A scalable framework for quantifying field-level agricultural carbon outcomes

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Title: A scalable framework for quantifying field-level agricultural carbon outcomes

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Abstract:

Agriculture contributes nearly a quarter of global greenhouse gas (GHG) emissions, which is motivating interest in certain farming practices that have the potential to reduce GHG emissions or sequester carbon in soil. The related GHG emission (including N_2O and CH_4) and changes in soil carbon stock are defined here as "**agricultural carbon outcomes**". Accurate quantification of agricultural carbon outcomes is the basis for achieving emission reductions for agriculture, but existing approaches for measuring carbon outcomes (including direct measurements, emission factors, process-based modeling) fall short of achieving the required accuracy and scalability necessary to support credible, verifiable, and cost-effective measurement and improvement of these carbon outcomes. Here we propose a foundational and scalable framework to quantify field-level carbon outcomes for farmland, which is based on the holistic carbon balance of the agroecosystem: **Agroecosystem Carbon Outcomes = Crops (*C*) × Management (*M*) × Environment (*E*)**. Following a comprehensive review of the scientific challenges associated with existing approaches, as well as their tradeoffs between cost and accuracy, we propose that the most viable path for the quantification of field-level carbon outcomes in agricultural land is through an effective integration of various approaches (e.g. diverse observations, sensor/in-situ data, modeling), defined as the "**system-of-systems" solution**. Such a "system-of-systems" solution should simultaneously comprise the following components: **(1)** scalable collection of ground truth data and cross-scale sensing of crop conditions (C), management practices (M), and environment (E) at the local field level; **(2)** advanced modeling with necessary processes to support the quantification of carbon outcomes**; (3)** systematic Model-Data Fusion (MDF), i.e. robust and efficient methods to integrate sensing data and models at each local farmland level; **(4)** high computation efficiency and artificial intelligence (AI) to scale to millions of individual fields with low cost; and **(5)** robust and multi-tier validation systems and infrastructures to ensure solution fidelity and true **scalability**, i.e. the **ability of a solution to perform robustly with accepted accuracy on all targeted fields**. In this regard, we provide here the detailed scientific rationale, current progress, and future R&D priorities to achieve different components of the "system-of-systems" solution, thus accomplishing the Crop×Management×Environment framework to quantify field-level agricultural carbon outcomes.

1. Introduction

Agriculture contributes about a quarter of global greenhouse gas (GHG) emissions, with approximately 14% directly from agricultural activities and 10% through clearing land to create new croplands and pastures (IPCC, 2014). In many countries with intensified crop production, such as the U.S., GHG emissions associated with soil and fertilizer management contribute to more than half of the total agricultural emissions (Clark et al., 2020). Reducing these emissions is critical for limiting global warming to the Paris Agreement of 1.5 °C or 2.0 °C (compared to preindustrial levels), and requires rapid adoption of multiple and coordinated solutions (Bossio et al., 2020; Fargione et al., 2018; Searchinger et al., 2019; Wollenberg et al., 2016). Certain farming practices have the potential to favorably impact GHG emissions and soil carbon stocks, here defined as "**agricultural carbon outcomes**". Quantifying "agricultural carbon outcomes" associated with specific agricultural practices is a major research challenge. These practices, which largely overlap with "conservation agriculture" practices, are alternatively referred to as "regenerative agricultural", "climate-smart" or "carbon farming" practices. They include but are not limited to no-till, cover cropping, precision nitrogen (N) fertilizer management, biochar and compost application, enhanced mineral weathering, new crop rotations, and agroforestry (Beerling et al., 2020; Fargione et al., 2018; Paustian et al., 2016). The urgency in combating climate change and achieving sustainable development has spurred climate-pledges by individual companies to cut their carbon footprints (Pineda & Faria 2019) and stimulate the growth of agricultural carbon markets to incentivize farmers to adopt these practices (Stubbs et al., 2021). Accurate quantification of carbon emissions and carbon removal resulting from adopting various practices is the basis for emission reductions and carbon markets in industry and agriculture. However, the existing scientific literature is not yet conclusive as to where, when, if, and by how much these practices might lead to genuine GHG reduction or carbon removal (Bradford et al., 2019; Ranganathan et al., 2020; Smith et al., 2020).

While some may debate the effectiveness of these practices for GHG reduction and carbon removal, various public and private sector initiatives are driving substantial investment in policy and incentivization programs to motivate agricultural carbon outcomes, driven by strong political, investor, corporate, and consumer pushes in the European Union, the U.S., China, and other nations (Oldfield et al., 2022; Novick et al., 2022). It is thus more urgent than ever for the scientific community to develop robust and scalable strategies for the credible quantification of agricultural carbon outcomes. These estimates will form the basis for assessment of the climate mitigation potential of these practices, and guide investment in incentivization tools, and perhaps more importantly, to ensure the market rewards mitigation actions fairly and accurately.

Here, we propose that field-level quantification of agricultural carbon outcomes is not only fundamental to a trustworthy, transparent, and cost-effective agricultural carbon market, but also critical to any other sustainability-oriented program for ecosystem services. The existing literature has illuminated the scientific and technical issues related to the rigor of these assessments of carbon outcomes in agricultural land (Paustian et al., 2019; Smith et al., 2020), but actionable roadmaps and pathways to quantify field-level carbon outcomes are scarce. From the scientific perspective, existing approaches, such as direct measurement (e.g. soil sampling), emission factors, and process-based modeling, face fundamental challenges that prohibit them from achieving the accuracy, scalability, and cost-effectiveness demanded by the society (Bradford et al., 2019; Ranganathan et al., 2020; Smith et al., 2020). Given the growing demand for solutions to the climate crisis, the market is eager to rely upon existing and/or outdated quantification methods for rapid deployment without sufficiently considering their accuracy or scalability. This poses a major risk for large-scale public and private investment in agricultural carbon markets, as the credibility of these markets and the quantification of their outcomes is foundational to their success. Thus there is an urgent need to develop the right scientific tools for quantifying carbon outcomes in working lands, in order to minimize the risks of large-scale public and private investment in initiatives that do not provide actual climate benefits.

In this regard, we provide a framework for scalably quantifying field-level agricultural carbon outcomes that addresses many of the issues and uncertainty associated with the status quo approaches. Specifically, we first discuss the criteria for a successful quantification solution (Section 2.1), then propose a new framework to scalably quantify field-level agroecosystem outcomes (Section 2.2), and lay out the underlying disciplinary foundation (Section 2.3), followed by identifying the scientific challenges in existing approaches (Section 2.4). We then present a "System-of-Systems" solution for achieving the field-level quantification of agricultural carbon outcome in an accurate, cost-effective and truly scalable way (Section 3). Finally, in Section 4 we propose an R&D agenda that can substantiate not only agricultural carbon markets but also sustainable indicators for agroecosystem management.

2. A foundational framework to scalably quantify field-level carbon outcomes for agroecosystems

2.1 Criteria for a successful quantification technology for field-level carbon outcomes

Effective carbon quantification technology applied at the field level must be accurate, scalable, and cost-effective. "Field-level accuracy" is needed if individual farmland's carbon outcomes may be monetized in the carbon market; it is also required for traceability of any aggregated carbon outcomes in supply-chain quantification (e.g. SCOPE 3 emission). "Scalable" here means that the quantification solution must have an independently verified uncertainty measure across all possible locations; in other words, showing that a solution works well at a few demonstration sites, as many existing Measurement-Reporting-and-Verification (MRV) efforts do, is not enough. Instead, true "scalability" means one method must demonstrate an acceptable accuracy of the solution at randomly selected 'real-world' sites. Another benefit of "scalability" is the potential to map the benefits across the landscape, so investments can be prioritized in places they are most likely to succeed. Though some practitioners argue that aggregated-level accuracy is sufficient because carbon markets have buyers who mostly purchase carbon credits* in bulk, we argue that aggregated-level accuracy, which is almost impossible to validate, must come from field-level accuracy. Finally, for any technology, there is a tradeoff between cost and accuracy, and the desired solution should be sufficiently cost-effective to achieve the needed accuracy (See Section 2.4).

<u>* Here insert a knowledge box:</u>

Carbon Credits: the amount of the reduction, avoidance, or sequestration of CO_2 or GHG equivalent due to the adoption of new practices, compared to the "business-as-usual" scenario (Stubbs et al., 2021). "One carbon credit represents one tonne of CO_2 removed from the atmosphere or the equivalent amount of a different GHG (CO_2e)." (Oldfields et al., 2021) There are a few key criteria to ensure high-quality "carbon credit": permanence/durability (i.e. accrued reduction or sequestration should last for a sufficiently long time), verifiability (i.e. carbon credits should be verified by third party based on registry's protocols), and additionality (i.e. carbon credits are generated due to the change in practices or adoption of new practices).

In particular, "additionality" from the Greenhouse Gas Protocol (Ranganathan et al., 2004) is related to "whether the project has resulted in emission reductions or removals in addition to what would have happened in the absence of the project". Thus, the "additionality" requirement means that carbon credit is quantified as the difference of carbon outcomes between counterfactual scenarios (e.g., with and without cover crops for the same field) (Figure 0). To better explain this point, we use a hypothetical corn-soybean rotation field in the U.S. Midwest to illustrate "carbon credits" that can be derived by adopting cover crops with a ten-year commitment (Figure 0). In the "business-as-usual" scenario, this field experiences SOC loss over time as many other fields in the U.S. Midwest (Thaler et al., 2021). Adding cover cropping may not reverse the overall declining trend of SOC in most cases, but can slow down the rate of SOC decline (Qin et al., in review). The difference of the ΔSOC between these two scenarios is the real carbon benefit (i.e. carbon credit) that the system generates in a period.

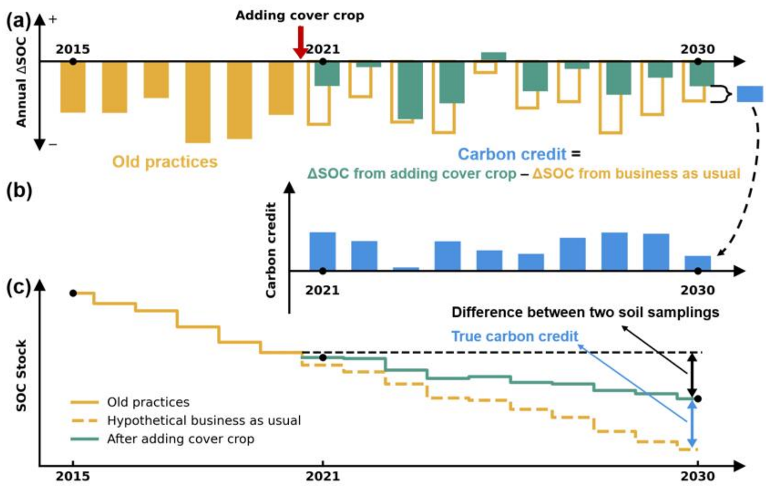

Figure 0. Illustration of the "additionality" concept for agricultural carbon credit, using a hypothetical corn-soybean rotation field in the U.S. Midwest as an example, assuming cover cropping is newly adopted in 2021 with a ten-year commitment. (a) Annual change in the SOC stock (i.e. ΔSOC) since 2015, with hypothetical scenarios from 2021 to 2030. (b) Generated annual carbon credit from 2021 to 2030. (c) Change in SOC stock over time.

2.2 A proposed framework of field-level carbon outcome quantification

Here we propose a foundational framework for the quantification of field-level carbon-related outcomes for farmland based on the holistic carbon balance of the agroecosystem, and captured in the following equation (Figure 1):

Agroecosystem Outcomes = Crops (*C*) × Management (*M*) × Environment (*E*) (Eq. 1).

Here, agroecosystem outcomes generically include crop productivity and various sustainability-related metrics (e.g. GHG emission, soil carbon sequestration, nutrient leaching); "agricultural carbon outcomes" refer to a specific group of agroecosystem outcomes that is related to the changes in GHG emission (including N_2O and CH_4) and/or soil carbon stock due to the change in agricultural practices. To calculate field-specific outcomes, three dimensions of information (***C***, ***M***, ***E***) as well as their interactions (i.e. two "×" in the equation) must be well represented at the field level. Specifically, ***E*** primarily refers to weather and soil information, which is often available as public, gridded products. However, these datasets may contain significant uncertainty at the field level (Potash et al., 2022; Zhou et al., 2022), and strategic soil sampling and local sensing may be needed to improve their accuracy. ***M*** primarily refers to farmers' management practices. Since certain "actions" determine the agricultural carbon outcomes, both monitoring and auditing of ***M*** are needed. The default methods to collect ***M*** information through farmer reporting are inefficient, error-prone, and leads to privacy concerns (Delay et al., 2020). Recent advancements in remote sensing and geospatial intelligence have unlocked an opportunity to generate accurate, unbiased, and verifiable estimates for ***M*** (see Section 3.1). ***C*** refers to location-specific crop information such as crop variety and interactions with ***M*** and ***E***, manifested in pheno-stages, maturity group, photosynthetic capacity, crop water use strategy, crop responses to stresses, etc. Obtaining ***C*** information at the field-level is extremely challenging, but missing this information and especially how ***C*** interacts with ***E*** and ***M***, can lead to large uncertainties in quantifying agroecosystem carbon credits (Figure 1b, also see Section 2.3). Finally, even when we have all the three types of information, the two "×" indicate that the outcome quantification requires us to quantify the interactions among ***C***, ***E***, and ***M***; and such quantification is usually achieved through process-based models (Section 2.4). Process-based models, in the current context of quantifying agroecosystem carbon outcomes, have also been referred to as "crop models" (more crop focused), "soil biogeochemistry models" (more soil focused), and "ecosystem models" (largely combining the above two). Despite a long history and rich literature, how to effectively use process-based models in field-level carbon outcome quantification remains unsettled in the scientific community (Riley et al., 2022ref), as existing approaches have large uncertainties (Section 2.3).

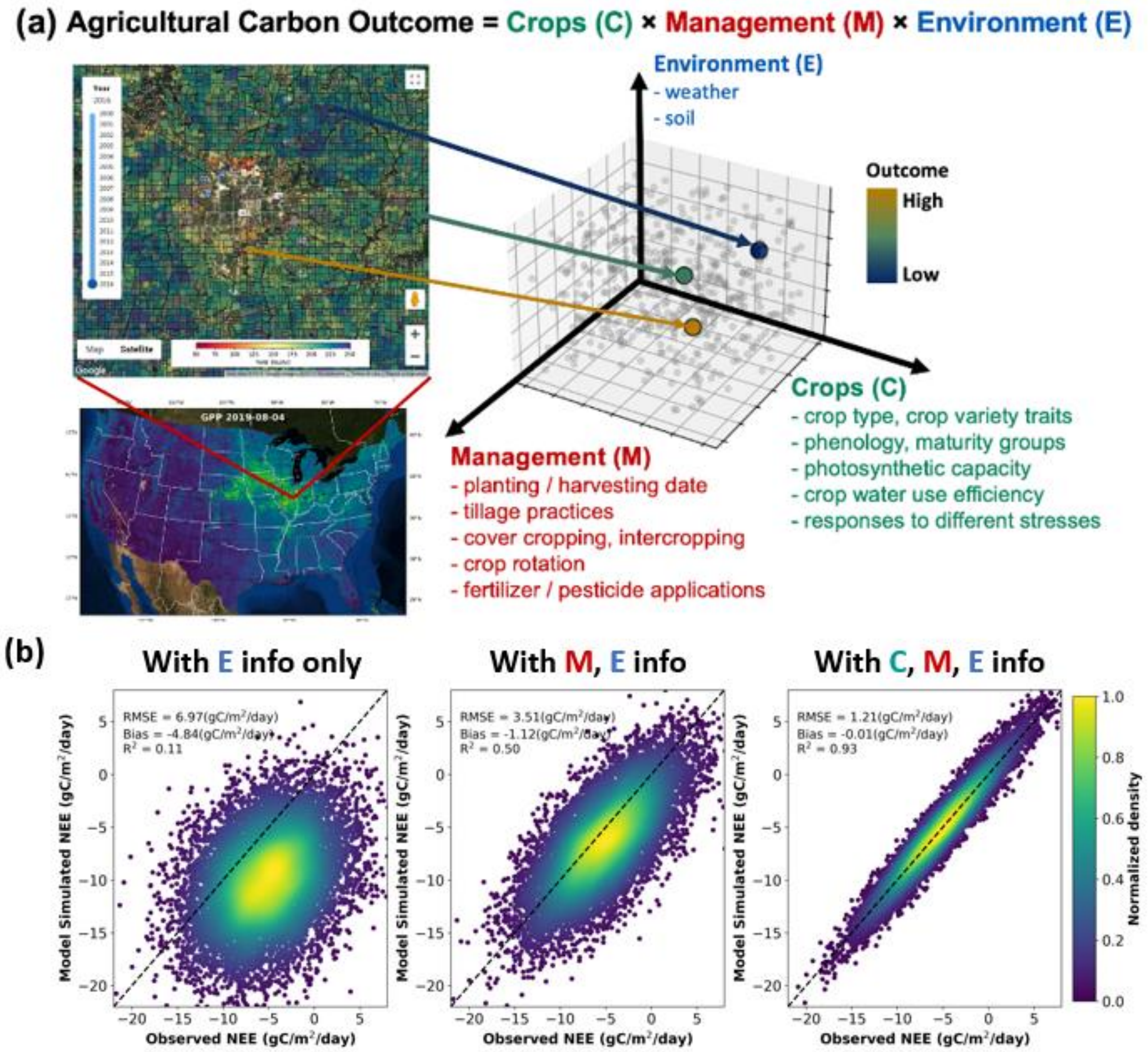

Figure 1. Conceptual diagram of quantifying agroecosystem carbon outcomes at the field level for agroecosystems. (a) Agricultural carbon outcome is determined by three factors, i.e. crop condition (***C***), management practices (***M***), and environment condition (***E***), as well as their interactions. (b) Accuracy of the quantification methods improves significantly as more information is constrained at the field level. The example shown here focuses on quantifying net ecosystem exchange (NEE), which is the net CO_2 exchange between land and atmosphere that can be measured directly with the eddy-covariance flux tower sites in the U.S. Midwest (Zhou et al., 2021a); the three scenarios refer to: (left) only using E information (i.e. weather and soil) as input in the carbon outcome quantification, (center) using both M (i.e. field-level management practices) and E information for the carbon outcome quantification, and (right) using C (i.e. photosynthesis, yield, leaf area index), M, E information together to drive or constrain the model.

2.3 A holistic view of farmland carbon balance and their connections to the GHG emissions - the disciplinary foundation for field-level carbon outcome quantification

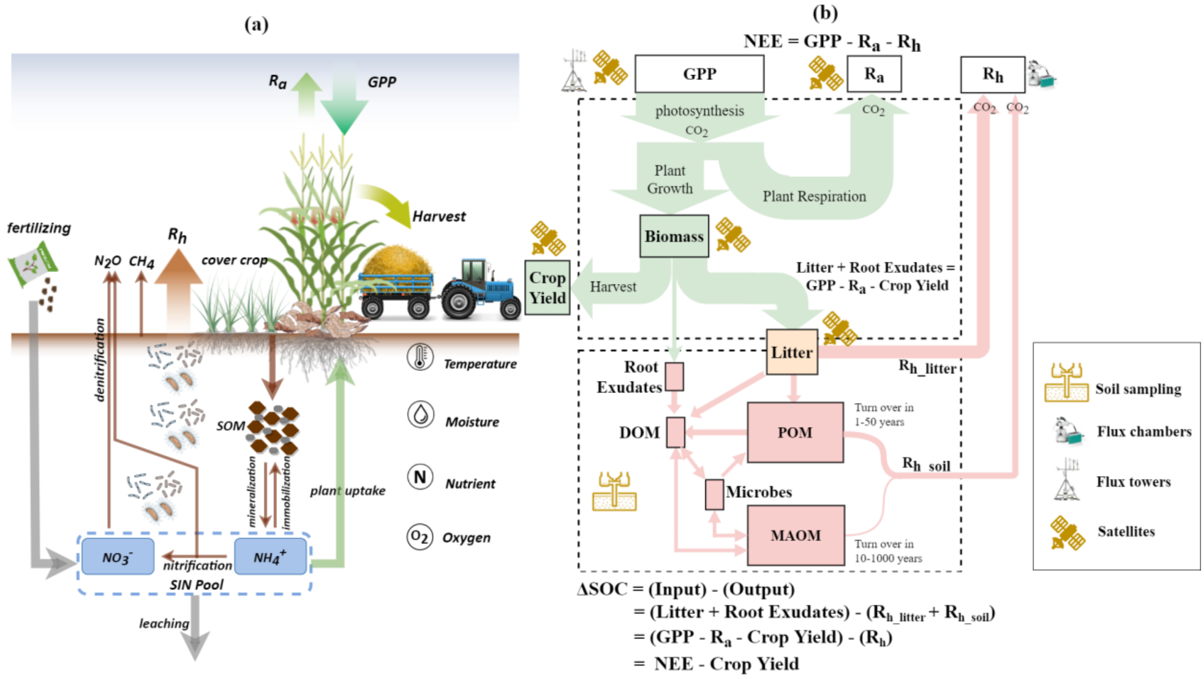

Figure 2. The holistic carbon and nitrogen balance and its linkage with greenhouse gas emissions over annual row cropping farmland (a) and a mass balance based approach to quantify the change of soil organic carbon (SOC) (b). GPP: gross primary productivity; Ra:autotrophic respiration; Rh: heterotrophic respiration; NEE: net ecosystem exchange; DOM: dissolved organic matter; POM: particulate organic matter; MAOM: mineral-associated organic matter.

A holistic perspective on farmland carbon balance is the foundation for carbon outcome quantification (Figure 2). From a systems perspective, the change of carbon storage in the system is determined by the mass balance of input and output carbon fluxes (Zhou et al., 2021a; Smith et al., 2008). Specifically for annual row cropping systems, soil organic carbon (SOC, note that litter is generically included in SOC here) is the only carbon storage pool, as other carbon pools from plants will be harvested at the end of growing season. For typical soils in farmland, carbon input is entirely from plant litter, including both aboveground and belowground litters and root exudates (Preece & Peñuelas, 2020; Williams et al., 2022). Addition of carbon through manure, composts, and biochar also contributes to the carbon input when they are applied. The carbon output is primarily heterotrophic respiration (Rh) from soil, with minor mass contribution from methane emission, dissolved organic matter (DOC) and dissolved inorganic carbon (DIC) leaching, photodegradation and soil erosion. At the annual scale, carbon input (i.e., plant litter and root exudates) can be calculated by plant photosynthesis (drawing CO_2 from atmosphere to plants) minus plant autotrophic respiration and harvested yield (or biomass), i.e. Litter + root exudates = GPP - Ra - Crop Yield (at annual scale) (Bernacchi et al., 2005). The carbon output (i.e., Rh) is controlled by a cascade of microbial decomposition of plant litter and transformation of different SOC pools with different residence times. Therefore, at the annual scale or longer term for annual row crops, the change of SOC (ΔSOC) can be quantified using the carbon mass balance approach as (Figure 2b):

$$
\begin{aligned}
\Delta SOC &= (Input) - (Output) \\
&= Litter - (Rh\_litter + Rh\_soil) - \xi \\
&= (GPP - Ra - Crop\ Yield) - Rh - \xi \\
&= - NEE - Crop\ Yield - \xi \qquad \text{(at annual scale)} \qquad \text{(Eq. 2)},
\end{aligned}
$$

in which - NEE = GPP - Ra - Rh, and ξ is the carbon leakage including CH_4 emission, DOC and DIC leaching from the field (ξ is a much smaller term compared with others in Eq.2, and in most cases can be neglected, though sometimes not). All the terms above are aggregated terms at the annual scale. Based on the definition of Chapin et al. (2006), NBP = - NEE - Crop Yield - ε, where NBP is net biome productivity. Eq. 2 is thus only valid at annual scale or longer time scales, when NBP can be used to approximate ΔSOC for annual cropping systems (≥annual scale). Biomass harvested besides Crop Yield is not common and rare in the U.S. Midwest row crop systems, and here we included it in the generic "Crop Yield" term. For agricultural soils, both carbon input and output vary from field to field due to the intrinsic heterogeneity embedded in ***C***, ***M***, ***E*** conditions, and accurate quantification of both carbon input and output at the field level is thus required for field-level carbon outcome quantification.

SOC dynamics can mediate emissions of other GHGs (N_2O and CH_4) from agricultural soils through several mechanisms (Figure 2a). Methanogenesis and many of the microbial processes responsible for N_2O production, such as denitrification (Butterbach-Bahl et al., 2013), represent heterotrophic metabolisms that rely on SOC as an energy source and a carbon source for biosynthesis. The decomposition of soil organic matter also plays an important role in supplying inorganic N as a substrate to fuel nitrification and denitrification, the two major N_2O source processes in agricultural systems (Figure 2a). Even in fertilized agricultural systems with large inputs of exogenous inorganic N, mineralization of organic N contained in SOM can continue to endogenously supply NH_4^+ for plant and microbial use (Mahal et al. 2019; Daly et al. 2021). Nitrogen mineralization rates are controlled largely by the C:N ratio of SOM (Booth et al. 2005, Yang et al. 2017a), with microbes excreting NH_4^+ into the soil when the C:N ratio of SOM is below-microbial stoichiometric requirements. As such, N_2O emissions tend to be higher in agricultural systems that generate low C:N ratio plant residues that decompose in the field, such as leguminous cover cropping systems (Basche et al. 2014). Soil oxygen consumption during SOM decomposition can also mediate N_2O and CH_4 emissions via the formation of anoxic soil microsites conducive for anaerobic processes, such as methanogenesis, denitrification, and dissimilatory nitrate reduction to NH_4^+ (DNRA), even in non-flooded soils (von Fischer and Hedin 2007; Yang et al. 2016; Yang et al. 2017b). These anaerobic processes can therefore be more important where higher quantity and quality SOC supports faster SOM decomposition rates (Parkin

1987), particularly when soil aggregation and high soil moisture limit the diffusive re-supply of oxygen into soil (Silver et al. 1999, Sey et al. 2008). Given that higher quantity and quality SOM can potentially lead to greater N_2O and CH_4 emissions through these distinct mechanisms, it is important to account for how SOC influences soil emissions of these other GHGs to capture fully the carbon outcomes of different agricultural systems and practices.

2.4 Issues in the existing quantification methods

Based on the above framework and disciplinary foundations, we can identify shortcomings of existing carbon outcome quantification methods, including: (1) direct measurements, such as soil sampling for SOC change (Norman & Allison, 1965; Smith, 2006; Wendt & Hauser, 2013), and eddy-covariance sensors to measure GHG emissions (Baldocchi et al., 2001; Baldocchi et al., 1988); (2) emission factor estimation, in which a fixed linear factor is used to approximate "carbon outcomes" based on different management practices (IPCC, 2019); and (3) process-based modeling (Ogle et al., 2010; Sándor et al., 2018).

Direct measurements have long been the primary tool for quantifying carbon outcomes, although they are in general cost-prohibitive and thus not scalable. Direct measurements, such as using soil sampling to measure changes in SOC storage or using eddy-covariance flux towers to measure carbon fluxes (e.g. photosynthesis and respiration), have significantly advanced our understanding of carbon cycling in the agroecosystems (Kucharik et al., 2001; Luo et al., 2017; Zhou et al., 2021a). However, it is impractical to collect direct measurements for every field due to the high financial and labor costs. As a mature technology, laboratory-based optical and Fourier transform infrared spectroscopy has significantly reduced the soil carbon testing cost (Gholizadeh et al., 2013; Margenot et al., 2016; Sanderman et al., 2020; Sanderman et al., 2021) and has been promoted by Global Soil Partnership of the UN Food & Agriculture Organisation (Shepherd et al., 2022). Meanwhile, emerging technologies such as in-situ spectroscopy (Wijewardane et al., 2020) or geophysical measurements (Doolittle & Brevik, 2014) can reduce sampling cost, but their accuracy is significantly lower than classical laboratory tests, thus limiting their potential utility. Directly using satellite or other remote sensing techniques (either multispectral or hyperspectral) to measure SOC carries some promise (Wang et al., 2022), but remains challenging in real field environment, due to the limitations including: (1) remote sensing data only detects surface-level soil carbon, not the whole soil profile (Jobbágy & Jackson, 2000); and (2) even for surface-level soil carbon estimation, crop residue and soil moisture have a large confounding impact on spectral signals, thus making the estimation of bare soil surface carbon concentration difficult in practice (Wang et al., 2022). Additionally, spatial variation within any given field can be larger than year-to-year changes in SOC, contributing to substantial uncertainty inherent in direct measurement of SOC stock (Maillard et al., 2017) (Figure 3). This makes soil sampling unfeasible as a short-term (i.e. annual) quantification method but rather one that sets the baseline (i.e. measure initial SOC stock) or periodic verification after 5+ years of practice changes (Smith 2004).

Moreover, direct measurement can not simultaneously measure changes in SOC under a practice change vs a counterfactual business-as-usual scenario, but both are needed for estimating carbon credits by definition (Figure 0). Direct measurements may be useful when paired experiments are properly implemented in the same field – an approach which has not historically been adopted by market systems. Using the cover crop adoption as an example (Figure 0), the "additionality" criterion for carbon credits requires us to know the SOC stock in the two scenarios, one with newly adopted cover cropping in which SOC stock can be directly measured, and the counterfactual scenario for "business-as-usual" in which SOC stock can no longer be measured directly, but can only be estimated through modeling. Because soil sampling cannot measure ΔSOC that involves a hypothetical "business-as-usual" scenario, the standard methods for assessing carbon credits are actually not able to directly quantify the realized carbon benefits (e.g. carbon credit). This issue also applies to other direct measurements (such as eddy-covariance flux measurements), as the "carbon credit" quantification always requires counterfactual scenarios for calculating the difference, and agricultural practice inevitably has such a challenge unless farmers are willing to carve out part of their field for two different practices to create the counterfactual scenarios.

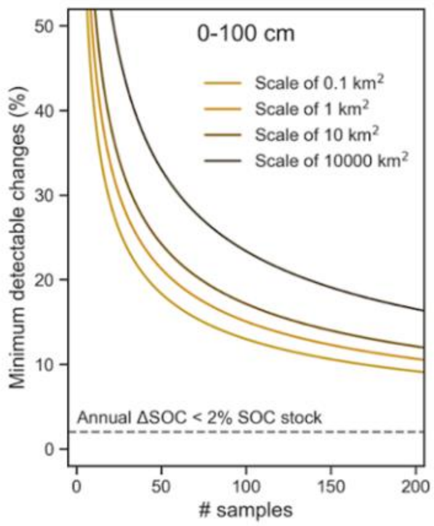

Figure 3. Soil sampling accuracy (i.e. minimum detectable change, in terms of relative change in the SOC stock) as a function of the number of soil samples and field sizes, which is much larger than the annual change of SOC stock in reality (Maillard et al., 2017).

Emission factor methods are the most widely used approaches in past IPCC reports (IPCC, 2019) and also the easiest method to use. While useful for large-scale carbon emission accounting, they suffer from the inability to capture spatial and temporal heterogeneity of ***E*** and ***C*** and cannot comprehensively track the dynamics embedded in the interactions between ***E***, ***C*** and ***M***. The assumption of the same (or a linear scaling of) emission or sequestration outcomes based on a particular "action" (***M***) across different fields is not only inaccurate, but may also disincentivize farmers from participating in a carbon market. Emission factor methods also assume constant crop conditions (***C***), while interannual/decadal variability in ***C*** could be significant. Emission factor methods thus can not be used for field-level carbon outcome quantification. For some recent efforts of applying process-based modeling to generate emission factors for more granular spatial and temporal scales (Cui et al., 2021; Wang et al., 2020), we treat that approach as "process-based modeling" in the next section.

Process-based modeling has been regarded as the most mechanistic method to quantify carbon outcomes. Since process-based models can simulate "business-as-usual" scenarios and other counterfactual scenarios, this approach arguably addresses the counterfactual issues of the direct measurement approach laid out above (Figure 0) and can allow direct calculation of the actual carbon benefit. Although there has been an increase in the use of process-based modeling as the main approaches to quantify agricultural carbon outcomes (e.g. Verra VM0042 and Climate Action Reserve Soil Enrichment Protocol) (Verra, 2020; CAR, 2022), existing modeling approaches have various critical gaps to address, especially related to the absence of necessary processes (see detailed discussion in Section 3.2) and the lack of constraints to reduce uncertainties in model parameters.

As to the latter point, few existing process-based models include observational constraints, especially when applied to locations beyond calibration/validation sites. The performance of process-based models is ultimately determined by two groups of parameters, i.e. **process-specific** and **location specific parameters**. **Process-specific parameters** usually do not vary over space and time (e.g. the maximum microbial denitrification rate, gaseous and aqueous diffusivities of O_2, and the energy yield of aerobic respiration), therefore can be obtained through calibration and validation based on extensive lab or field experiment data. In contrast, **location-specific parameters** vary at different locations. Location-specific parameters are fundamental to the scalability of process-based models. For example, photosynthetic capacity is a variable that is spatially and temporally variant with a key control on the photosynthesis process, unfortunately such a major carbon-related process is missing in most process-based models currently used for agricultural carbon quantification. For the limited number of models that include this photosynthetic process explicitly, they are still using crop-specific or even plant-functional-type-specific values of photosynthetic capacity (i.e. maximum carboxylation rate; Vc,max) given a lack of spatial information; using a uniform photosynthetic capacity in space and time (the common practice for now) can lead to 21% error in estimating photosynthesis (Luo et al., 2019). More broadly speaking, **location-specific parameters** also include local information of model inputs, such as weather, soil properties, and management practices at the field level, without which the field-level accuracy is impossible to achieve. The lack of location-specific information for both model input and model constraints thus is the largest uncertainty in quantifying field-level carbon outcomes (Figure 1b).

We also need to be cautious of "infinite model improvement", which is common among academicians. We agree that any model used for operational carbon outcomes quantification should have necessary complexity and processes (see more discussions in Section 3.4), and theoretical advances in science should be ultimately incorporated into existing models to improve representations of relevant processes. However, we need to acknowledge that models with more detailed mechanistic representations are not always better than simpler models in practice. When evaluating the appropriate model structures for agricultural carbon outcomes, we should focus on two fundamental questions: (1) Is a specific process indispensable for simulating the specific outcome and also achieving the desired accuracy? (2) Is there sufficient data to parameterize that specific process at both field and regional scales? If the answer to either question is no, then including the new process may not necessarily benefit the quantification of carbon outcome for now.

3. "System-of-Systems" Solutions represent the most viable pathway

For any technology used for carbon outcome quantification, there is a tradeoff between cost and accuracy (Figure 4). Although no clear criterion has been established so far to accept or reject a technology, for any quantification technology to be scalable, its per-acre operational cost must be meaningfully lower or significantly lower than the expected monetized carbon values from adopting climate-smart practices. In the current U.S. agriculture carbon market with a carbon price of roughly US \$20/t CO_2e, for example, this criterion, based on the DOE ARPA-E estimation (DOE ARPA-E: DE-FOA-0002250, 2020), means costs should be significantly lower than \$10/acre/year for soil carbon and \$50/acre/year for N_2O quantification for large-scale deployment, including installation, calibration, operation, and hardware lifetime and at the same time, the technology should be able to achieve less than 20% error at the field level (DOE ARPA-E: DE-FOA-0002250, 2020). No single existing technology can meet both of these expectations. Instead, we propose that a more viable path for quantification of field-level carbon outcomes in agricultural soils is through an integration of sampling, sensing, and modeling, defined as the "**System-of-Systems" solution**.

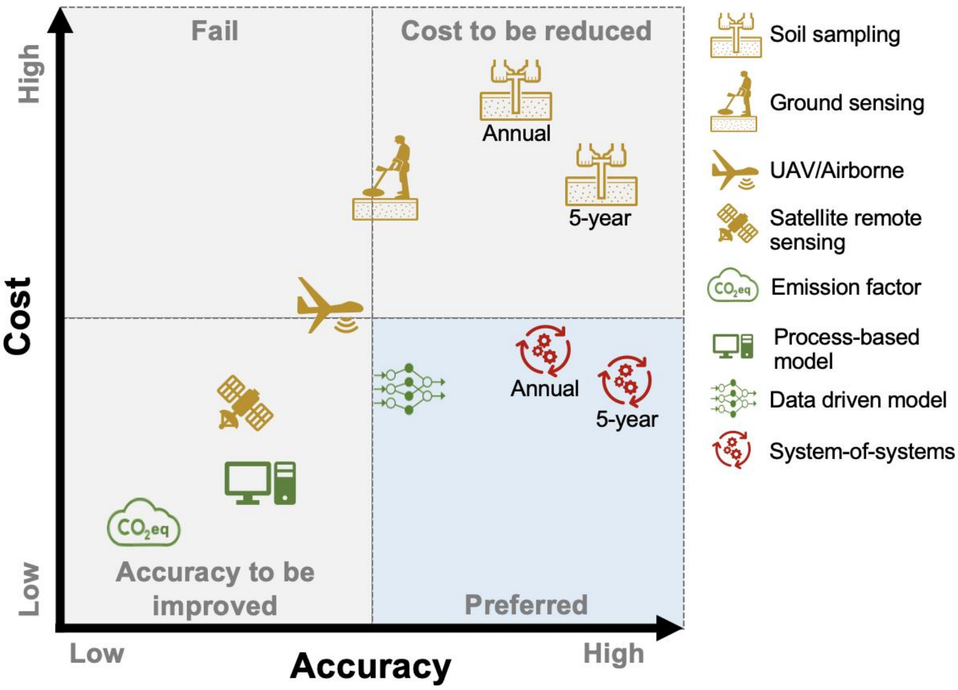

Figure 4. How different technological solutions for quantifying field-level carbon outcomes fit in the accuracy and cost diagram.

The "System-of-Systems" concept means that the complex problem of quantifying agroecosystem carbon outcomes cannot be solved by using a single sensor or a model alone, but only can be solved by effectively integrating various approaches (e.g. diverse observations, sensor/in-situ data, modeling). Such a "System-of-Systems" solution should simultaneously comprise the following features (Figure 5): **(1)** scalable collection of ground truth data and cross-scale sensing of ***C***, ***M***, and ***E*** at the local field level; **(2)** advanced modeling with necessary processes to support the quantification of carbon outcomes**; (3)** systematic Model-Data Fusion (MDF), i.e. robust and efficient methods to integrate sensing data and models at each local farmland level; **(4)** high computation efficiency and AI to scale to millions of individual fields with low cost; **(5)** robust and multi-tier validation systems and infrastructures to test model/solution's **scalability**, defined as the **ability of a solution to perform robustly with accepted accuracy on all targeted fields**. Thus the "System-of-Systems" solution is a holistic framework including multiple sub-systems for sensing, monitoring, modeling, and model-data fusion, targeting to assure field-level accuracy, scalability, and cost-effectiveness.

The "System-of-Systems" approach is so far the only pathway to implement the mass-balance approach to quantify SOC changes, which requires various localized observations and the integration of observations/data with models to accurately estimate each term in the mass-balance equation and achieve the field-level accuracy. Compared with existing approaches (Section 2.4), there are several advantages of using the mass-balance approach to quantify the change of SOC. First, all of the carbon budget terms (NEE, GPP, Ra, Rh, and Crop yield) are measurable, although some being costly, and can be used to verify model accuracy and provide a basis for confidence. Second, all the carbon budget terms can be measured and verified at relatively short time scales, i.e. from sub-hourly scale (e.g. NEE, GPP, Ra, Rh) to annual time scale (e.g. Crop yield), which enables the quantification of annual change of SOC. In contrast, soil sampling is generally not able to detect annual changes, as the uncertainty of soil sampling is usually much larger than the annual change of SOC. Third, those carbon budget terms (GPP, Ra, Crop Yield) for calculating the carbon input to soil (i.e. litter) can be estimated using advanced remote sensing technologies (see Section 3.1), which offers an efficient and scalable way to achieve the field-level observational constraints in a large region due to the ubiquitous coverage of remote sensing technologies. Fourth, the carbon mass balance approach provides a holistic picture of the overall carbon budget of farmland soils, which enables a mechanistic understanding of differential impacts of management practices on SOC from field to field and from year to year, thereby could help farmers to improve their management practices along with the changing climate.

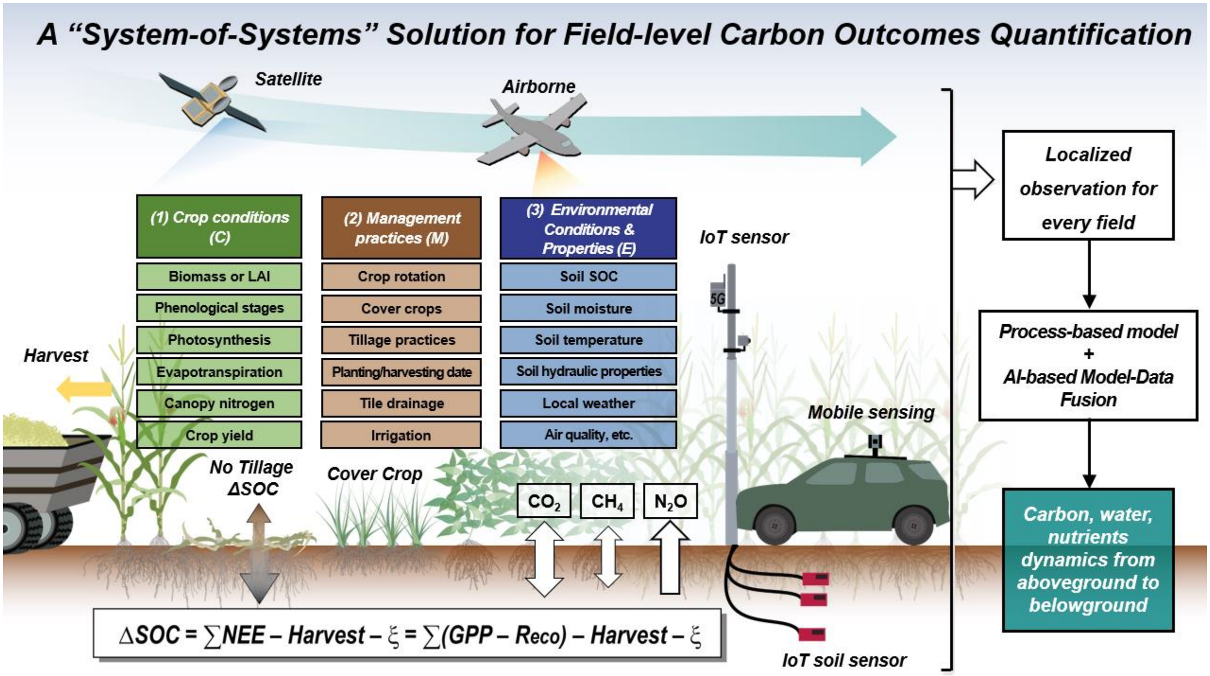

Figure 5. Illustration of a "System-of-Systems" solution for quantifying field-level carbon outcome, including above and belowground processes. The "System-of-Systems" solution includes sensing, monitoring, modeling, and model-data fusion, targeting to assure field-level accuracy, scalability, and cost-effectiveness. ξ represents carbon loss from various sources, which is usually very small (<0.5%) and thus can be neglected in most cases.

3.1 Scalable collection of ground truth data and cross-scale sensing of field-level information

Scalably sensing/estimating local information of $\boldsymbol{C}$, $\boldsymbol{E}$, and $\boldsymbol{M}$ at the field level is the first step of a "System-of-Systems" solution, which involves two seemingly different but inherently connected tasks: (1) ground truth collection, and (2) cross-scale sensing. Ground truth here is broadly defined as information that is collected on the ground to train, constrain or validate models. Agricultural ground truth is scarce and expensive to collect. For example, the carbon flux data requires eddy-covariance flux towers, which are generally costly to set up (~$100K needed to set up) and operate. **The need for ground truth data is non-negotiable and should be a major investment with public funding** (see Section 4). However, we also have to face the reality that even with low-cost sensing technology or crowdsourcing efforts, one cannot collect ground truth for every field. Instead, we propose to develop cross-scale sensing approaches, especially those enabled by remote sensing, to scale-up "ground truth" collection to large scales.

Cross-scale sensing can be demonstrated by the most recent development of deriving field-level photosynthesis information. Photosynthesis is the only term for land carbon input and also the largest carbon budget term (Beer et al., 2010). Ecosystem photosynthesis (i.e. GPP) is the primary driver for crop litter (i.e. carbon input to the SOC) and thus significantly contributes to the long-term change in SOC, as demonstrated in Section 2.3. Correctly quantifying photosynthesis at the field level puts significant constraint and reduces uncertainty on simulating crop carbon dynamics, crop litter (including both aboveground and belowground) and soil carbon dynamics (Li et al., 2021; Peng et al., 2018; Zhou et al., 2021b). A recent breakthrough in the remote sensing of photosynthesis was made possible by full integration of leaf-level chamber/sensor measurements, canopy-level hyperspectral sensing (especially solar-induced fluorescence, SIF) (Berry 2018; Kimm et al., 2021; Porcar-Castell et al., 2021), and regional-scale mapping through satellite fusion data (Figure 6) (Jiang et al., 2021; Luo et al., 2018). The cross-scale sensing here is guided by the domain knowledge of plant physiology, radiative transfer modeling, and hyperspectral theories; ground truth data - in particular, leaf-level samples and eddy-covariance flux tower data - are extensively used in the model development stage, but once the translation from ground-truth data to satellite-scale signals can be robustly developed, satellite fusion data can expand the photosynthesis information for every single field every day since 2000 to present (Jiang et al., 2021).

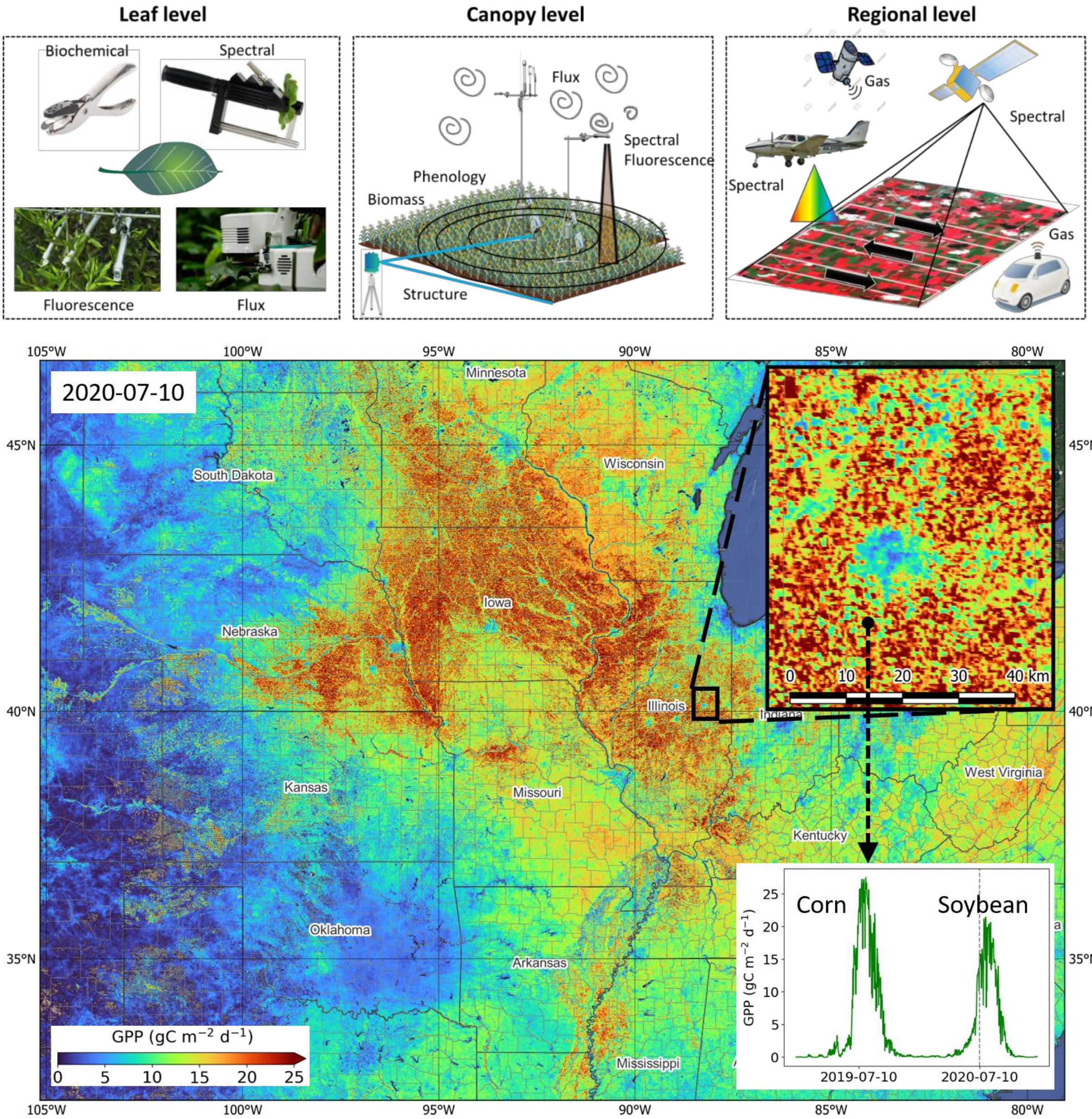

Figure 6. Cross-scale sensing to generate photosynthesis information at the field level. (Top) The cross-scale sensing from leaf to canopy, and to regional levels for estimating photosynthesis. (Bottom) A snapshot of field-level estimation of photosynthesis on 07-10-2020, derived from the large-scale SLOPE photosynthesis data at daily frequency (Jiang et al., 2021), showing field-level Champaign County pattern and a field-level daily time series of photosynthesis.

Another advance in cross-scale sensing is the use of intermediate sensing to augment traditional ground truth collection, and enable the scaling from leaf-level or plot-level ground measurements to coarse satellite pixel size - a classic problem in the area of remote sensing. A typical example is the use of airborne hyperspectral imaging (AHI). Hyperspectral imaging can provide estimates of certain soil and plant traits with high accuracy (Wang et al., 2022), although its application for scalable mapping has been limited by its high cost. A novel use of AHI is to treat AHI data as an intermediate bridge between ground truth collection and satellite scale-up. A general procedure is to first develop robust methods to translate AHI signals with targeted estimates (i.e. surface crop residue, surface SOC, cover crop biomass) based on data from intensive lab and field experiments; and then to use AHI as a strategic sampler to selectively "sample" over space and time, serving as a bridge from granular resolution of ground truth to large satellite pixels; and finally, to use satellite data overlaid with the AHI sampled area to translate satellite multispectral signals along with environmental variables into plant and soil trait estimation, thus deriving targeted ***C***, ***M***, ***E*** variables ubiquitously using satellite data. Though similar approaches have achieved success in mapping forests canopy biogeochemistry (Asner et al., 2016, 2017), they have rarely been used in agroecosystems. Once advanced and automated pipelines are established to conduct AHI collection and data processing (Wang et al., 2021; Zhou et al., in review a), AHI can be applied to estimate crop canopy nitrogen content, cover crop biomass, and crop residue fraction and tillage practices. Figure 7 demonstrates how AHI is used to scale up the estimation of crop residue fraction and tillage intensity at the regional scale. Other sensing approaches, such as mobile vehicle sensing (Yan & Ryu, 2021), IoT sensing network and robotics (Elijah et al., 2018; Tzounis et al., 2017), could also achieve a similar function to augment ground truth collection and enable satellite scaling-up to regional scales. Table 1 provides a non-inclusive list of different critical ***C***, ***M***, ***E*** variables that currently have been estimated using cross-scale sensing technologies.

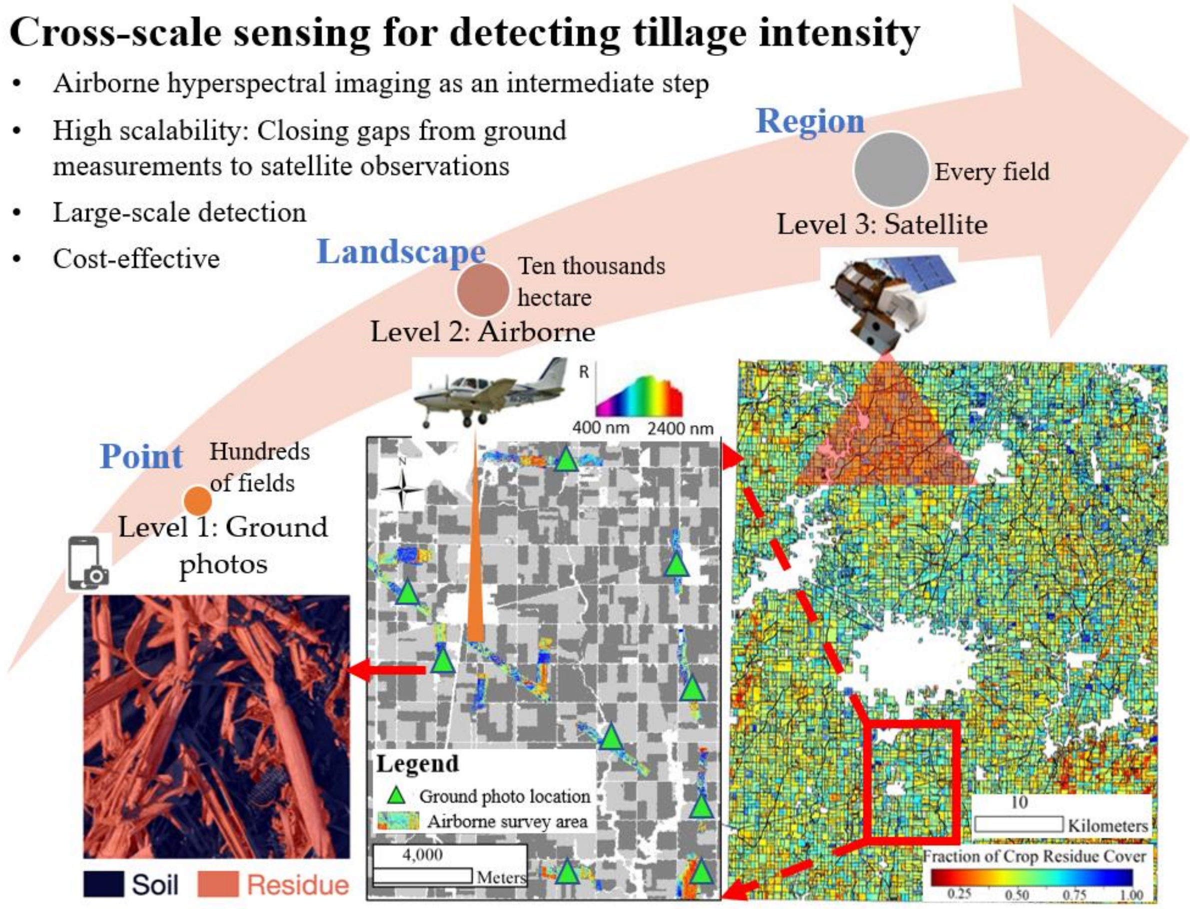

Figure 7. Cross-scale sensing to quantify regional high-resolution tillage intensity. Ground truth of crop residue cover was obtained through ground photos and computer vision-aided image segmentation. Then, airborne hyperspectral imaging along with machine learning was applied to upscale ground point measurements to landscape scale. Finally, massive airborne hyperspectral survey derived residue cover data were integrated with multi-source satellite fusion data to derive regional information of residue cover and tillage intensity.

Table 1. Major C, M, E variables that we can or will be able to derive based on cross-scale sensing technology.

	Variables	Typical upscaling framework	Methodology Maturity	Use Cases	References
C	Crop types	Mobile vehicle or survey -> satellite	High	Model input	(Cai et al., 2018; Johnson, 2019)
	Photosynthesis (i.e. GPP)	Flux tower -> satellite	High	Model constraint	(Ryu et al., 2019; Jiang et al., 2021; Wu et al., 2019)
	Agroecosystem water use (e.g. ET)	Flux tower -> satellite	High	Model constraint	(Anderson et al., 2011; Jiang et al., 2020)
	Leaf Area Index (LAI)	Ground data -> satellite	High	Model constraint	(Luo et al., 2018; Viña et al., 2011)
	Crop Yield	Ground data -> satellite	Medium	Model constraint	(Cai et al., 2019; Guan et al., 2017,2022; Lobell et al., 2015)
	Leaf traits (e.g., Photosynthetic capacity, nitrogen content, chlorophyll content)	Ground data -> airborne -> satellite	Low	Model input/constraint	(Serbin et al., 2015; Wang et al., 2021)
M	Planting & Harvest date	Ground data -> satellite	Medium	Model input	(Weiss et al., 2020)
	Tile Drainage	Ground/airborne surveys -> satellite	Low	Model input	(Khanal et al., 2017)
	Tillage practices	Ground data -> airborne -> satellite	Medium	Model input	(Daughtry et al., 2006; Wang et al., in review a)
	Cover crop adoption/growth outcome	Ground data -> airborne -> satellite	Medium	Model input/constraint	(Thieme et al., 2020; Wang et al., in review b; Zhou et al., in review b)
	Irrigation availability (e.g. existence of a center pivot)	Ground data -> satellite	Low	Model input	(Salmon et al., 2015; Xie & Lark, 2021)
	Irrigation water amount	Model-Data Fusion	Low	Model input	(López Valencia et al., 2020; Zhang et al., in review)
	Nitrogen fertilizer use	Currently challenging to acquire from remote sensing, with satellite-based NH3 possibly shed some lights	Low	Model input	

E	Local weather and its forecast	IoT sensors -> integrating with weather forecasting	High	Model input	(Tzounis et al., 2017)
	Soil properties (e.g., soil types, soil hydraulic properties, soil moisture, soil organic carbon)	Ground data -> satellite	Low	Model constraints	(Entekhabi et al., 2010; Croft et al., 2012; Wang et al., 2022)

3.2 Advanced modeling with necessary processes to support the quantification of carbon outcomes

The "System-of-Systems" solution heavily relies on advanced process-based models to simulate the complex carbon, nutrient, water and energy cycles on farmland. There are many process-based models with different levels of complexity available in the scientific community. We envision that these modeling approach would benefit from following the three protocols below:

(1) Have sufficient and necessary processes represented. Coupled carbon-nutrient-water-energy cycling over farmland is the foundation for field-level carbon outcome quantification, thus models should include a sufficient number of mechanistic pathways that clearly track the input, output and storage of water, carbon and nutrient in crop lands under the interference of agricultural management. For the plant component, simulating the responses of crop carbon uptake and water use to different abiotic and biotic stresses is necessary as they largely determine the crop production and carbon input to the soil. From this perspective, proper representation of canopy energy balance, stomatal conductance, uptake and transport of water and nutrients from soil to canopy are needed to mechanistically simulate the crop carbon and nutrient uptake and crop water use (Peng, et al., 2020). Many of the existing process-based models may lack critical processes or use over-simplified processes to model specific carbon outcomes. One obvious example, following our prior discussion on the importance of the holistic carbon budget of agroecosystems, is that most existing process-based models lack sufficient mechanisms that can model plant carbon processes as emergent phenomenon (including GPP, Ra, Rh, and litterfall), resulting in significant errors when quantifying the downstream ΔSOC. For example, lack of explicit modeling of photosynthesis (Farquhar et al., 1980; Wu et al., 2016), plant stomatal responses to environmental stresses (Buckley & Mott, 2013), and reproductive processes for yield (Peng et al., 2018) can cause huge uncertainty of the modeled carbon input to the soil pools, contributing significant error to the simulated ΔSOC. For the belowground part, soil temperature, water, oxygen, and pH dynamics, biogeochemical reactions related to carbon, nitrogen and phosphorus cycling, microbial activities and their regulation on SOM formation and stabilization as well as GHG emissions are core processes that need to be simulated. For example, recent studies identified two distinct pathways of SOM stabilization from litter decomposition, i.e. the DOM-microbial pathway (non-structural or soluble compound in the litter) in the early stage of decomposition, and the physical transfer pathway (brittle litter residue) in the final stage of decomposition (Cotrufo et al., 2015). This work emphasized the importance of dissolved organic matter (DOM) and microbial activities, and necromass in stabilizing SOM (Cotrufo et al., 2015). Having those mechanisms and their interactions with related environmental drivers (such as soil temperature, oxygen, moisture, and nutrient conditions) well represented in the soil carbon models is essential to accurately simulate the dynamics of SOC and its physical fractionations. Besides these biophysical and biogeochemical processes, representing the farming management practices and their impacts on coupled carbon-nutrient-water-energy cycling over farmland is critically needed to quantify the carbon outcomes.

(2) Maximum use of mechanistic processes representation. Many existing models use multiplication factors (Schimel et al., 2001), law of the minimum (Ågren et al., 2012), and empirically-derived response functions (Azizi-Rad et al., 2022), all of which are ad hoc by nature, to simulate biogeochemical and biogeophysical processes. One consequence of these non-mechanistic modeling approaches is that different researchers applying the same method to a given process will obtain different mathematical representations, which then lead to a loose foundation to implement that particular process in these models. Moreover, non-mechanistic representation which lacks support from physical laws also limits the generality and scalability of the model simulations, especially when a model is used to extrapolate beyond the environmental and management conditions under which the model is previously developed or calibrated. For example, many models use the empirically-derived soil water stress functions to depict the down-regulation of crop carbon uptake and water use under water stress conditions, which causes inconsistencies and discrepancies in multi-model intercomparison simulations (Egea et al., 2011; Grant et al., 2006; Verhoef & Egea, 2014). A more mechanistic way to account for crop soil water stress would be to explicitly represent the plant-hydraulic-stomatal-photosynthetic coordination from soils to plant, and to atmosphere (Grant, 2001). Similarly, most models formulate soil carbon decomposition by assuming different controlling factors, e.g. temperature, moisture, chemical composition, and soil mineral content, interact multiplicatively, while the biogeochemical processes that lead to decomposition are intertwined following specific mechanistic pathways (Tang & Riley, 2017). Another example is how the impacts of different tillage practices are represented on soil physical and biogeochemical processes. From a mechanistic perspective, tillage directly changes the mixing of soil and crop residue as well as soil structure, which then affect soil biogeochemistry and crop performance through various mechanistic pathways (Grant, 2001). As such, all other impacts on water, energy, carbon and nutrient cycles from tillage are then simulated as an emergent outcome in a coherent way. In contrast, some models represent the effect of tillage as direct modification of evaporation fluxes, and decomposition rates based on multiplication factors derived from empirical data (You et al., 2022; Yu et al., 2020), which introduces excessive parametric uncertainty and strong context dependence on the empirical data used for model parameterization.

(3) Simulate as many measurable variables as we can, such that the model simulation can be thoroughly validated, and measurable constraints can be easily incorporated to further improve the model simulation. For example, as discussed in Section 2.3, GPP largely determines the carbon input to the soil (through litter and root exudates), and crop yields are major carbon outputs from cropland, thus models with observational constraints from ground or satellite measured GPP and/or crop yields will unsurprisingly outperform models without such constraints. From a mass-balance perspective (Eq. 2, Figure 2), GPP could serve as a particularly strong constraint for quantifying litter and root exudates, two critical carbon cycle components that have significant spatial heterogeneity but are hard to measure (Figure 8). Another example is the recent paradigm shift from using conceptual and non-measurable SOC pools to using measurable SOC fractions for SOC simulation in process-based models (Abramoff et al., 2018; Abramoff et al., 2022; Cotrufo et al., 2013; Robertson et al., 2019; Zhang et al., 2021). SOM is a complex mixture of materials with heterogeneous origins, chemical compounds, microbial accessibility, and turnover rates (Schmidt et al., 2011). Physical fractionation of SOM differentiate particulate organic matter (POM) and mineral-associated organic matter (MAOM, stabilized and exchangeable), which all are measurable in the laboratory and have different characteristic residence times (Cotrufo et al., 2019; Lavallee et al., 2020; Lugato et al., 2021). Beyond the change in total SOC, quantifying the changes and distributions of POM and MAOM may help address the permanence issue of soil carbon credit. However, most previous soil carbon models simulate SOM dynamics as non-measurable fluxes between conceptually defined and non-measurable soil carbon pools (Robertson et al., 2019). Only if POM and MAOM are properly conceptualized and represented in the models can they be used to simulate the changes of those SOM fractions and can measured SOM fractionation data be used as direct constraints for models (Guo et al., 2022).

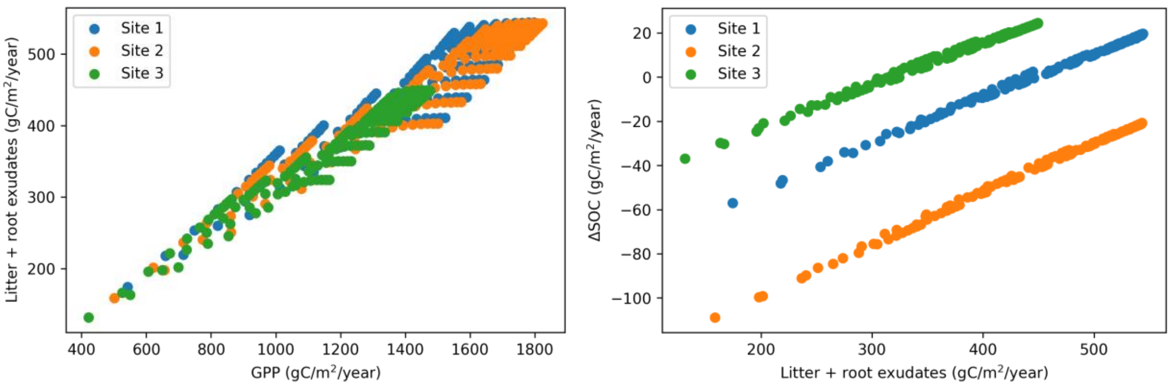

Figure 8. GPP is closely linked with soil carbon input, i.e. litter and root exudates, and thus directly affect change of SOC (Grant, 2001). This site-level sensitivity analysis is conducted over three sites with different environmental and soil conditions in northern (Site 1), central (Site 2) and southern (Site 3) Illinois using the ecosys model (Zhou et al., 2022).

3.3 Model-Data Fusion with accuracy and robustness at individual fields

Model-data fusion (MDF) here refers to a set of techniques that reduce the uncertainty of states and parameters of process-based models or data-driven models (e.g. statistical model or neural networks) using local information (i.e. field-level ***C***, ***M***, ***E*** data) to obtain improved estimation of carbon outcomes (Fer et al., 2018). MDF also has the ability to evolve by incorporating new sensors/sensing data or new model developments to this framework.

MDF is the core part of the "System-of-Systems" solution, with the basic rationale that available observations can only see part of a system, but a model that has the necessary processes can leverage available observations to help constrain the overall system and thus improve prediction accuracy for the processes that observations do not see. The most successful example of MDF is weather forecast - the integration of weather models with satellite observation - leading to its everyday use by different industries (Bonavita et al., 2016; Geer et al., 2018). MDF is not a new concept in earth science and ecological studies (Fer et al., 2021; Luo et al., 2011), as methods such as Bayesian Inference, Data Assimilation, and Emergent Constraint have been extensively used to improve various predictions at some sites, watersheds, or relatively coarse spatial grids (Dietze et al., 2018; Kalnay, 2003; Reichle, 2008; Wang et al. 2020); however, the use of MDF for field-level carbon outcome quantification has many new requirements.

We propose a new MDF approach to enable MDF being conducted at every individual field level, while also clarifying critical components of carbon cycle to inform both science and management practices. Essentially, for every field in a targeted region, cross-scale sensing (Section 3.1) provides high-resolution and spatially-explicit ***C***, ***M***, ***E*** observations, which are then used as either inputs or constraints for a model with necessary processes represented (Section 3.2), and a set of **location-specific parameters** will be constrained for every field. By doing so, carbon outcome quantification allows the uncertainty quantification at every field, and model verification at every field is also made possible when extra carbon-related observations can be used as independent validation data. This MDF approach to enable high-resolution and spatially-explicit model constraining represents a major advance over any of the existing quantification protocols (Climate Action Reserve, 2020b; Verra, 2020) that only require validation at the regional scale. This new MDF approach fulfills the model validation needed to test whether a model or a solution has true scalability, which was defined earlier as the ability of a model to perform robustly with accepted accuracy on all targeted fields. Only models that can reproduce the accepted 'accuracy' at any random fields can be used as an accepted MRV tool for agricultural carbon outcome quantification.

Meanwhile, such a new MDF calls for new computational techniques, as the conventional implementation of MDF techniques (e.g. Bayesian Inference, Data Assimilation) would be too computationally expensive to handle the field-level MDF. Take Champaign county in Illinois alone as an example, it has ~ 12,000 fields in active cultivation; and the state of Illinois has ~ 1,000,000 fields in active cultivation; conducting intensive MDF using traditional implementation for each of these fields is infeasible. Moving to AI-based solutions and fully leveraging GPU computing to facilitate efficient and effective scale-up of the field-scale MDF over a broad region is the only path forward, which will be discussed further in Section 3.4.

3.4 High computation efficiency and AI to enable scaling to millions of individual fields

Scaling a System-of-Systems solution to all the individual fields with similar accuracy and at a low cost is a twofold problem: (1) cross-scale sensing to generate rich ***C***, ***M***, ***E*** information for constraining various aspects of agricultural carbon cycles (Peng et al., 2020) (as discussed in Section 3.1); and (2) scalable application of MDF over millions of individual fields (as discussed in Section 3.3). To reduce the computation cost to scale up, both problems require the inclusion of AI and a transition from CPU-heavy to GPU-heavy models on supercomputing or cloud-computing platforms for massive deployment. Below we will specifically discuss three pathways to help realize the upscaling of MDF, spanning across a spectrum of different levels of integrating process-based models with AI.

Pathway 1: The most straightforward path to reduce model uncertainty is to use MDF to constrain model parameters. However, the high computational cost of parameter optimization limits the scaling of MDF. A feasible bypass without massive re-coding is to leverage deep learning algorithms and develop GPU-based surrogate models. Forward inference of neural network-based surrogates can be orders of magnitude faster than CPU-based process-based models, making them particularly suitable for parameter calibration (Brajard et al., 2021; Fer et al., 2018). Successful applications have been reported in hydrologic (Tsai et al. 2021) and Earth system models (Asher et al., 2015; Lu & Ricciuto, 2019), this strategy is also practiced in other complex systems such as agroecosystem (Zhou et al., 2021b) and climate models (Couvreux et al., 2021).

Traditional parameter optimization algorithms work by iteratively searching for the optimal parameter combination to minimize an objective function (e.g., RMSE), but may get stuck at random local optima where multiple parameter combinations correspond to identical model outputs. If parameters are calibrated for individual pixels, this ill-posed issue may lead to a discrete spatial distribution of the target parameters. Recently, neural network-based parameter learning methods have demonstrated promising possibilities to address this issue without a searching procedure (Reichstein et al., 2019; Schneider et al., 2017). For example, the differentiable parameter learning framework developed by Tsai et al., (2021) enables the inference of model parameters by an unsupervised parameter learning network, which was automatically constrained by the surrogate network to produce reasonable parameter combinations in the training phase. Compared to the traditional SCE-UA method (Duan et al., 1992) in calibrating the Variable Infiltration Capacity (VIC) model, the parameter learning network estimates physically more sensible parameter sets with continuous spatial patterns because the inputs of the parameter network (e.g., forcings) are themselves spatially coherent. Although AI-based surrogate models provide a pathway for the MDF upscaling, the objectives of further research should not be limited to speeding up the parameter calibration procedure but to exploring generalized pathways for estimating interpretable and reasonable model parameters.

Pathway 2: The second pathway is a hybrid modeling approach to integrate machine learning (black box) and mechanistic modeling (glass box) in one integrated modeling system to achieve computational efficiency, prediction accuracy and model transferability. Knowledge-Guided machine learning (KGML) is one such approach that learns complex patterns from data while incorporating domain-specific knowledge, such as physical rules (e.g. mass conservation), causality (e.g. dependency structure between variables) and nature of variables (e.g. states vs fluxes), informed by process-based models (Reichstein et al., 2019). Preliminary success has been achieved in many topics including streamflow prediction (Jia et al., 2021), lake phosphorus (Hanson et al., 2020) and temperature estimation (Jia et al., 2021; Read et al., 2019), and GHG emission modeling (Liu et al., 2022). In particular, the KGML-ag model developed by Liu et al. (2022) incorporated knowledge from the ecosys model into a GRU (Gated Recurrent Unit, one kind of recurrent neural network for representing time series) model and outperformed both the ecosys model and pure GRU model in predicting the complex temporal dynamics of N_2O fluxes (**Figure 9**). Combining KGML with Meta-learning may increase model transferability by accelerating hyper-parameter learnings that account for spatial heterogeneity (e.g. those in different watersheds) (Chen et al., 2022). Despite this early success, efforts to develop hybrid models are still in its nascent stage. Scaling field-level KGML for carbon accounting across millions of fields would require innovative approaches to assimilate multimodal remote and in-situ sensing data, possibly by assimilating these data via low-dimensional embeddings to constrain neural networks. Future research should also address multi-objective learnings, because existing KGML models are mostly mono-objective (e.g., simulating CO2, CH_4 and N_2O individually) and lack synergistic considerations for the coupling of soil biogeochemistry.

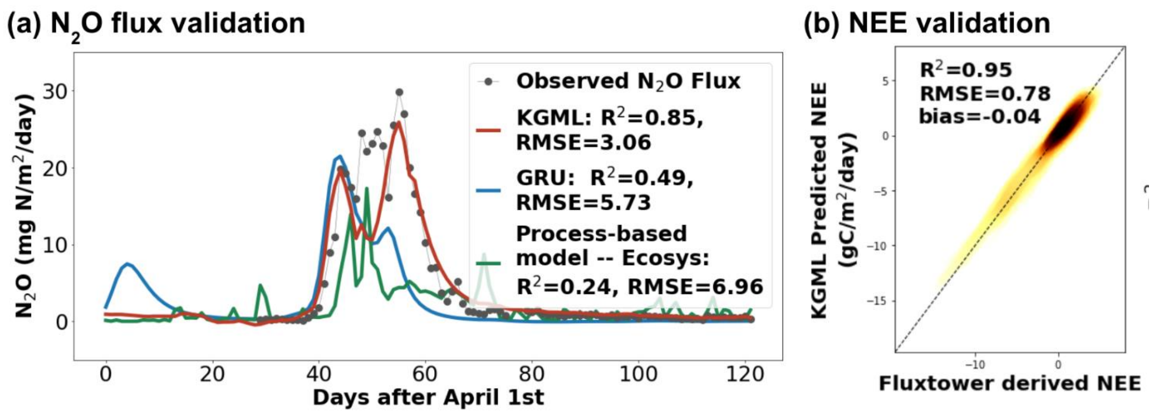

Figure 9. N_2O and CO_2 fluxes estimated by two KGML models. (a) KGML outperforms the process-based model and pure ML model in simulating N_2O fluxes. (b) Out-of-sample validation of KGML predicted net ecosystem exchange (NEE) with 11 flux tower observations.

Pathway 3: Fully upgrading existing agroecosystem models to GPU-accelerated systems requires intensive code redesign and rewrite, thus requiring longer coordinated efforts with dedicated funding support (Bauer et al., 2021; Irrgang et al., 2021). Based on previous explorations for Earth System Models (ESMs) (Bauer et al., 2021; Irrgang et al., 2021) and specific challenges in agricultural carbon outcome quantification (described in Section 2.4), the ideal GPU-accelerated agroecosystem models should have the following characteristics: (1) each submodule should have the same or higher level of performance and interpretability as in the original model; (2) working freely in the GPU environment and be flexible enough to adapt to hardware improvements; and (3) enabling the assimilation of generic data ensemble from multiple sources with different scales (e.g. the cross-sensing data described in 3.1) for efficiently training/validating/finetuning and on-time correcting. Progress is faster in upgrading modules with relatively known physical rules, such as climate and hydrology than in biogeochemistry or human disturbance (Irrgang et al., 2021). For example, previous efforts on rewriting domain-specific language to adapt the GPU-accelerated systems succeeded in weather modeling (e.g. COSMO) (F. Thaler et al., 2019) and climate modeling (e.g. CESM) (Zhang et al., 2020). An extensive effort is currently underway to adapt DOE ESMD/E3SM with modern machine learning techniques to next-generation architectures that are capable of GPU computing and generic data assimilation (Alexander et al., 2020). The recently proposed concept of neural earth system modeling (e.g. NESYM) (Irrgang et al., 2021), aiming for a deep and interpretable integration of AI into ESMs, might be the closest solution for upgrading agroecosystem models as well. One profound step for such upgrading is to replace every submodule of the process-based model with a ML surrogate, and to train those surrogates jointly with real-world observations. However, proceeding in this direction needs to conquer the challenge of mapping highly non-linear processes involving partial differential equations (PDEs) with different coefficients at different spatial and temporal resolutions. One solution that has shown some early success in predicting global atmospheric circulations (Pathak et al., 2022) is Fourier Neural Operator (FNO) (Li et al., 2020), a neural network specifically designed for solving an entire family of PDEs by learning mappings between functions in infinite-dimensional spaces (i.e., functions are discretized in an arbitrary way). However, FNO is only one kind of "black box" neutral solver for PDEs. To be adopted in agroecosystem simulations, FNO needs to combine with other famous machine learning models (e.g. RNN, GNN, transformer) to consider the connections and heterogeneity in space and time, and needs knowledge-guided constraints to provide predictions following physical/biogeochemical rules.

3.5 Three-tier validation system: ensuring model fidelity and true scalability

Model fidelity is critical for establishing trust in any carbon outcome quantification. Model validation, a procedure to benchmark model simulation with independent, high-quality observational data, is the only way to build model fidelity. The new MDF approach of high-resolution and spatially-explicit model constraining essentially proposes a more strict way to test model **scalability**, defined as the **ability of a model to perform robustly with accepted accuracy on all targeted fields**. "Scalability" of a model or a solution should not only be demonstrated by model performance at a limited number of sites with rich data, where extensive parameter calibration is allowed; a true test of model "scalability" should be also demonstrated at many random sites, where only limited measurements are available. The latter is what a real-world application entails - we are required to quantify the carbon outcomes at any given field. To achieve the above goal to fully validate the **model scalability**, a three-tier validation approach is needed, and results from these three tiers should be reported to the community for fair and transparent comparison. It is worth mentioning that at all the three tiers of sites, cross-scale sensing technology should be able to provide already rich remote-sensing based observations, which should provide the necessary model inputs, model constraints for MDF.

Tier 1 - Super sites: This tier includes sites that have collected a complete suite of measurements data that can be regarded as gold-standard datasets (Novick et al., 2022). An ideal super site should include measurements that cover from biogeophysics (profiles of temperature, and moisture, energy fluxes) to biogeochemistry (carbon and nutrient fluxes and state variables), i.e. a dataset that is sufficient to recreate the soil-plant-atmosphere continuum, and evaluate/benchmark the major ecosystem processes simulated by models. Thus a typical super site should at least include EC flux tower, extensive and deep soil samples, ground-level remote sensing, and various other advanced measurements (automatic chambers for N_2O). Existing examples of research infrastructure that already supports many of these "gold-standard" data variables include the USDA Long-Term Agroecosystem Research (LTAR) network, some National Ecological Observatory Network (NEON) sites, and AmeriFlux sites on cropland and pasture land (Baldocchi et al., 2001). Further, the recently launched U.S. Department of Energy ARPA-E SMARTFARM sites have been collecting soil, crop, and GHG fluxes data with even greater spatial and temporal resolutions (ARPA-E, 2019) (Figure 10), enabling a new generation of R&D development such as high-resolution remote sensing monitoring, or novel modeling methods that can capture granular dynamics such as hot-spot and hot-moment patterns of GHG emissions.

Tier 1 super sites would enable detailed model calibration and out-of-sample validation by virtue of the fact that gold-standard datasets capture whole ecosystem flux (e.g. NEE, GPP), soil carbon flux and stock, plant biomass etc. What would make the Tier 1 super sites more useful is to add **paired experiments** with detailed measurements for the pairs. For example, setting up two neighboring sites (e.g. weather and soil conditions should be similar) with one growing crop cover and the other not, and keeping other management practices the same or similar enough, the difference of measurements could provide strong scientific evidences and thus validation data for quantifying the carbon outcome of different management practices. Successful examples of paired experiments with EC flux measurements have been demonstrated in rice methane emission using alternate wetting

(Runkle et al., 2019). Super sites also provide further validation for the cross-scale sensed ***C***, ***M***, ***E*** variables.

Tier 2 - Intermediate sites: This tier includes an extensive number of sites that only have a few key ground measurements (e.g. soil samples for soil texture and SOC, crop yield, leaf samples) but do not have a complete suite of observations as the Tier 1 super sites. Using these ground measurements and also remotely sensed observations, MDF can be conducted, and validation can still be made directly to compare the simulated crop yield, SOC stock and SOC changes with ground observations. When doing model validation at the Tier 2 sites, only basic information about site location and management history will be provided, and the modeling team should report their simulation results for independent comparison with observations.

Tier 3 - Scaling sites: This tier includes virtually any site or field which requires carbon outcome quantification. Little or no ground measurements are available at these sites. This tier of sites thus represents the real-world situation for operational use. However, due to the cross-scale sensing technologies (Section 3.1), all random fields will still have a suite of remotely sensed ***C***, ***M***, ***E*** data available to enable MDF and quantify both carbon outcomes and associated uncertainty at all these fields. Model verification at every field is also made possible when extra remotely sensed observations can be used as independent validation data. It is worth noting that Tier 3 almost entirely relies on remotely sensed ***C***, ***M***, ***E*** information, which highlights the importance of cross-scale sensing to enable such a new MDF approach.

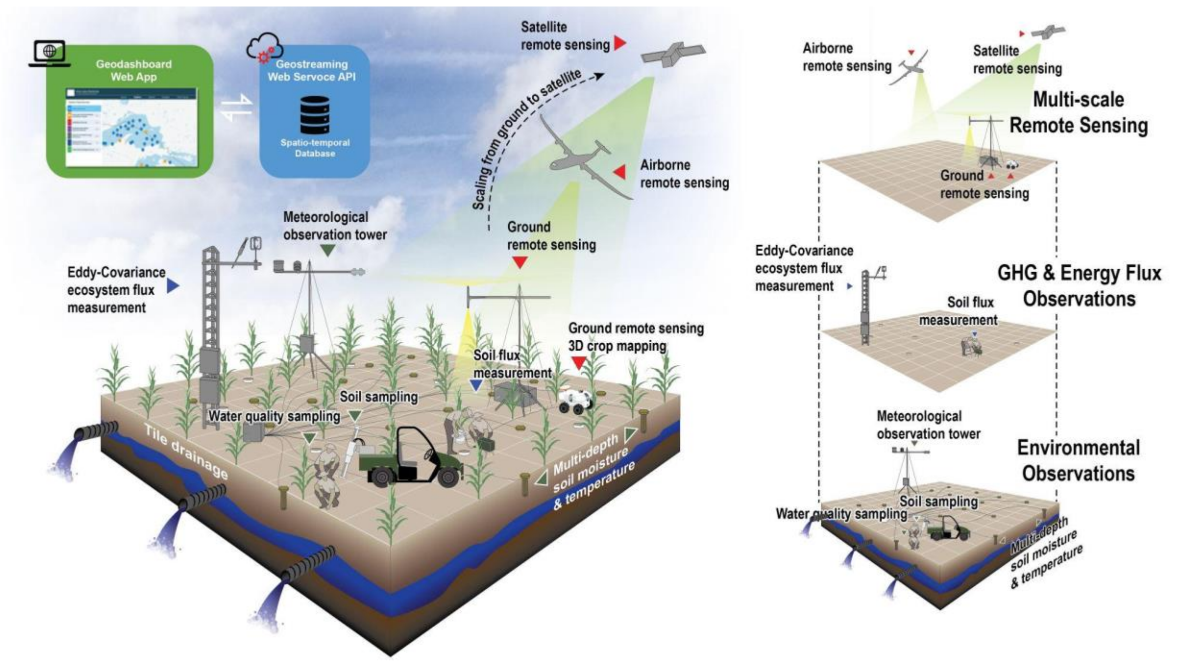

Figure 10. Example of the Tier 1 super site: using the ARPA-E SMARTFARM Phase 1 site at Champaign, Illinois, managed by University of Illinois Urbana Champaign.

4. Financial investment for R&D to substantiate agricultural carbon market and sustainable agroecosystems

Looking forward, the "System-of-Systems" solution will be the most promising technology for field-level carbon outcome quantification. One of the biggest advantages of the "System-of-Systems" solution is that it is an inclusive framework that can embrace new technology and has the potential to ingest new scientific discoveries and information, and thus can continue to evolve with the whole scientific community and technology trends. While prototypes of such a "System-of-Systems" solution emerge for certain crop types and geography (Zhou et al., 2021a), this integrated system consists of several components that are still at their early stages, thus requiring considerable R&D investment by government and industry. Coincidentally, these investments will build the foundation for the next generation of precision agriculture whose scope has been expanded from increasing productivity and efficiency with site-specific management (Yan et al., 2020), to the integration of sensing, big-data analytics and automation for guiding sustainable farming (Tautges et al., 2019). However, technical advances alone are insufficient for substantiating the agricultural carbon market or agricultural sustainability more broadly; success will also rely on synergies among citizens, researchers, corporations, NGOs and governments to remove scientific and practical hurdles.

First and foremost, we should fully acknowledge that agricultural carbon outcomes are deeply rooted in complex agroecosystems, and a holistic **system** view of carbon, nutrient, energy, and water cycles strongly coupled with human management should be the guiding principle. Aboveground and belowground processes of carbon cycle collectively determine the SOC change (Section 2.3), thus only focusing on changes in soil carbon pools while neglecting other critical carbon processes (e.g. over-emphasis of soil sampling at the cost of other flux measurements) may lead to limited success. The tight connection of carbon cycle with other biogeochemical cycles (including redox and elemental stoichiometry) and water cycle also highlights the importance of soil moisture, soil oxygen and chemical characterization of litter, which links SOC with the GHG missions (N_2O and CH_4). Many unknowns about these above linkages exist (e.g. mechanisms that drive N_2O emission with hot-spot and hot-moments) (Butterbach-Bahl et al., 2013). Coordinated research on understanding the holistic carbon-nutrient-water cycles for agroecosystems is a priority that could be effectively pursued by effectively leveraging the Integrated Model-Observation-Experiment (ModEx) Paradigm (Geernaert et al., 2018; U.S. DOE, 2021). ModEx promotes the idea that models should be developed with the current best knowledge and corroborated with observational and experimental data, and models are then used to identify opportunities for additional field and lab-based research to fill gaps in further understanding system structure and function. Iterative feedback between models and experiments advances the overall progress in this area.

Second, we should use community efforts to develop unified protocols that guide measurements and modeling schemes to understand and reduce the uncertainty of carbon outcome quantification. Such protocols must be established through collective effort to achieve scientific rigor and transparency. Existing efforts led by certification organizations such as Verra (Verra, 2020) and Climate Action Reserve (Climate Action Reserve, 2020a) are important and valued, but tend to be simplistic, conservative, and not always well-adapted to the nuances of production agriculture, given the limited empirical data and insufficient MRV tools (Oldfield et al., 2021). To successfully establish climate-smart commodity and agricultural carbon markets, a concerted effort of more advanced field work, data collection, and modeling assessment will be necessary. It is anticipated that debate will intensify as more disciplines and stakeholders become involved in the new phase of protocol development and validation, especially when the necessary rigor requires technical sophistication beyond traditional quantification approaches (Badgley et al., 2022; Novick et al., 2022). To foster open and constructive conversations that increase credibility and the public's confidence in carbon outcome quantification methods, three principles must be emphasized. First, **the quantification uncertainty of field-level carbon outcomes must be emphasized, and especially for the carbon credit market the uncertainty of the calculated carbon credit should be reflected in its price or policy design (e.g. insurance)** to ensure that the incentivized impact is not over- or under-compensated. For example, the standard deviation of a MRV system can be used to discount the value of credits generated (Kim & McCarl, 2009). This is an essential requirement for the protocol to be usable, not just a subjective technical preference. Second, **validation is the only way to report system-wide uncertainty**. No exemption should be made for any quantification tool, even if the tool is widely used or peer-reviewed. There are some academic-based model intercomparison MIP efforts (Eyring et al., 2016; Rosenzweig et al., 2013) that can shed light on how to set up such validations, but given the transaction purpose of carbon credits, a high bar must be set for acceptable model performance. **Third, demonstrating performance at the scale of an individual field is critical.** Due to the challenges of achieving scalability, some practitioners suggest compromise by focusing on the aggregated accuracy of quantified carbon credit (Oldfields et al., 2021). We argue that aggregated accuracy, which is almost impossible to validate, must come from field-level accuracy.

Next, **establishing high-quality and comprehensive datasets and inter-comparison infrastructure for developing, calibrating, and validating MRV systems** is essential to building stakeholder trust in these technologies. The high-quality and comprehensive dataset to represent the three Tier validation system (Section 3.4) should ensure site representativeness to include different soil, weather, crop, and management types, and be open-source but compiled under a protocol of community-wide acceptance. An analogy is the ImageNet database (Deng et al., 2009; Russakovsky et al., 2015) for computer vision and AI research, with which new algorithms will be benchmarked to show their progress in visual object recognition. Establishing an "ImageNet for Agriculture" is certainly more challenging given the complexity of carbon quantification. Due to the often large uncertainty associated with agricultural measurements, protocols for standardized data collection, and processing techniques must be carefully evaluated and imposed. Some long-term experiment and observation networks that have collected a complete suite of ***C, M, E*** variables (i.e. super tites) have the great potential to provide high-quality and comprehensive data. Lastly, a large number of controlled experiment sites can be used to test the model scalability. These sites often have limited amounts of ground measurements but represent the real-world conditions for operational use.

Further investment in high-quality data collection should prioritize experiments that can help understand the carbon outcomes associated with different bundles of carbon-outcome-related practices, such as the combination of no-till and cover crop, as well as measurements that can disentangle the opaque "black box" of complex plant-soil-microbe interactions (Yan et al., 2020). In addition, deep sampling of soils beyond the typical surface sampling depths (e.g. 0-30cm) is necessary to accurately quantify the extent of SOC changes (Tautges et al., 2019) and to corroborate estimates by models. Developing cyberinfrastructure to ensure archiving and sharing of the scientific data is also highly important and should be an investment priority. Such cyberinfrastructure development should be guided by the FAIR guiding principle (i.e. Findaility, Accessibility, Interoperability, and Reusa of digital assets) for the collected scientific data management and stewardship (Wilkinson et al., 2016), with a thorough consideration of privacy protection of farmer data.

Finally, while our discussion has mainly focused on agricultural carbon outcomes, it is important to note the myriad environmental and economic co-benefits (e.g. improving soil health, reducing water use and air pollution, and increasing climate resilience), which in turn can bring further benefits to carbon mitigation programs *per se*. Some recent case studies have demonstrated that, given the relatively low carbon credit price, participation of farmers may be primarily driven by these co-benefits (ARPA-E, 2019; Deng et al., 2009). The "System-of-Systems" framework proposed in this perspective can be extended to assist the accounting of these co-benefits, and inform sustainable agroecosystem management by holistically studying the often coupled carbon, water, and nutrient cycles and human activities, a topic itself at the frontier of Earth system science.

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