**An Online Supervised Monitoring and Evaluation System for E3SM/ELM Model Simulation** - An E3SM NGD white paper submitted by Dali Wang.

**Background, motivation, and alignment with E3SM strategic vision**

The majority of Earth system model evaluation and data analysis are in the post-simulation mode and these efforts are plagued by the intensive IO operations and time-consuming human interaction to identify the possible results from massive datasets. While there are several efforts that adapt in-situ data visualization and analysis on high performance computing platforms, these efforts mainly focus on in-situ infrastructure establishment and static workflow developments [1-5]. These in-situ data analysis systems can be further improved with the incorporation of model-specific data processing workflow to facilitate E3SM model result verification and performance evaluation. Recent advances in AI technologies, especially recurrent neural network, deep reinforcement learning, and continuous control, provide new opportunities for online model result verification and performance evaluation with policy-based human interfaces [6-8]. In this effort, we propose to develop an in-situ, supervised monitoring and evaluation system for E3SM/ELM model on the coming leadership computers, such as the Summit at ORNL.

**Proposed research and approach**

Deep reinforcement learning has a large advantage over traditional dynamic programming and genetic algorithm to represent complicated decision-making processes [9-10], therefore, we plan to design a reinforcement learning procedure and train a two-layer neural network using E3SM/ELM simulation results and to determine the correlations between input parameters, intermediate model results and the model outputs in a predefined temporal-spatial window.

This research would involve three main tasks: 1) a real-time simulation data sampling component, 2) an automated deep reinforcement learning system, and 3) an online model verification and prediction component.

*Task 1 – a real-time simulation data sampling component:* Global E3SM/ELM simulation requires hundreds of CPU cores, we will further improve our data analysis framework for E3SM/ELM [11-14] to conduct compiler-based code instrumentation and to automatically collect and sample the model variables in real-time on high performance computers. Within the sampling system, a collection of ELM model variables (such as air or soil temperature, photosynthesis intensity, maintenance respiration, carbon flux, etc.) along with model inputs (such as time, location, plant functional types, precipitation, and nitrogen decomposition etc.) are collected and transported into a deep reinforcement learning system using either Graphic Processing Unit (GPU) or Tensor Processing Unit (TPU) on the coming Summit at ORNL.

*Task 2 – an automated deep reinforcement learning system:* We will develop a two-layer deep neural networks for reinforcement learning process using guided policy method [15,16]. We will use the collected model variables to train the model using predefined rules and labels associated with special events (such as drought season or strong storms) or typical ecosystem function patterns (such as diurnal cycles, and seasonal phenology), therefore, it is a supervised learning process to establish the neural network. Considering the strong temporal relationship between the ELM model variables, a long short-term memory (LSTM) recurrent neural network (RNN) approaches and other deep learning methods will also be tested on high end computers [17-19]. The output nodes will be designed to represent several key ecosystem variables with either short term variances (such as canopy flux, and growth respiration) or longer-term variance (such as carbon pool and fine root biomass). Since the E3SM/ELM is a global simulation, we can establish a comprehensive training and cross-validation datasets for ELM model at different scale, i.e., grid cell, soil column, and vegetation etc.

*Task 3 – an online model verification and predication component:* We will use the deep reinforcement learning system, trained in the tasks 2, to verify the model results during the simulation. If the ELM model configuration is valid, the simulation result will align well with the online AI model prediction. Otherwise, the AI model will flag the mismatch and potentially terminate or steer the simulation if some critical conditions are triggered. This model verification component will also use the underlying in-situ infrastructure for data communication with the real time model simulation. The online model verification component can provide a computationally-light approach to validate the functional relationship between E3SM/ELM submodules, key ecosystem function, and model variables inside a specific subroutine. Therefore, it can be further developed as a surrogate model for E3SM/ELM model uncertainty quantification [20] and be integrated into another NGD efforts lead by Dr. Ricciuto. It can also be used to perform parameterization for E3SM/ELM model tuning and optimization.

**Timeline:** These three tasks will be conducted in three stages, each lasting approximately 18 months, with 6-month overlap in staged execution of these tasks to optimize efforts across the E3SM team members and domain science expert collaborators throughout the three-year project.

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