**Title:** Toward spatiotemporally resolved methane emissions for modeling and upscaling research **Authors/Affiliations:** Housen Chu¹ (hchu@lbl.gov), Gavin McNicol², Qing Zhu¹, Avni Malhotra³, Camilo Rey-Sanchez⁴, David Durden⁵, Stefan Metzger⁵, ¹Climate & Division, Ecosystem Sciences Division, Lawrence Berkeley National Laboratory; ²Department of Earth and Environmental Sciences, University of Illinois Chicago; ³Biological Sciences Division, Pacific Northwest National Laboratory; ⁴Department of Marine Earth and Atmospheric Sciences, North Carolina State University; ⁵National Ecological Observatory Network, Battelle; ⁴Department of Atmospheric and Oceanic Sciences, University of Wisconsin–Madison

## **Focal Areas**

- Key uncertainties and knowledge gaps where new methodology, infrastructure, or technology can advance predictive understanding of the methane cycle.
- The importance of how the combination of data across spatial or temporal scales or scientific domains may lead to new scientific insights, either within or across fields.

# **Science or Technological Challenge**

Networks of eddy-covariance towers, such as AmeriFlux and FLUXNET, provide large datasets of ecosystem energy, water, and carbon fluxes, enabling upscaling from sparse observations to regional/global flux predictions<sup>1</sup>. Recently, the FLUXNET-CH4 initiative harmonized methane flux data from 81 sites, primarily wetlands, aiming to provide bottom-up upscaled methane fluxes<sup>2</sup>. While eddy-covariance data are recognized for their rich temporal information, their spatial dynamics are often overlooked and remain a primary source of uncertainties<sup>3–5</sup>. Briefly, the source area contributing to the flux at each time (i.e., flux footprint) varies depending on the effective measurement height, underlying surface characteristics, and turbulent state of the atmosphere. This spatiotemporal dynamic nature poses a critical challenge, particularly at sites with heterogeneous underlying sources/sinks such as wetlands. Hot spots and moments of methane emissions can form due to fine-scale variability driven by subsurface biogeochemistry, hydrologic gradient, salinity, nutrient availability, soil characteristics, vegetation types, and microtopography. The spatiotemporally dynamic footprints and sources/sinks jointly could lead to ~14%-25% biases<sup>6-8</sup> in area-integrated methane emissions and up to 83% in an extreme case<sup>9</sup>. While recognizing the spatiotemporal dynamics, it remains challenging to incorporate the footprint information into the modeling and upscaling framework.

## Rationale

Numerous research studies have attempted to address this "footprint" challenge, mostly in single-site studies with specific considerations of site characteristics and underlying processes. Attempts also varied regarding additional data requirements (e.g., chamber flux<sup>7</sup>, paired towers<sup>8</sup>, spatial surface characteristics<sup>5,6</sup>, wavelet-based flux calculation<sup>5</sup>) and core model types/structures (e.g., biophysical<sup>10</sup>, statistical model<sup>6,8,11,12</sup>, vegetation index-based<sup>13</sup>, machine learning<sup>5</sup>, hybrid approach<sup>4,5,14</sup>). While deemed promising individually, there have been limited attempts to benchmark the proposed approaches across sites, particularly for methane fluxes. We attributed the research latency to the following challenges. First, flux-decomposing research mostly began with pre-identified/hypothesized hot spots or spatial gradients. Yet, eddy-covariance flux data

contain rich temporal information reflecting a combination of complex and dynamic processes over different timescales. Thus, spatial flux information is masked and confounded by temporal variability, hindering spatially-explicit investigations. Second, the additional data requirements remain a significant hurdle. For example, very few eddy-covariance wetland sites have co-located, continuous, and representative chamber measurements<sup>15</sup> (e.g., over vegetation, soil, and open water) that help constrain or validate the flux decomposition. Also, fine-resolution (both temporally and spatially) surface characteristics, such as vegetation indices, surface temperature, and soil moisture, are rarely available. Third, most approaches require prior knowledge of the methane flux's controlling mechanisms, which might vary across wetlands or land cover types within the site, further complicating the generalization of approaches across sites. A few studies have proposed a machine-learning-based approach to derive environmental response functions, which combine observations, processes, and data mining to express the spatiotemporal flux<sup>4,5</sup>. This approach uses a universal model across a site's flux footprints and reconciles observed spatiotemporal dynamics based on temporal and spatial covariates. A hybrid approach was proposed, built upon this framework, to incorporate the machine-learned spatiotemporal dynamics into a process-based model<sup>14</sup>. It extracts multi-dimensional processes from the environment constrained by knowledge-based processes and creates georeferenced maps and process benchmarks for geostatistics, model evaluation, and upscaling.

## Narrative

We propose future synthesis to build a robust, scalable workflow to decompose methane fluxes measured using the eddy-covariance technique, producing the spatiotemporally resolved, debiased ecosystem methane emissions for modeling and upscaling research. Machine learning can help fill the workflow's technical and data gaps discussed earlier. First, a recent study proposed a simplistic approach to derive a hot spot flux map based mainly on eddy-covariance data<sup>16</sup>. The method can better identify and delineate potential hot spots and their flux contributions when paired with a knowledge-based land cover map. Machine-learning-based classification can be a surrogate or a means for accurate, fine-scale wetland land-cover classifications across sites<sup>17</sup>. Second, several new constellations of satellites, e.g., PlanetScope and HydroSat, are becoming available and shedding light on fine spatiotemporal surface characteristics in the foreseeable future. Machine-learning approaches can help generate robust downscaled, fine-resolution surface characteristics before the desired retrievals become available<sup>18</sup>. We also advocated future efforts to collect and synthesize chamber fluxes for providing ground-truth validation<sup>15</sup>. Third, while machine learning has demonstrated the potential to learn and simulate the spatiotemporal flux dynamics, many previous studies still adopted a process-based core model for decomposing the spatial fluxes. We suggested that machine-learning methods can serve as a data-exploring tool to detect relationships and interactions that help unveil new microbiological and biogeochemical processes. Further research should also explore the potential of a hybrid modeling approach, taking advantage of process-based and machine-learning models, attributing the spatial variability, and informing site design and validation studies.

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