Title: Improving Predictability of Methane Emissions from Terrestrial Ecosystems and Terrestrial-Aquatic Interfaces through Machine Learning Approaches

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Focal Area(s): This white paper addresses how artificial intelligence (AI) or machine learning (ML) algorithms can improve the predictability of and reduce uncertainties in methane (CH_4) fluxes by integrating complementary data collected at broad spatial and temporal scales (Focal Areas 3 and 4). We will also address how AI/ML approaches can transfer the knowledge gained from fine (microsite)-scale measurements to field-scale observations and regional- and global-scale budgets (Focal Area 5).

Science or Technological Challenge: We will focus on processes related to methane (CH_4) productions and consumptions in terrestrial ecosystems and terrestrial-aquatic interfaces. We will address several data-model integration challenges that directly support BER priorities in enhancing representation of ecosystem processes to improve predictive models. Process-based Earth System Models like E3SM lack representations of complex, non-linear processes related to hot-spots and hot-moments in CH_4 fluxes due to poor understanding of underlying mechanisms related to productions and oxidations of CH_4 (Xu et al., 2016). AI/ML approaches can be used to learn patterns in the data and model errors and use them to inform model structures and equations and correct process-based model errors. Complex, non-linear processes regulating CH_4 dynamics are difficult to unravel and represent in process-based models. Some such correlations may be spurious and not helpful to inform model structure, but AI/ML can help expand human understanding of predictor-response relationships across broad spatial and temporal scales, which, when combined with researcher knowledge, experience, and judgment, can increase our capability to glean insight from complex data. Thus, we can use AI to advance an integrated, robust, and scale-aware predictive understanding of interacting biogeochemical, hydrological and biophysical processes that enable developing a new paradigm for improved predictability of CH_4 fluxes.

Rationale: Narrowing uncertainty in the regional and global CH_4 budgets is essential for defining necessary policies for climate change mitigation. Significant challenges in reducing uncertainties in the regional and global CH_4 budgets arise from our incomplete understanding of different underlying processes related to production, consumption, and net fluxes of CH_4 from terrestrial and terrestrial-aquatic interfaces. AI-enabled predictability of methane emissions can close this research gap by cross-scale integration of measurements from multiple sources and disciplines. Insights obtained from laboratory-scale measurements (e.g., dynamics of methanogens or methanotrophs) can inform field-scale observations (e.g., methane fluxes at the biosphere-atmosphere boundary), which could explain patterns in remotely sensed measurements (e.g., the atmospheric concentration of CH_4 at the regional and global scale).

Narrative: The growing volume of data collected across multiple scales and disciplines offers opportunities to improve AI-enabled predictability of CH_4 fluxes from terrestrial and wetland ecosystems.

Use AI to synthesize automated methane flux measurements and high-frequency sensor data: Technological advances will allow quantification of CH_4 fluxes at sub-daily resolutions (*e.g.*, eddy-covariance data and automated chamber data for soil and ecosystem fluxes). Coupling these measurements with *in-situ* sensors for soil temperature and moisture can help us identify covarying patterns with seasonal variations and synoptic (i.e., intra-seasonal) oscillations in redox conditions. In 2018, AmeriFlux launched an "Action Theme Year" called Year of Methane (https://ameriflux.lbl.gov/year-of-methane/year-of-methane/), which brought together the CH_4 flux community to synthesize high-frequency measurements of CH_4 fluxes at the ecosystem scale across FluxNet sites (Knox et al., 2019). Parallel synthesis activities elsewhere resulted in comprehensive datasets of CH_4 fluxes from terrestrial ecosystems (e.g., boreal and arctic sites, Kuhn et al., 2021) and terrestrial-aquatic interfaces like coastal wetlands (e.g., see Coastal Carbon CH_4 working group, https://serc.si.edu/methane-working-group). Integrating AI/ML algorithms with these continuous measurements at the ecosystem scale and other community databases like COSORE can identify contributions of different ecosystem components (soil, plant) in the net fluxes of CH_4 at the biosphere-atmosphere interface (Bond-Lamberty et al., 2020; Megonigal et al., 2008).

Leverage multi-disciplinary data collected at various spatial and temporal scales to unravel competing mechanisms: Competing processes related to productions and consumptions (or oxidations) of CH_4 can regulate net CH_4 fluxes (Conrad, 1989). State-of-art techniques like isotope pool dilution (von Fischer et al., 2002) and gas push-pull technique (Urmann et al., 2005) are now available to separate net CH_4 fluxes in gross rates of productions and consumptions in the field. Omics data available from observational networks like MONET (Molecular Observation Network) and NEON (National Ecological Observation Network) can inform spatial variations in microbial functional groups related to CH_4 production (methanogens) and oxidation (methanotrophs) at the continental scale (Xu et al., 2015, Sihi et al., 2021b). Geochemical factors like redox-sensitive elements or alternative electron acceptors (e.g., iron) can further regulate net CH_4 fluxes by influencing the rates of anaerobic oxidation of CH_4 in ecosystems across broad environmental gradients (Blazewicz et al., 2012; Ettwig et al., 2016; Sulman et al., 2022; Teh et al., 2008; Zheng et al., 2019). Synthesis of knowledge obtained from laboratory-scale studies can further quantify the potential effects of microbial, geochemical, and biophysical (redox) processes on observed CH_4 fluxes in the field. Leveraging laboratory, field, and air-borne measurements across multiple DOE-funded projects (NGEE-Tropics/Arctic, AmeriFlux, SPRUCE, and COMPASS) can improve our understanding of CH_4 cycle processes in critical ecosystems. AI/ML algorithms can upscale these fine (microsite)-scale measurements of underlying processes to large-scale fluxes by integrating spatial heterogeneity of covarying factors. We expect that implementing explainable ML approaches into the MODEX (Model-Experimental Coupling) framework can improve prediction of hot spots and hot moments **(**Sihi et al., 2021a**)** and reduce uncertainty in regional (Zona et al., 2016) and global CH_4 budget (https://www.globalcarbonproject.org/methanebudget/).

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