#### Knowledge-based Artificial Intelligence for Agroecosystem Carbon Budget and Crop Yield Estimation

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July 3, 2023

#### Abstract

Improving the estimation of CO<sub>2</sub> exchange between the atmosphere and terrestrial ecosystems is critical to reducing the large uncertainty in the global carbon budget. Large amounts of the atmospheric CO<sub>2</sub> assimilated by plants return to the atmosphere by ecosystem respiration (Reco), including plant autotrophic respiration (Ra) and soil microbial heterotrophic respiration (Rh). However, Ra and Rh are challenging to be estimated at large regional scales because of the limited understanding of the complex interactions among physical, chemical, and biological processes and the resulting high spatio-temporal dynamics. Traditional approaches for estimating Reco including process-based (PB) models are limited by human knowledge resulting in limited accuracy and efficiency. Accumulation of the in situ observation of net ecosystem exchange (NEE), weather, and soil, and satellite data of GPP, LAI and soil moisture make it possible for applying data driven machine learning (ML) approaches. But the ML model approach has disadvantages of omission of domain knowledge and lack of interpretability. Here we propose a novel knowledge guided machine learning (KGML) method for predicting daily Ra and Rh in the US crop fields. With Gated Recurrent Unit (GRU) as the basis, we develop the KGML models constructing the hierarchical structure of ML with a mass balance constraint. The KGML models were pre-trained using synthetic data generated by an advanced agroecosystem model, ecosys, and re-trained with real-world FLUXNET observation data. We extrapolate the best KGML model to crop fields over the US with the help of satellite data, reanalysis climate forcings, and soil database to reveal the spatio-temporal variations and key controlling factors. We believe this study advances the interpretable machine learning concept for carbon cycle estimation and will shed light on many other process-based biogeochemistry research.

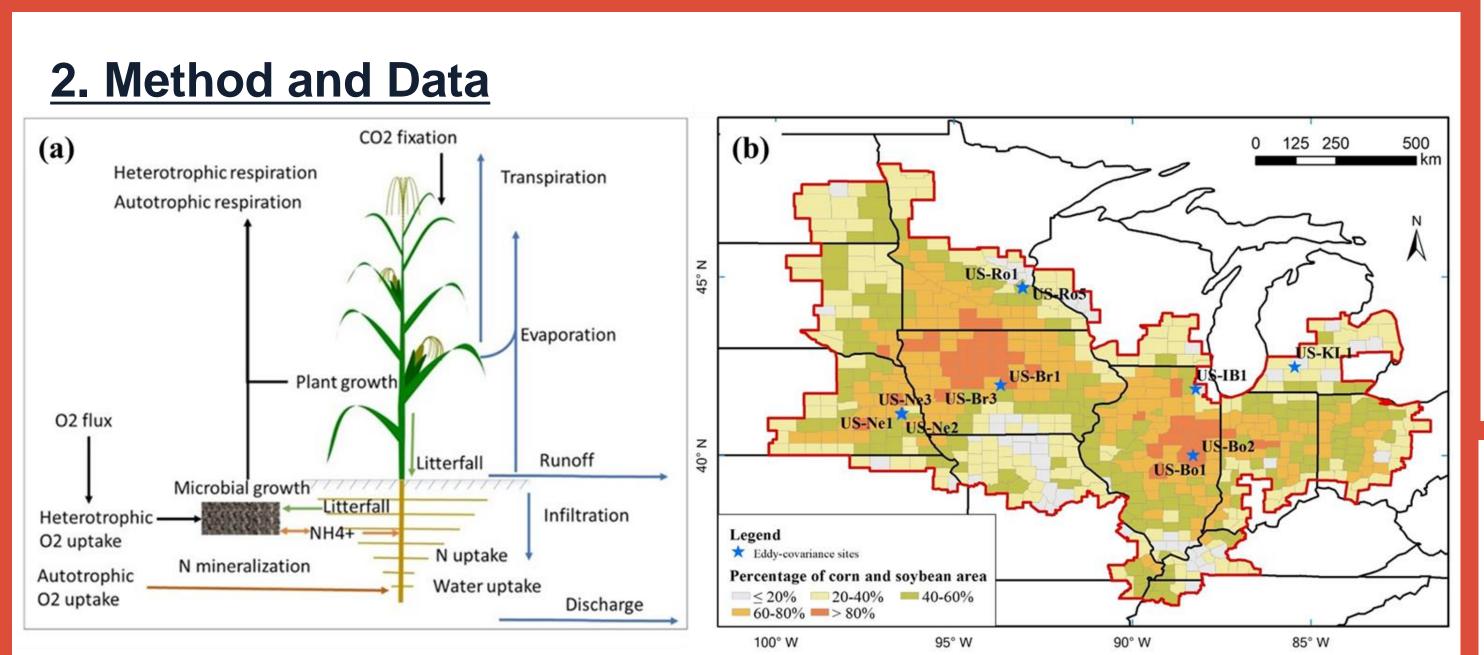
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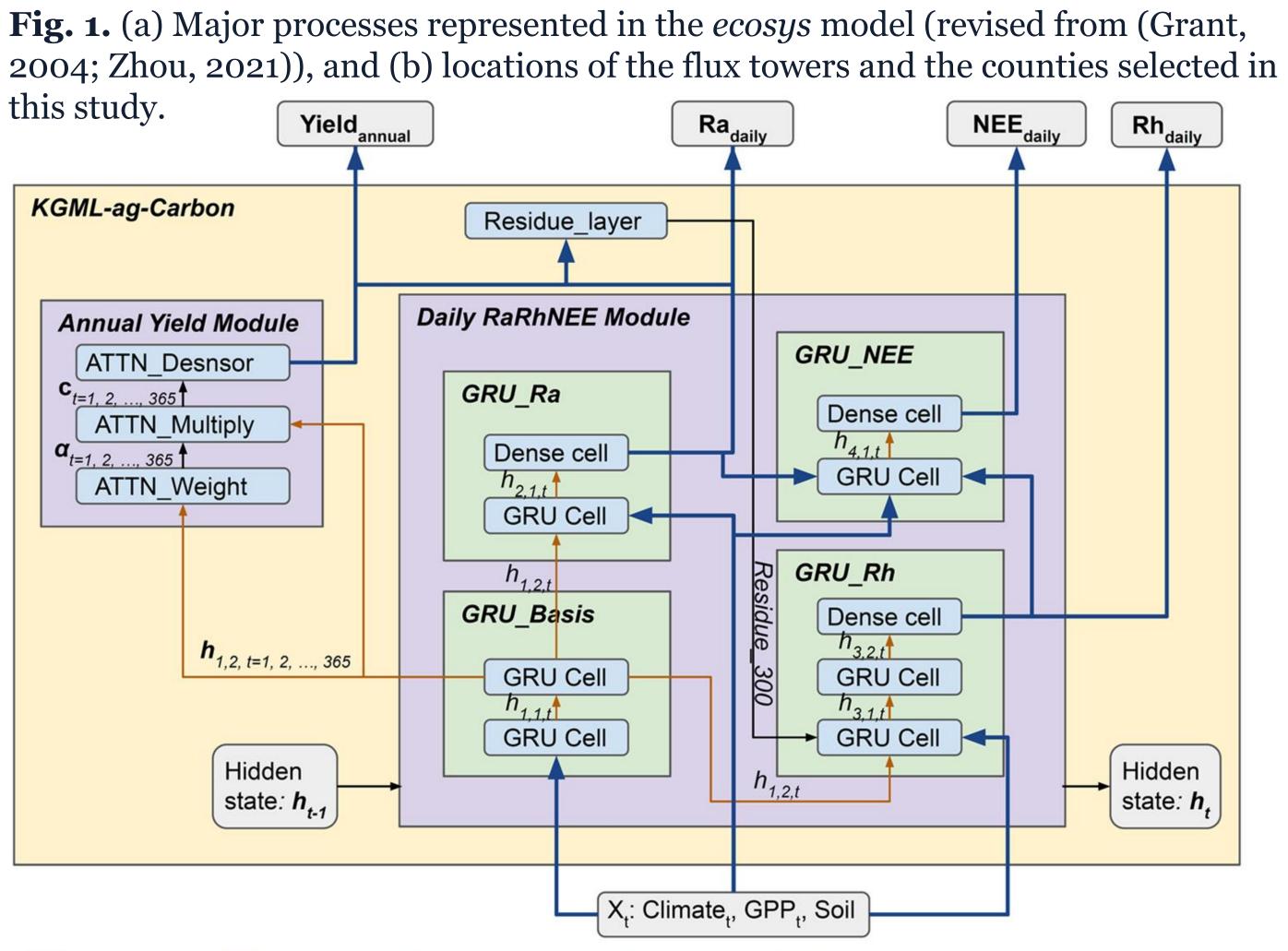
# Licheng Liu<sup>#</sup>, Wang Zhou<sup>#</sup>, Kaiyu Guan<sup>\*</sup>, Bin Peng, Chongya Jiang, Jinyun Tang, Sheng Wang, Robert Grant, Symon Mezbahuddin, Xiaowei Jia, **Shaoming Xu, Vipin Kumar, Zhenong Jin\***

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### **1. Introduction**

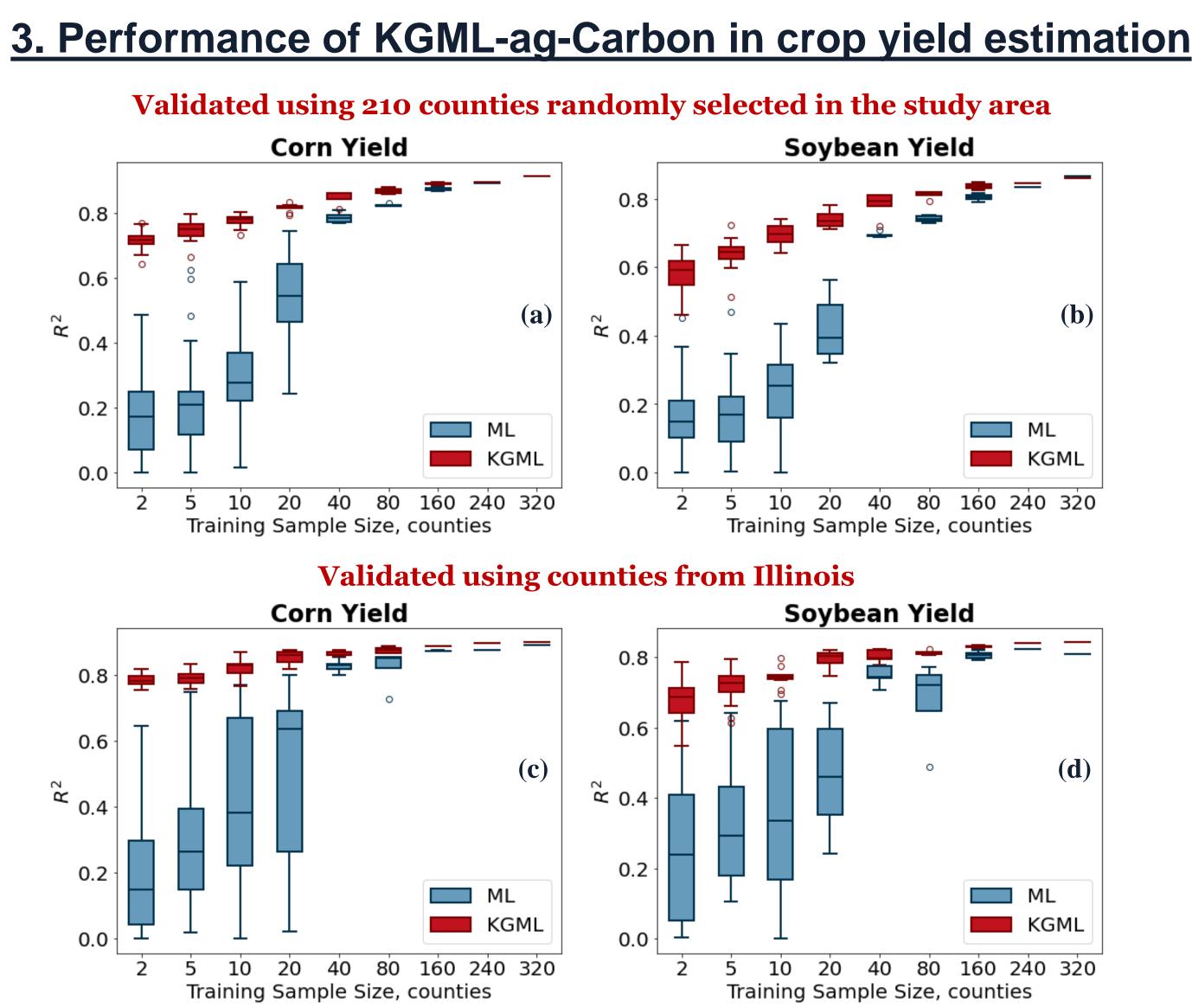
- Accurate estimation of carbon budgets is vital to assessing the climate change mitigation potentials of terrestrial ecosystems. Cropland carbon budgets play an important role in regional carbon budgets over cropland dominates the landscape such as the U.S. Midwest.
- However, there is still no reliable product on cropland carbon budget with high spatial and temporal resolutions over the U.S. Midwest.
- Empirical studies use flux tower observations to quantify different components of cropland carbon budget at local scale, such as net ecosystem exchange (NEE), but it is difficult to scale local observations up to regional scales.
- Process-based models can simulate individual components of cropland carbon budget, but are lacking effective constraints from observations.
- Although there is an increasing interest in leveraging recent advances in machine learning, capturing this opportunity requires going beyond the ML limitations, including limited generalizability to out-of-sample scenarios, demand for massive training data, and low interpretability due to the "black-box" use of ML
- To fill this gap, we used the knowledge-based artificial intelligence to integrated the advanced ecosystem model, ecosys, with a new remotely-sensed daily ecosystem gross primary production (GPP) observations to estimate the crop yield, ecosystem respiration (Reco), and NEE at field scale in the U.S. Midwestern cropland.





Input/output ML layer GRU submodule Module Model → Input/output transfer → *h* transfer with 20% dropout → Internal state transfer

**Fig. 2.** The structural of knowledge-based machine learning for agricultural carbon budget estimation (KGML-ag-Carbon) developed in this study. KGML-ag-Carbon model would be carefully trained by including knowledge constraints before regional extrapolation.



**Fig. 3.** The performance of KGML-ag-Carbon and pure machine learning (ML) in crop yield estimation. (a) and (b) were the model performance validated using 210 counties randomly selected in the study area for corn and soybean, respectively, and (c) and (d) were the model performance validated using the counties from Illinois for corn and soybean, respectively.

### 4. Carbon fluxes estimation over the U.S. Midwestern cropland

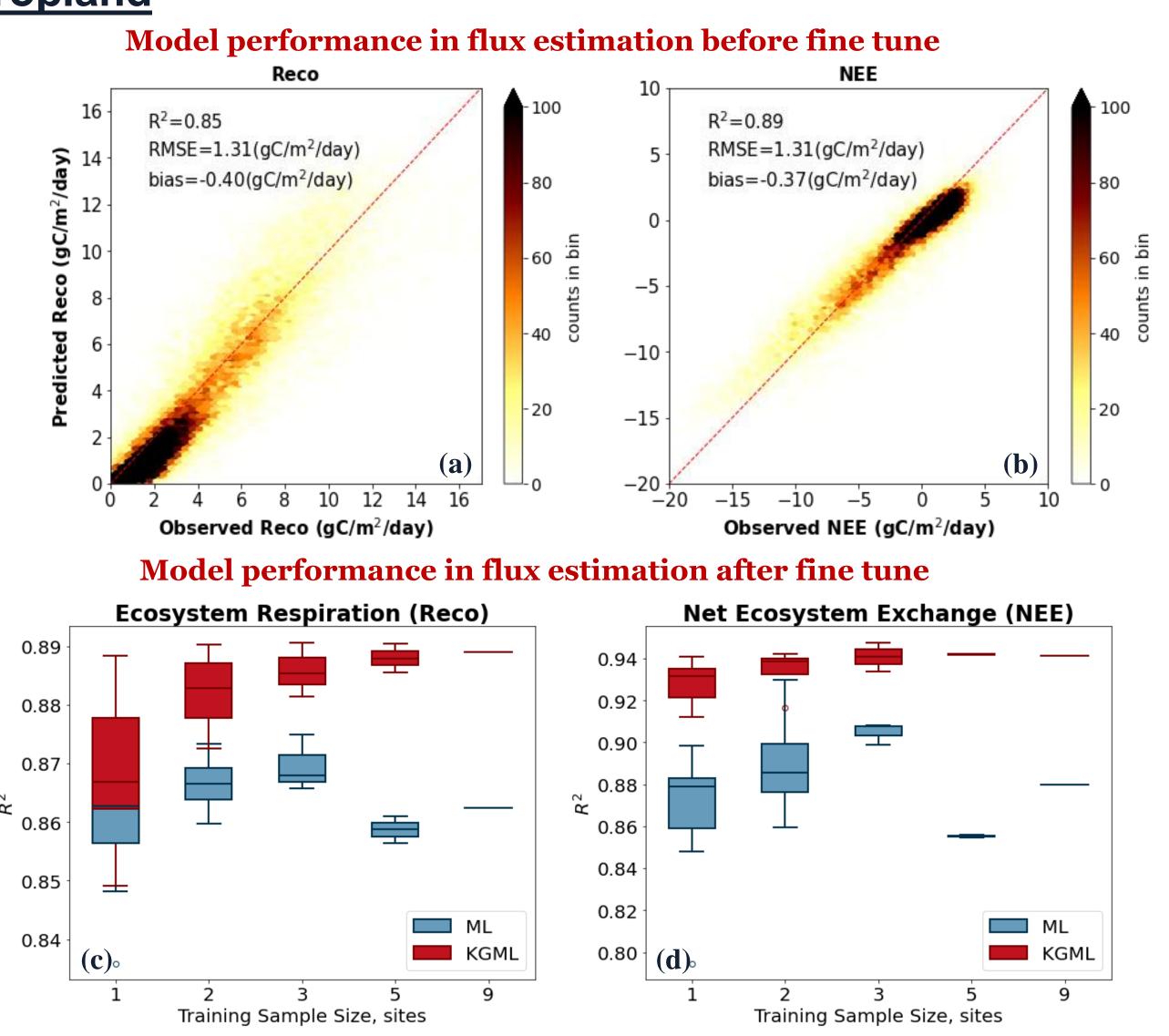


Fig. 4. The performance of KGML-ag-Carbon and pure machine learning (ML) in carbon fluxes (Reco and NEE) estimations. (a) and (b) were the KGML-ag-Carbon performance at 11 fluxtower sites before fine tuning, and (c) and (d) were the model performance for KGML and ML at US-Br1 and US-Br3 with different number of sites for fine tuning (or training), respectively.

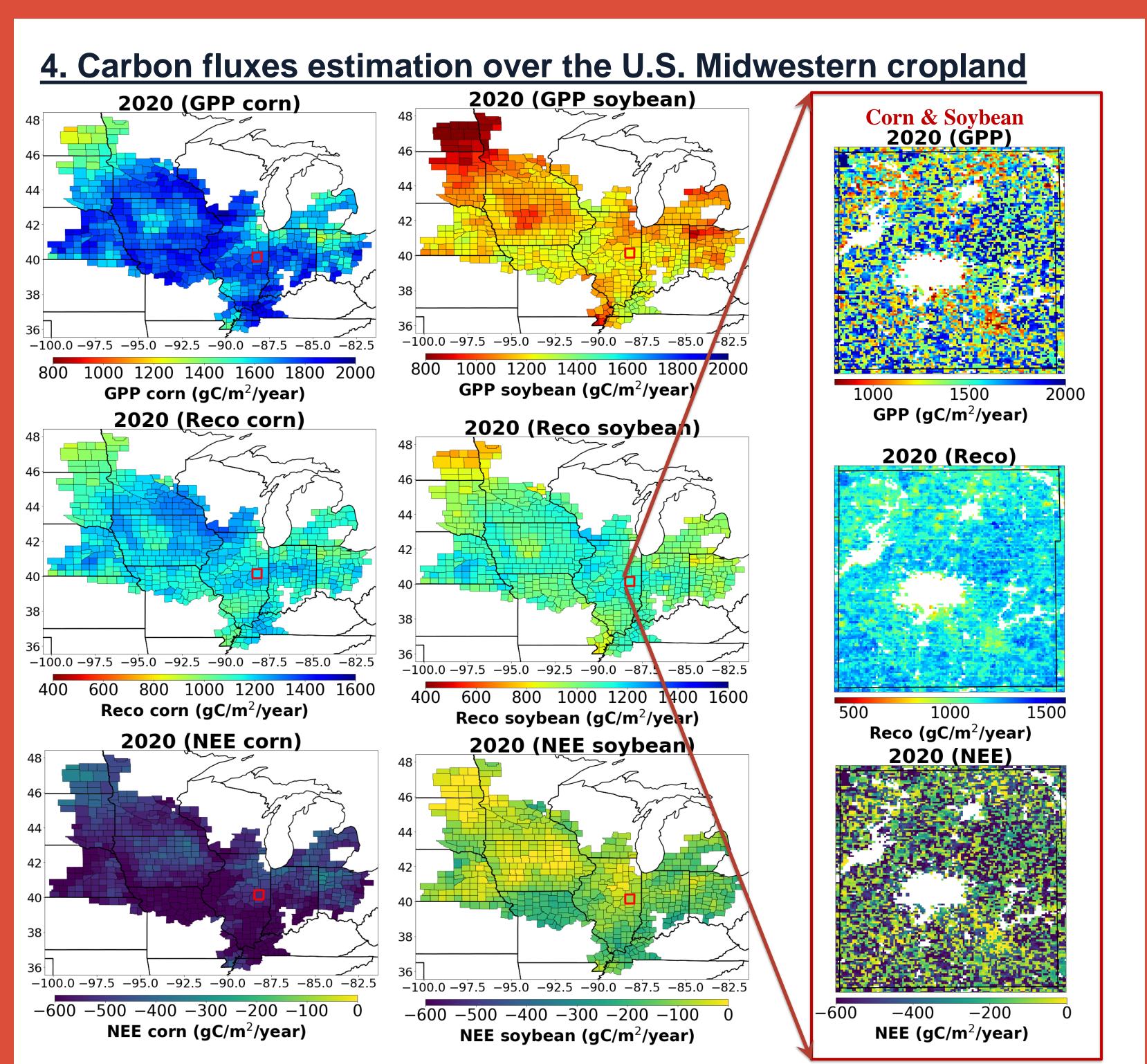


Fig. 5. An example of NIRv-based GPP and KGML-ag-Carbon estimated carbon fluxes (Reco and NEE) in 2020.

## **5.** Conclusion

- ecosystem model, and remotely-sensed GPP observations.
- cropland eddy-covariance sites in the U.S. Midwest.
- and temporal resolution

## 6. References and Acknowledgements

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Built an AI-based field scale carbon budget (Yield, Reco, NEE) estimation framework (KGML-ag-Carbon) by integrating knowledge-based artificial intelligence, advanced

Validated the performance of KGML-ag-Carbon in corn and soybean yield and carbon fluxes estimations using the crop yield from USDA NASS at county scale, and Reco and NEE at 11

An efficient and reliable tool to estimate crop carbon and detailed components in high spatial

It has potential to evaluate soil, climate and management influences on carbon credit in field level and therefore guide farmers and policy makers to make right decisions The final product can feedback to process-based model for calibration and testing

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