Enhancing Photosynthesis Simulation Performance in ESMs with Machine Learning-Assisted Solvers

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***Abstract*—When simulating vegetation dynamics, photosynthesis accounts for a large fraction of the computational cost in most Earth System Models (ESMs). This is largely since photosynthesis is represented as a system of nonlinear equations, and the solution requires the use of an initial guess followed by many iterations of the numerical solver to obtain a solution. We use machine learning (ML) to replicate the response surface of the model's numerical solver to improve the choice of initial guess, therefore requiring fewer iterations to obtain a final solution. We implemented this test on the leaf-level calculations as well as at the canopy scale, and for both we observed fewer iterations of the photosynthesis solver when a ML-based initial guess was implemented. The model tested here is the Energy Exascale Earth System Model - Land Model (ELM). The ML-based algorithms used here are trained on simulations from the model itself and used only to improve the initial guess for the solver; therefore, the model maintains its own set of physics to obtain the final solution. This work shows novel ways to utilize ML-based methods to improve the performance of numerical solvers in ESMs.**

Keywords—photosynthesis, numerical solver, machine learning, Earth System Model

I. Introduction

In Earth System Modeling, simulating the complex dynamics of vegetation, particularly photosynthesis, presents a significant computational challenge (Bonan and Doney 2018). This challenge is magnified when working with models like the Energy Exascale Earth System Model - Land Model (ELM), which incorporates numerous processes across different scales (Golaz et al., 2022). Photosynthesis, a core component of vegetation dynamics, is typically represented as a system of nonlinear equations (Collatz et al., 1992; Massoud et al., 2019). Solving these equations requires iterative methods, where the solution is gradually refined through successive approximations (Fig. 1). The computational cost of these iterative solutions can be substantial (Ricciuto et al., 2018; Lu et al., 2018; Massoud 2019), especially when the simulations are extended over large spatial domains or long temporal scales.

The computational burden is particularly pronounced in high-resolution simulations that span continental or global scales, where the data outputs can reach petabytes in size (Abdulah et al., 2024). For single-site simulations, the data generated can already be on the order of gigabytes. The sheer volume of data and the iterative nature of the numerical solvers impose significant demands on computational resources (Mengaldo et al., 2019). As Earth System Models become more sophisticated, there is a pressing need to enhance the efficiency of these simulations to make them more feasible and accessible for comprehensive climate studies.

To address this challenge, we propose the integration of machine learning (ML) techniques into the solver process, specifically targeting the initial guess in the iterative solution of photosynthesis equations. Traditional numerical solvers begin with an initial guess, which is then iteratively refined to reach the final solution. The quality of this initial guess is crucial; a poor initial guess can lead to a higher number of iterations, thereby increasing the computational cost (Tromeur-Dervout and Vassilevski 2006; Ye et al., 2020). By employing ML to generate a more accurate initial guess (Fig. 2), we hypothesize that the total number of iterations required by the solver can be significantly reduced, leading to faster and more efficient simulations.

In this study, we focus on two scales within ELM: the leaf-level and the canopy-scale (Zhu et al., 2019, 2020; Bisht et al.,

2024). At both scales, we evaluate the performance of ML-based initial guesses compared to traditional methods. Our approach leverages a large catalog of model simulations, using the data to train neural networks that can predict optimal starting points for the solver. The potential benefits of this approach are substantial, particularly in reducing the computational costs associated with large-scale, long-term simulations.

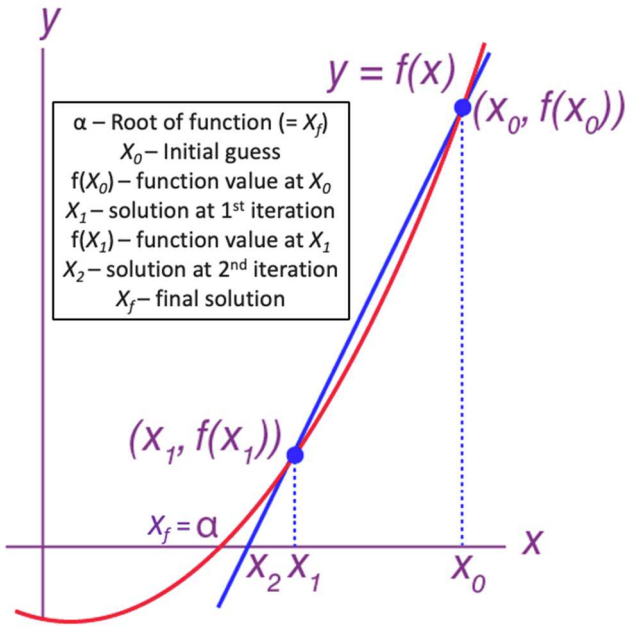

Fig. 1. Schematic of Iterative Root Finding in the Photosynthesis Solver. The process begins with an initial guess x_0, where the function value is $f(x_0)$. After the first iteration, the solution is updated to x_1 with the corresponding function value $f(x_1)$. The process continues with the solution advancing to x_2 and $f(x_2)$ after the second iteration. This iterative procedure continues until the final solution x_f is reached, where $x_f = \alpha$, after n iterations. This schematic illustrates the multiple iterations required to converge to the final solution in the nonlinear photosynthesis equations.

The results from our study demonstrate that the ML-based approach can indeed reduce the number of iterations required in the solver, with varying degrees of success depending on the scale. For leaf-level simulations, we observed a significant reduction in computational cost, while at the canopy scale, the improvements were more modest. These findings suggest that while ML-based methods hold promise for enhancing solver efficiency, further refinement and adaptation are necessary to fully realize their potential, particularly at larger scales.

This paper contributes to the growing body of research exploring the intersection of machine learning and Earth System Modeling (Greer et al., 2021; Pawar and San 2022; Chen et al., 2023; Massoud et al., 2023), offering novel insights into how data-driven techniques can be harnessed to accelerate complex simulations (Eyring et al., 2024). As the demand for more detailed and accurate climate models continues to grow, the integration of ML into these models offers a pathway toward more efficient and scalable simulations, paving the way for more comprehensive climate studies.

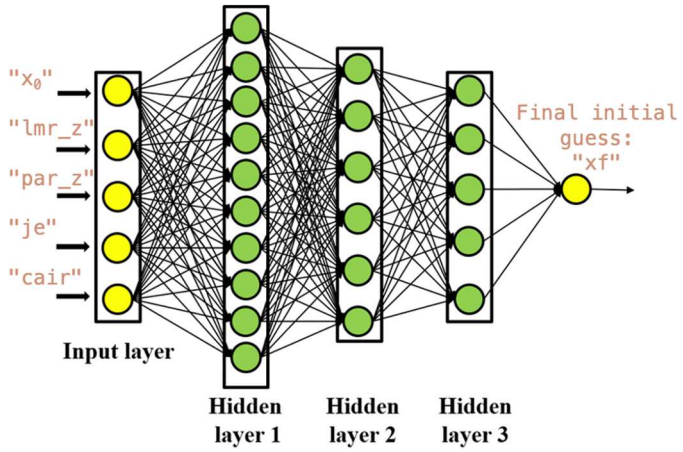

Fig. 2. Schematic of a hypothetical Neural Network structure used to improve the initial guess for the photosynthesis solver. The neural network (NN) takes as inputs various variables from the original model simulation, including the initial guess "x_0", leaf maintenance respiration "lmr_z", and other relevant parameters. The output of the NN is the predicted final solution "x_f", which is then used as the new initial guess "x_0" for the numerical solver. The model subsequently applies its own physical equations to converge on the actual final solution "x_f". The goal of this approach is to provide an initial guess that is closer to the true final solution, thereby reducing the total number of iterations needed for the solver to converge.

II. The Energy Exascale Earth System Model (E3SM)

The Energy Exascale Earth System Model (E3SM) is a state-of-the-science Earth system model developed by the United States Department of Energy (DOE) to advance our understanding of the complex interactions between climate and energy systems. E3SM is designed to operate at exascale computing levels, enabling high-resolution simulations that capture critical processes influencing energy production, water resources, and climate dynamics across regional and global scales.

Within the E3SM framework, the land surface is represented by the E3SM Land Model (ELM). ELM is a comprehensive model that simulates the fundamental processes governing carbon, water, energy, and nutrient cycles across terrestrial ecosystems. It integrates various land surface processes, including vegetation dynamics, soil hydrology, and biogeochemistry, as well as the effects of land-use changes (Lawrence et al., 2019). This integration within a single modeling framework allows ELM to provide detailed predictions of land-atmosphere interactions under a wide range of climate scenarios. ELM's robust capabilities are essential for advancing climate science, particularly in projecting the impacts of climate change on terrestrial ecosystems. By utilizing exascale computing, ELM enhances the accuracy and resolution of these projections, making it a valuable tool for informing policy and decision-making at both regional and global levels.

In this study, we applied the ELM component of E3SM at the temperate forests of the southeastern United States for the years 1850-2005, specifically focusing on the evergreen Duke Forest. The simulations were driven by meteorological data and other site-specific characteristics, including stoichiometry, allometry, and soil properties, derived from the Free-Air CO_2 Enrichment (FACE) experiments (Walker et al., 2014, 2019). This site provides a representative setting for testing the model's

performance in simulating photosynthesis and other key land surface processes under varying environmental conditions.

III. Background and Motivation

A. Computational Bottlenecks

The motivation for this work arises from the pressing need to improve the computational efficiency of photosynthesis simulations in ESMs. As models grow more complex and the demand for high-resolution, long-term simulations increases, the computational burden associated with these simulations has become a significant bottleneck. Reducing the number of iterations required in the numerical solver presents a promising avenue for mitigating this challenge.

In recent years, machine learning (ML) has emerged as a powerful tool for enhancing various aspects of Earth System Modeling. ML techniques, particularly neural networks, excel at identifying patterns in large datasets and making predictions based on those patterns. This capability makes ML an ideal candidate for improving the initial guess in numerical solvers, thereby reducing the number of iterations needed to achieve convergence.

B. Potential Paths Forward

Previous studies have explored the use of simpler statistical methods, such as multi-linear regression (MLR), to improve solver performance by refining the initial guess. While these methods have shown some success, they often lack the flexibility and accuracy required for more complex, nonlinear problems like photosynthesis. Neural networks, with their ability to capture complex, nonlinear relationships, offer a more robust alternative.

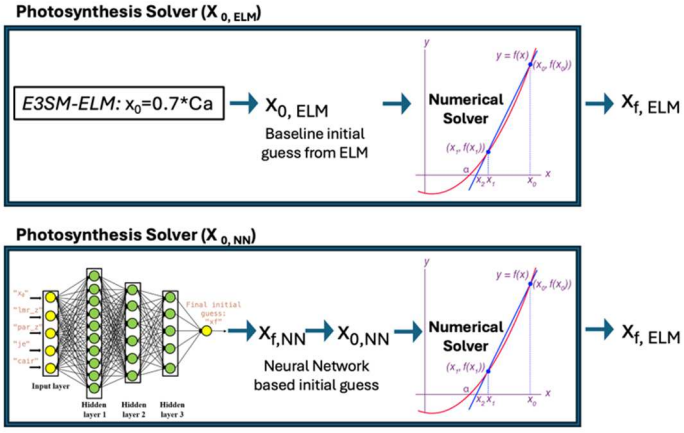

Fig. 3. Schematic Flow Diagram Comparing the Original and Neural Network (NN)-Based Initial Guesses for the Photosynthesis Solver. The top panel illustrates the process in the original ELM model, where the initial guess x_0=0.7×Ca is input into the numerical solver. After a certain number of iterations, the solver converges to the final solution x_f, denoted as $x_{f,ELM}$. The bottom panel depicts the process using the NN-based approach, where the output of the NN ($x_{f,NN}$) is used as the new initial guess ($x_{0,NN}$). This initial guess enters the same numerical solver, which then converges to the same final solution $x_{f,ELM}$ regardless of which initial guess was used. The key difference is that the NN-based initial guess is intended to be closer to the true final solution, thereby reducing the total number of iterations required by the solver.

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This study seeks to build on these earlier efforts by leveraging a large catalog of model simulations to train neural networks specifically designed to improve the initial guess for the photosynthesis solver in the ELM model (Fig. 3). By doing so, we aim to significantly reduce the computational cost associated with these simulations, making high-resolution, long-term simulations more feasible.

TABLE I. Table of Parameters for Leaf-level Simulations

Input / Output	Parameters used for Leaf-level Simulations		
	Parameter Symbol	*Parameter Name*	*Unit*
Input	x_0	initial guess of the solution	µmol $CO_2/m^2/s$
Input	lmr_z	leaf maintenance respiration rate	µmol $CO_2/m^2/s$
Input	par_z	par absorbed per unit LAI for canopy layer	W/m^2
Input	rh_can	canopy air relative humidity	-
Input	gb_mol	leaf boundary layer conductance	µmol $H_2O/m^2/s$
Input	je	electron transport rate	µmol electrons/m^2/s
Input	cair	atmospheric CO_2 partial pressure	Pa
Output	x_f	final value of the solution	µmol $CO_2/m^2/s$

The scale of the data involved in this work is substantial, with single-site simulations generating gigabytes of data and continental or global simulations potentially reaching terabytes in size. This large-scale data availability presents both a challenge and an opportunity. On one hand, it necessitates the use of advanced data management and processing techniques. On the other, it provides a rich dataset for training ML models that can generalize well across different scales and environmental conditions.

TABLE II. Table of Parameters for Canopy-Scale Simulations

Input / Output	Parameters used for Canopy-Scale Simulations		
	Parameter Symbol	*Parameter Name*	*Unit*
Input	t_veg_0	initial guess of the solution	K
Input	forc_lwrad	downward infrared (longwave) radiation	W/m^2
Input	forc_t	atmospheric temperature	K
Input	forc_u	atmospheric wind speed (east)	m/s
Input	forc_pco2	partial pressure of CO_2	Pa
Input	sabv	solar radiation absorbed by vegetation	W/m^2
Input	t_grnd	Ground surface temperature	K
Output	t_veg_f	final value of the solution	K

IV. Proposed Neural Network Based Initial Guess

In this section, we outline the approach of utilizing Neural Networks (NNs) to generate improved initial guesses for the photosynthesis solver in the ELM model. The method was applied at both the leaf level and the canopy scale, with the goal

of reducing the number of iterations required for the solver to converge to a final solution. By integrating NNs, which are trained on a large dataset of model simulations, we aim to enhance the efficiency of the solver by providing a more accurate starting point.

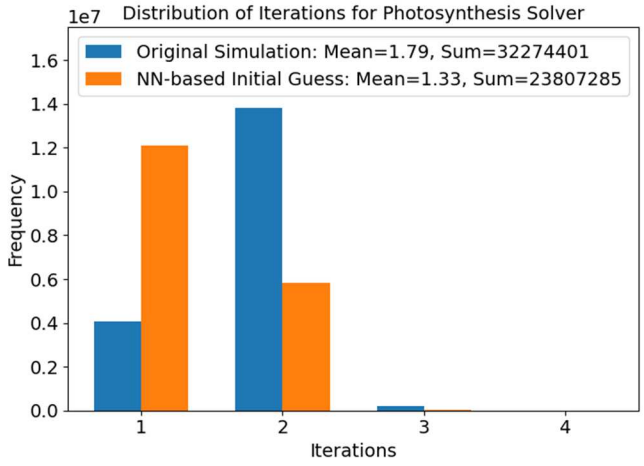

Fig. 4. Bar plots depicting the total number of iterations required for solving the photosynthesis model at the leaf level across different simulations. The "Original Simulation" category refers to simulations using the original model setup, while the "NN-based Initial Guess" category represents simulations utilizing a neural network-based initial guess for the photosynthesis solver. The data illustrate that simulations incorporating the NN-based initial guess generally require fewer iterations compared to the baseline approach.

A. *Leaf-level Photosynthesis Simulations*

At the leaf level, photosynthesis is modeled through a set of nonlinear equations that require an iterative solution. Traditionally, the ELM model uses an initial guess x_0=0.7×Ca, where Ca represents the internal CO_2 concentration of the leaf. This initial guess is then processed through a numerical solver that iteratively adjusts the solution until convergence is achieved at the final value $x_{f,ELM}$.

To improve this process, we developed a NN model that uses the inputs listed in Table 1. Included in the inputs is the original initial guess ($x_{0,ELM}$), which provides the NN with additional information that can be helpful in finding the final solution. The output of the NN model is the predicted final solution ($x_{f,NN}$), which is then used as the initial guess ($x_{0,NN}$) for the numerical solver.

B. *Canopy-scale Photosynthesis Simulations*

At the canopy scale, photosynthesis becomes increasingly complex due to the interaction of various environmental factors. In the ELM model, the canopy photosynthesis process is intricately linked to the transfer of energy within the canopy, which includes terms such as evapotranspiration, sensible heat flux, and temperature distributions within the canopy. Traditionally, the model approaches this by using an initial guess t_veg_0 derived from predefined physical equations, and then iteratively refines this guess until a final solution t_veg_f is obtained, which balances the energy transfer equations.

For the canopy-scale application, the NN model was trained using the inputs shown in Table 2. The NN's output is the predicted final solution $t\_veg_{f,NN}$, which is then used as the initial guess $t\_veg_{0,NN}$ in the solver. The solver, utilizing the NN-based guess, proceeds through its iterative process to arrive at the final solution t_veg_f, as it would using the original model-based initial guess. Although the NN-based approach showed promise in reducing the total number of iterations, further refinements in the network architecture and training data could potentially enhance performance at the canopy scale.

V. Reducing Total Iterations in the Solver

A primary goal of this study was to determine whether using a neural network (NN)-based initial guess could reduce the total number of iterations required by the photosynthesis solver in the ELM model. This section reports on the results of the analysis, and quantifies the reduction in the total number of iterations needed for each set of simulations.

A. *Reducing Leaf-level Solver Iterations*

Fig. 4 displays histograms comparing the total number of iterations required by the photosynthesis solver in the leaf-level simulations. The baseline simulation required a total of 3,227,440 iterations. When the NN-based initial guess was implemented, the total number of iterations was reduced to 2,380,728, resulting in a significant savings of 26.23%, demonstrating the effectiveness of the NN-based approach in improving computational efficiency at the leaf level. For both sets of simulations, most solutions required 1 or 2 iterations, but overall, the accumulated benefits of the NN-based initial guess had significant impacts to the overall efficiency of the solver.

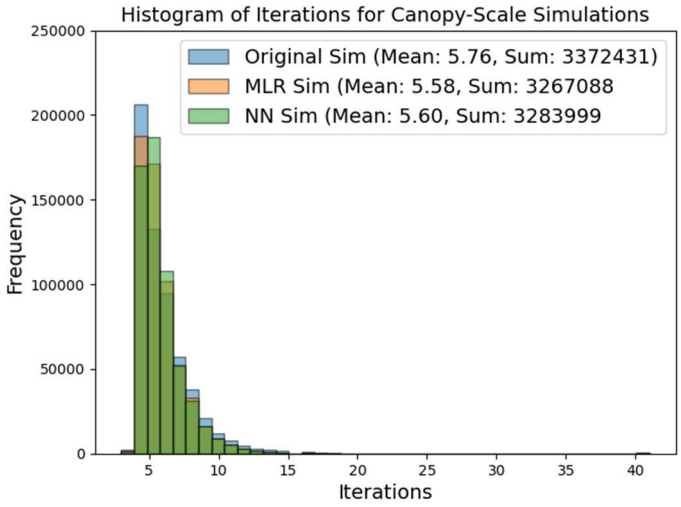

Fig. 5. Bar plots illustrating the total number of iterations required for solving the photosynthesis model at the canopy scale. The "Original" category denotes simulations using the original model setup, while "MLR" refers to simulations with a multi-linear regression-based initial guess, and "NN" indicates simulations employing a neural network-based initial guess. The results demonstrate that both MLR and NN-based initial guesses generally lead to fewer iterations compared to the original model simulations.

B. *Reducing Canopy-scale Solver Iterations*

Fig. 5 presents histograms of iteration counts for the canopy-scale simulations. The baseline simulation required 3,372,431 iterations using the original initial guess. The introduction of the

NN-based initial guess reduced this number to 3,283,999 iterations, yielding a savings of 2.62%. Interestingly, a multi-linear regression (MLR)-based initial guess provided an even greater reduction, with the total iterations decreasing to 3,267,088, corresponding to a 3.12% savings. These results indicate that while the NN-based approach is beneficial, the complexity of canopy-scale processes may necessitate further refinement of the NN model to maximize efficiency gains.

C. Percentage Reduction in Iterations

Table 3 summarizes the percentage reduction in the total number of iterations for both leaf-level and canopy-scale simulations. As shown, the NN-based initial guess yields a substantial reduction in iterations at the leaf level (26.23%), with modest improvements observed at the canopy scale (2.62%). The MLR-based initial guess provides a slightly better reduction at the canopy scale (3.12%). These modest improvements, reported based on our simulations for the historical period of ~150 years, can lead to significant computational efficiency for climate projection simulations that are often conducted in ensembles for 100-300 years in the future. These findings highlight the potential of NN-based methods to enhance computational performance in Earth System Models while also identifying areas for further research and optimization.

TABLE III. PERCENTAGE SAVINGS IN NUMBER OF ITERATIONS

Simulation	*# of Iterations*	*% Savings*
Leaf-Level		
Original	3,227,440	N/A
NN	2,380,728	26.23%
Canopy-Scale		
Original	3,372,431	N/A
MLR	3,267,088	3.12%
NN	3,283,999	2.62%

VI. POTENTIAL IMPROVEMENTS IN FUTURE WORK

This study demonstrates the capability of neural networks to reduce solver iterations in ELM, but several enhancements could further strengthen the approach. First, understanding the influence of individual features on prediction quality is crucial, and future work will include methods like Shapley values or sensitivity analysis to reveal the contributions of each input feature. Such insights could improve model interpretability and guide adjustments to enhance performance.

In addition, while this paper reports reductions in solver iterations as a percentage, future work will translate these savings into wall-clock time to provide a more direct measure of computational efficiency. This will involve a breakdown of computational resource usage, including memory and processing demands, to better capture the impact of iteration reduction on overall performance.

Although ELM does not use widely known heuristics for generating initial guesses, it does provide a default estimate (e.g., x_0=0.7×Ca for leaf-level photosynthesis). While our neural network approach has demonstrated improvements over this default, further comparisons with traditional heuristic methods, should they become available, will offer a more comprehensive benchmark.

Moreover, to address the relevance of this approach for Big Data applications, future work will apply this methodology to larger spatial and temporal scales. Expanding to higher-resolution simulations aligns this research with Big Data challenges, enhancing its applicability to exascale computing environments and complex, large-scale Earth system modeling.

Another area for improvement lies in the description of the neural network itself. A more detailed account of the network architecture, including its layers, activation functions, and training procedures, will be provided in future studies. This increased transparency will support reproducibility and help researchers understand the underlying mechanisms contributing to performance improvements.

At the canopy scale, the neural network achieved a 2.62% reduction in solver iterations, which was slightly lower than the 3.12% improvement achieved by multilinear regression. This difference suggests that canopy-level complexity may require more advanced model architectures or hybrid approaches. Future work will consider additional environmental factors, explore hyperparameter tuning, and potentially integrate more sophisticated network designs to address these challenges.

Lastly, the introduction of machine learning into numerical solvers presents potential challenges in robustness and generalization. Future studies will therefore include robustness testing across diverse datasets and environmental conditions to ensure the model's adaptability. These planned improvements will enhance the model's reliability, scalability, and utility for Earth system modeling at exascale computing scales.

CONCLUSIONS

This study explored the use of machine learning (ML) to accelerate the performance of the photosynthesis solver in the E3SM Land Model (ELM) by improving the initial guess required for iterative solutions. By implementing a neural network (NN)-based initial guess, we observed a significant reduction in the total number of iterations required at the leaf level, achieving a 26.23% savings. At the canopy scale, the NN-based approach also led to a reduction in iterations, though the improvement was more modest (2.62%), and a traditional multi-linear regression (MLR) approach yielded slightly better results (3.12%).

These findings underscore the potential of ML-based methods to enhance computational efficiency in Earth System Models, particularly in complex model parameterizations like the one used for photosynthesis simulations. While the NN-based approach was highly effective at the leaf level, the canopy scale results suggest that further refinement of the neural network model may be necessary to fully realize its potential in more complex scenarios. Overall, this work demonstrates a promising avenue for integrating ML techniques into the modeling workflow, offering new opportunities to optimize performance and reduce computational costs in large-scale climate simulations.

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