## A hybrid approach to improve Earth system model predictions of CH<sub>4</sub> emissions from northern peatlands

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**Focal Areas:** Application of AI-based surrogate modeling approaches; Earth system modeling; model optimization and calibration

Scientific and Technical Challenge: The accurate prediction of CH<sub>4</sub> emissions from northern peatland systems is crucial for understanding the role of terrestrial ecosystems and their feedbacks to the global carbon cycle. However, simulating CH<sub>4</sub> emissions is challenging as peatlands are complex ecosystems that contain a range of interacting processes including vegetation productivity and litter inputs, hydrology, microbial decomposition, and different pathways for the production and consumption of CH<sub>4</sub>. In particular, those interactions are nonlinear and vary strongly across space and over time. Meanwhile, global environmental changes (i.e. climate change and elevated CO2) add complexity to the CH<sub>4</sub> modeling. Capturing all variations and future climate scenarios into reliable peatland models of CH<sub>4</sub> fluxes is a challenge that needs to be addressed.

Rationale: There is a clear need for improved models to accurately predict CH<sub>4</sub> fluxes given the significant impact that these emissions can have on the global climate. Although there are a number of CH<sub>4</sub> observation sites, data from manipulative treatments are limited. The Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment introduced whole ecosystem warming and elevated CO<sub>2</sub> treatments into an ombrotrophic bog in northern Minnesota, and initial results have indicated strong increases in CO<sub>2</sub> and CH<sub>4</sub> fluxes with warming (Hanson et al., 2020). The warming response of CH<sub>4</sub> flux is highly sensitive to water table position, as evidenced by a 2021 drought that strongly reduces CH<sub>4</sub> emissions. It is currently unclear whether the results from SPRUCE are representative of other wetland systems, because the SPRUCE treatments take the system far beyond what can be determined from the range of natural variability at other sites (Helbig et al. 2022). Additionally, running model experiments with ELM-SPRUCE to cover large spatial domains or parametric uncertainty is computationally expensive. Our proposed approach uses AI methods to extend our peatland model ELM-SPRUCE to other wetlands using neural network-based surrogate modeling approaches. Our approach will provide high-resolution maps of CH<sub>4</sub> fluxes and their uncertainties over northern peatlands in North America under historical and future climate conditions.

## **Narrative:**

**Aim 1**: Develop a hybrid modular vegetation and hydrology framework in which we could replace expensive model components in ELM-SPRUCE with surrogate AI-based representations. Simulating GPP and canopy-scale fluxes requires an hourly or smaller timestep and requires a computationally demanding solution. We may use model output to train a neural network representation that can predict these fluxes at any desired temporal resolution as a function of meteorological drivers and 2 key model state variables: Soil moisture and leaf area index. This module may then be replaced with this surrogate model that is much faster to evaluate. A second surrogate model representation will be developed for predicting soil moisture, temperature, and water table position. Predicting these variables requires knowledge about past states and drivers, a recurrent neural network is likely a good choice for making these predictions. We could use an interpretable LSTM (iLSTM; Lu et al. 2022a) to incorporate these memory effects and to provide physical insights about key drivers. The two surrogate models may be connected to the physically based ELM model of vegetation allocation and turnover to predict LAI and litterfall. This submodel is computationally inexpensive and may be simulated at daily or greater timesteps. This combined modeling system would provide estimates of litterfall, nutrient demand and soil conditions for the decomposition model (Aim 2).

Aim 2: Develop physical and surrogate representations of decomposition and CH<sub>4</sub> models. We can use the standalone version of the Microbe model (Xu et al., 2015; Riccuto et al. 2021) that is currently connected to ELM-SPRUCE to predict CH<sub>4</sub> production through hydrogenotrophic and acetoclastic methanogenesis, oxidation, and flux to the atmosphere through plant transport, diffusion, and ebullition. The associated decomposition model will also estimate nutrient mineralization that can be coupled to the vegetation allocation model (Aim 1). It would be computationally feasible to perform a large ensemble of Microbe model simulations, capturing the impacts under a wide range of temperature and moisture conditions, soil carbon distributions, litter inputs, and parametric uncertainty on CH<sub>4</sub> fluxes predicted by the model. This large ensemble could be used to train a surrogate model. It is unclear which machine learning or AI method will work best for this surrogate model, and we might explore multiple methods considering both spatial and temporal properties of the simulated fields.

Aim 3: Model calibration and regional simulation. We can calibrate the hybrid model in Aim 1 coupled with the surrogate Microbe model in Aim 2 to obtain posterior parameter distributions for SPRUCE and AmeriFlux sites given CH<sub>4</sub> flux observations. We can use Markov Chain Monte Carlo (MCMC) to obtain these distributions and may also explore using invertible neural networks (Lu et al. 2022b) to improve the efficiency of the calibration process. Scaling the results to boreal North American peatlands can be done at high resolution using the Peat-ML product (Melton et al. 2022) or other similar products to define peatland areas and initial peatland carbon stocks. Downscaled DAYMET data is available for historical simulations, and we could also perform future simulations using downscaled outputs from CMIP6 Earth system models (Rastogi et al., 2021). Historical and future projections of CH<sub>4</sub> fluxes and their uncertainties could be made available to the broader community for further analysis.

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