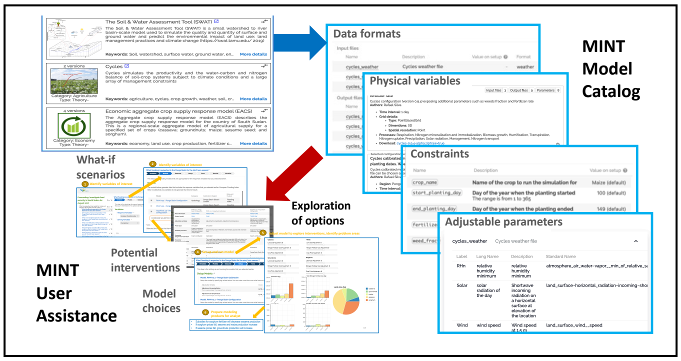

Fig. 1. Overview of Metadata in the MINT Model Catalog.

C. *Creating Model Ensembles in MINT*

Figure 2 gives an overview of how MINT handles model components and model execution. Modeling experts interact with the Model Insertion Checker (MIC) to easily create containers of their model code and any datasets that are needed to run that configuration [3]. The Desktop Application for Model Execution (DAME) environment allows users to test models in their local environment [4]. DAME also allows any MINT user to do small model runs as they are learning to use a model or testing a model component. MINT model services query MINT data services to retrieve available datasets from its Data Catalog, and to run data transformations that convert raw datasets into formats that specific models require.

Through MINT's user interface, users receive intelligent assistance to select and set up models. In this interface, users can specify many values for the adjustable parameters of models, as well as different initial conditions for example through alternative input datasets. MINT then generates ensembles of models that contain a model execution for each combination of the values specified by users. Users can run small model ensembles in a local server, for testing and exploration purposes. Once users are ready to generate large model ensembles, MINT can execute them on HPC facilities. Once model ensembles are executed, the results are registered in the MINT Data Catalog, so they are available for all users. This enables the use of model results as inputs to other models.

III. Running Models at Scale

MINT is installed at the Texas Advanced Computing Center (TACC). Model ensemble jobs are created through the MINT web-based user interface, and then submitted to the Tapis secure API for management of remote computing workloads [5] and the Slurm cluster management and job scheduling system [6].

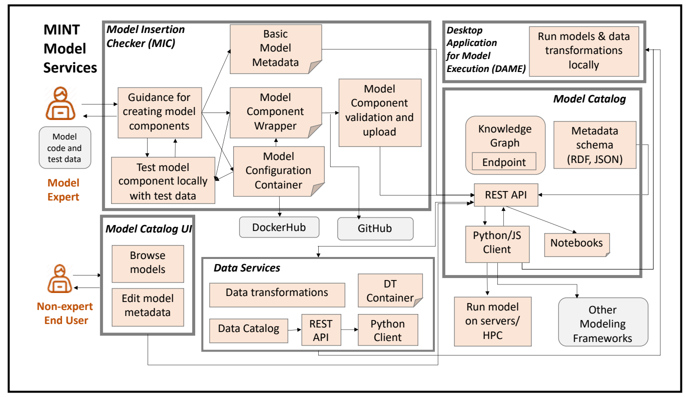

Fig. 2. Overview of MINT Model Services.

We are able to run MINT model ensembles on Stampede2 [7], the flagship supercomputer of the Extreme Science and Engineering Discovery Environment (XSEDE) network, serving thousands of researchers across the US. With 18 petaflops of peak performance, Stampede2 features 4,200 Knights Landing (KNL) nodes — the second generation of processors based on Intel's Many Integrated Core (MIC) architecture — and 1,736 Intel Xeon Skylake nodes.

In our work to date, we have been able to run model ensembles with over 14,600 model runs for an agriculture model. These ensembles explore scenarios for planting different crops, planting dates, fertilizer amounts, and rainfall.

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