



*3rd International Crop  
Modelling Symposium*

# Crop Modelling for Agriculture and Food Security under Global Change



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**ORAL**

**SESSION 1 – SCIENTIFIC AND  
METHODOLOGICAL ADVANCES  
IN CROP MODELLING**



## Scientific and Methodological Advances in Crop Modelling

### Revealing carbon-water trade-offs in Daisy crop model using Pareto-based calibration

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**Multi-objective optimisation; Biomass; Net Ecosystem Exchange; Evapotranspiration; Stomatal coupling**

#### Introduction

Crop models now integrate advanced processes such as biochemical photosynthesis and stomatal conductance, which link carbon and water fluxes. However, calibration is even more challenging, as fitting one output can create errors in others. Widely used in hydrology compared to crop modelling, multi-objective optimisation algorithms handle conflicting objectives by exploring trade-offs using Pareto-based sampling approach. Beyond identifying optimal parameter sets, they also provide valuable insights into model behaviour, revealing structural limitations or equifinality.

#### Materials and Methods

This research was conducted on four growing seasons of winter wheat, with detailed flux and biomass data measured at BE-Lon site, Belgium. The Daisy sol-plant-atmosphere model was applied in an hourly setup with site-specific meteorological, soil and crop inputs. It included the Soil-Vegetation-Atmosphere-Transfer (SVAT) module which couples the biochemical photosynthesis model (de Pury and Farquhar, 1997) with the surface energy balance through the stomatal conductance (Plauborg et al., 2010).

Influential parameters were selected based on a previous global sensitivity analysis performed on the same dataset. Regarding model calibration, we used the Speed-constrained Multi-objective Particle Swarm Optimisation (SMPSO) algorithm, seeking trade-offs among three objectives: dry matter (DM), Net Ecosystem Exchange (NEE) and latent heat flux (LE). The relative Root Mean Square Error (rRMSE) was used as objective function (F) for these three variables to enable fair comparison between them.

#### Results and Discussion

The Pareto analysis revealed clear trade-offs, especially between dry matter and NEE, indicating structural issues or biases in measurements (Fig. 1). While dry matter and NEE were reasonably simulated (RMSE = 0.948 t ha<sup>-1</sup> for DM; 1.49 gC m<sup>-2</sup> d<sup>-1</sup> for daily NEE), discrepancies pointed to problems in estimation of heterotrophic respiration and observational uncertainties. LE fluxes were poorly captured (RMSE = 30.7 W m<sup>-2</sup> using daily fluxes), with the model underestimating variability and failing during high temperature and VPD periods. These shortcomings were linked to simplifications in evapotranspiration modelling and an inability to reproduce stomatal decoupling during heatwaves, i.e. when plants increase transpiration to promote leaf cooling (Marchin et al., 2023).

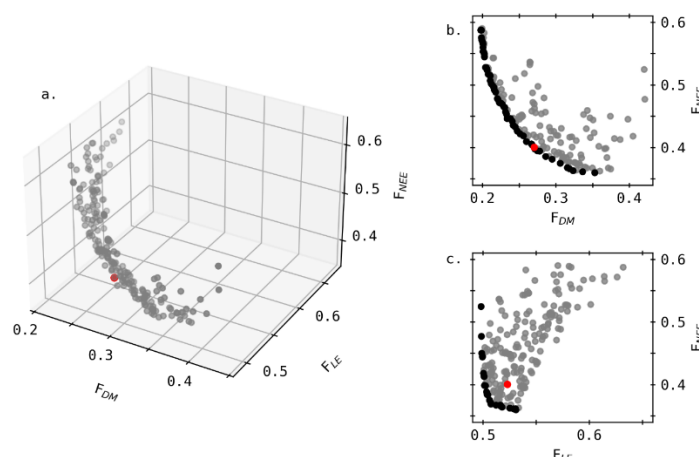


Figure 1. Non-dominated solutions in the objective space: (a) 3D Pareto front, and 2D projections considering (b) DM and NEE, or (c) LE and NEE

## Conclusions

The Pareto-based calibration proved useful for identifying parameter sets balancing carbon and water exchanges, but also for diagnosing structural weaknesses and guiding improvements in crop modelling. This study underlines the need to move beyond the simplified FAO56 approach and to better capture stomatal regulation under heat and high atmospheric demand. A deeper understanding and integration of stomatal decoupling mechanisms would enhance crop models' ability to simulate plants responses to heatwaves, which are expected to become more frequent with climate change.

## Acknowledgements

This research was conducted within the framework of the ICOS Wallonia project, which is supported by the Service Public de Wallonie, Belgium. Researchers were funded by the Federation Wallonie Bruxelles (FWB).

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## Crop yield prediction of kimchi cabbage based on model-informed machine learning approaches

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**Keywords:** climate change, process-based crop model, machine learning, hybrid modeling, *Brassica rapa*

### Introduction

Temperate vegetable crops such as kimchi cabbage are increasingly vulnerable to climate variability, underscoring the need for accurate yield prediction to support climate adaptation strategies and ensure stable production. Process-based crop models (PBMs) provide a structured framework to simulate potential growth, but they often fail to capture discrepancies between simulated and observed yields due to environmental and management constraints.

### Materials and Methods

Fresh weight measurements of kimchi cabbage were collected biweekly from 17 farms with varying planting dates in Taebaek, Gangneung, and Pyeongchang, the main highland production regions of South Korea. A hybrid modeling framework was developed by integrating the K-cabbage PBM with three machine learning (ML) algorithms: random forest (RF), XGBoost (XGB), and deep neural networks (DNNs). Eight feature subsets were evaluated, incorporating mean temperature, growing degree days (GDD), cumulative precipitation, and PBM-derived potential yield estimates. Model performance was assessed using root mean square error (RMSE) and Nash–Sutcliffe efficiency (NSE).

### Results and Discussion

RF and XGB consistently outperformed DNNs, producing higher NSE and lower RMSE values. The highest predictive accuracy was achieved when cumulative precipitation and PBM-based yield estimates were included as predictors, highlighting the value of combining climate and model-derived features. These results emphasize that both algorithm choice and feature selection critically affect ML performance in yield prediction.

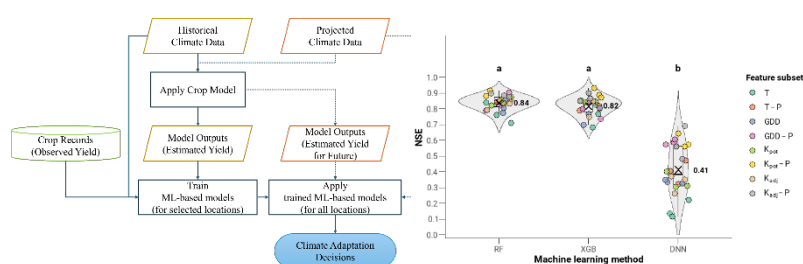


Figure 1. Hybrid modeling framework and comparative performance of machine learning approaches for kimchi cabbage yield prediction.



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## Conclusions

This study demonstrates that integrating PBMs with ML algorithms, informed by farm-level observations of climate and crop growth, enhances the prediction of actual kimchi cabbage yield. The approach provides a promising framework for advancing crop yield forecasting under climate variability and can inform broader applications in climate-resilient agriculture.

## Acknowledgements

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## How can microclimate simulation enhance plant growth modelling in complex environments?

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**Keywords:** Soil-Plant-Atmosphere Continuum, Computational Fluid Dynamics, Agrivoltaics, Energy & water budgets.

### Introduction

To face climate change, plants are increasingly cultivated in complex environments, such as within agrivoltaic systems, in agroforestry configurations, downstream vegetative hedgerows, or in urban landscapes. Designing such agricultural systems requires investigating the influence of spatially heterogeneous and temporally varying microclimates on soil-plant-air energy and water exchanges, ultimately on plant temperature and soil water content. Current state-of-the-art crop models often lack detailed microclimate representation. They either operate on daily time steps and spatial averages – oversimplifying the microclimate complexity – or are highly detailed, like Functional Structural Plant Models, making them difficult to couple with fine-scale microclimate models. This study introduces an approach that couples a Computational Fluid Dynamics (CFD) solver – designed to simulate airflow, radiation, and temperature distributions within complex environments – with a Soil-Plant-Atmosphere Continuum (SPAC) model, which leverages the CFD outputs to more accurately assess plant thermal and water status.

### Materials and Methods

The simulation framework involves a fluid solver – comprising wind speed resolution, turbulence modelling, as well as air temperature and air specific humidity transports – a radiation model, which resolves short-wave and long-wave radiation, and the SPAC model from (Tuzet et al., 2003). This coupling is integrated in the highly parallelized CFD software *code\_saturne*, which is well-suited to atmospheric applications. The feasible spatial scale ranges from 10m<sup>2</sup> to 5000m<sup>2</sup>, and the temporal scale spans from short simulations lasting a few minutes to extended simulations covering several days.

The fluid solver and the radiation model resolve 3D governing equations on 3D meshes which aim at representing specific situations, for example trees blocking wind flow, or photovoltaic panels obstructing sky exposure. Wind speed, air temperature, and specific humidity are derived using the Unsteady Reynolds-Average Navier-Stokes (U-RANS) equations, while short-wave and long-wave radiation are determined using the Discrete Ordinate Method (DOM). An innovative approach is employed to implicitly consider obstacles (e.g. hedgerows, trees, or photovoltaic panels) without representing them directly in the mesh, which would otherwise be computationally demanding. As described by (Katul et al., 2004) for trees or (Vernier et al., 2025) for photovoltaic panels, obstacles' impact on the microclimate can be modelled through source and sink terms directly implemented locally in the governing equations.

The considered SPAC model is composed of a plant layer assumed to be vertically homogeneous and located above a soil surface layer and a deep soil layer. It acts as the bottom boundary condition for the fluid, temperature, and radiation solvers by deriving plant-air and soil-air exchanges based on the local microclimate conditions retrieved from the CFD outcomes. The level of incident radiation at the plant canopy top is given by the DOM radiation model, then a Beer-Lambert law drives the quantity of short-wave and long-wave radiation absorbed by the plant layer and transmitted to the soil surface layer. Next, stomatal conductance is calculated:  $g_{CO_2} = g_0 + a f_{\Psi} / (c_i - \Gamma)$ , where  $g_0$  is the minimum value of stomatal conductance at light compensation point,  $a$  is an empirical coefficient,  $c_i$  is the intercellular-space CO<sub>2</sub> concentration, and  $\Gamma$  is the CO<sub>2</sub> compensation point. It depends on short-wave radiation and ambient temperature





through the assimilation rate  $A$ , which is derived from Farquhar's photosynthesis model, and soil water content through the water stress factor  $f_{\psi}$ . Together with plant aerodynamic and boundary layer resistances – which depend on simulated wind speed and turbulent fluxes at the plant canopy top – the stomatal conductance enables the estimation of plant latent and sensible heat fluxes, and ultimately, plant temperature and evapotranspiration.

## Results and Discussion

The simulated plant and soil energy and water exchanges are firstly evaluated in open-field conditions using data from ICOS, the Integrated Carbon Observation System: the overall RMSE, regarding energy exchanges, is lower than  $40 \text{ W/m}^2$ . Then, the estimations of solar and infrared radiation, as well as plant temperature are compared to measurements conducted at an experimental agrivoltaics power plant (e.g. photovoltaic panels above crops): plant temperature relative RMSE is lower than 15%. This demonstrates the capability of our model to accurately estimate plant thermal and water states in complex environments.

A key strength of the model lies in its ability to examine the impact of several obstacles, as exhibited in *Figure 1*, and so for many weather conditions: frost events, strong winds, heatwaves, or droughts. In this study, the impact of specific obstacles on plant temperature is investigated. While some obstacles – such as photovoltaic panels – would cast shadow, other obstacles – such as hedgerows – would attenuate wind speed. These two microclimate alterations lead to a reduction of evapotranspiration either by decreasing stomatal conductance, or by increasing aerodynamic and boundary layer resistances. This improved water conservation in the soil contributes to a greater plant resilience under dry conditions. Attenuating wind speed on sunny, yet cold, spring days can increase plant temperature by approximately  $5^{\circ}\text{C}$ , thereby boosting photosynthesis. On the contrary, under white frost conditions, it may exacerbate the risk of freezing, whereas photovoltaic panels can act as a radiation shelter, helping to protect plants from frost damage. Another strength of the model is its small time step, which enables capturing the temporal dynamics of stomatal conductance and photosynthesis rates in response to temporally varying microclimates. This approach not only considers light fluctuations – including the potential delay in plant response – but, also estimates extreme plant temperatures and water stress, along with their impacts on photosynthesis.

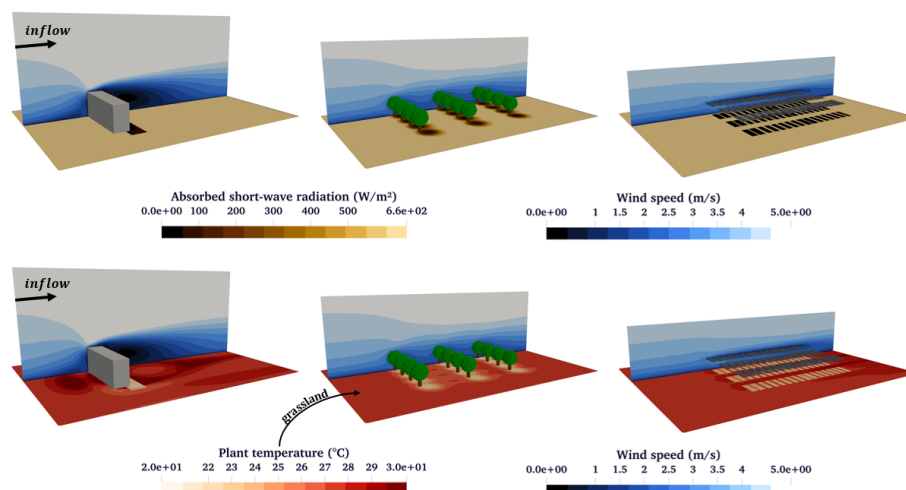


Figure 1. Simulated microclimate and the impact on plant temperature in complex environments: downstream a rectangular building (left), in an idealized agroforestry configuration (center), and within an agrivoltaic power plant (right).



## Conclusions

The coupling of CFD, radiation modelling, and a SPAC model enables simulating plant-air interactions in complex environments, notably those presenting spatial heterogeneity caused by obstacles. This paves the way to a better understanding of the impact of obstacles on plant photosynthesis and abiotic stresses. For instance, this model can help optimize agrivoltaic layouts by compensating for the reduction in photosynthesis caused by shading through heat and water stress mitigation.

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## Modeling perennial fruit trees with DSSAT-CSM: integration and evaluation of TREETRO

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**Keywords:** *Citrus sinensis* (L.), decision support, computer model.

### Introduction

The Decision Support System for Agrotechnology Transfer (DSSAT; Hoogenboom et al., 2024; 2019) is a leading crop modeling platform. However, despite its comprehensive set of models, it still does not include a perennial fruit tree module. Previous studies indicate that the Cropping System Model (CSM)-CROPGRO (Boote et al., 2018) within DSSAT provides a suitable basis for perennial fruit tree simulations, inspiring the TREETRO model (Morgan et al., 2003).

The initial TREETRO version, adapted from the CSM-CROPGRO-Tomato in DSSAT v4.4, due to its transplanted-fruit structure (Boote et al., 2012), showed potential but was never formally released. CROPGRO itself is a versatile modeling framework, featuring hourly simulations of leaf-level photosynthesis, a detailed soil-plant nitrogen balance, and routines for vegetative growth and reproductive development (Boote et al., 2018).

This study aimed to adapt, calibrate, and evaluate CROPGRO to strengthen TREETRO's conceptual development, as an opportunity to improve simulations of fruit tree systems, particularly sweet orange.

### Materials and Methods

Data from previously published experiments were used, including geographic location, phenological dates, planting density, scion/rootstock combinations, biomass data, weather and soil information. Multiple genetic parameters in the species and cultivar files were modified during the initial development process. Parameter values were set after a comprehensive literature review, ensuring that each coefficient reflected specific physiological and developmental traits of the sweet orange species.

Integration of the TREETRO code into the latest DSSAT-CSM version required further modifications. These changes were related to phenological routines, adjustments to represent the perennial nature of the crop, and structural updates to ensure consistency. To evaluate the impact of each modification, plant growth responses were tested by examining biomass allocation and developmental dynamics.

### Results and Discussion

After model adaptation and parameter calibration, TREETRO successfully reproduced the patterns of plant development and biomass accumulation across leaves, stems, and roots (Fig 1a). The simulated biomass partitioning among organs remained within the ranges reported in the literature (10-24% for leaves, 39-65% for stems and branches and 22-40% for roots). To estimate fresh fruit weight, a specific equation for dry matter content was derived and integrated into TREETRO.

Fruit size, expressed as unit weight over time, was reproduced by the model, capturing the temporal trajectory of fruit development (Fig 1b). After calibration of the cultivar file, the simulated fruit number aligned closely with experimental observations, demonstrating the model's ability to represent both fruit size and yield components. Consequently, total fruit yield was also reliably estimated. However, further improvements are still needed, particularly regarding the crop's response to drought stress and nutrient dynamics.





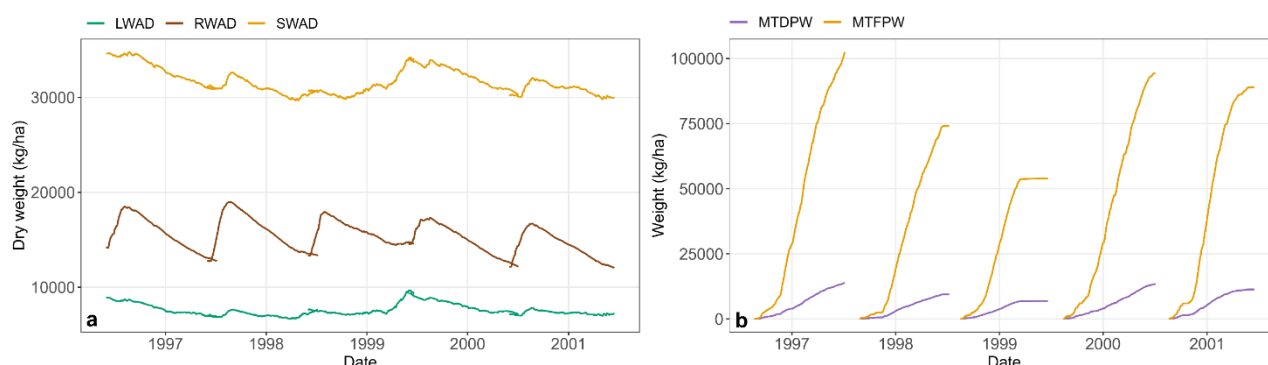


Figure 1. Leaf (LWAD), stem (SWAD) and root (RWAD) dry weight (a) of sweet orange Hamlin. Mature fruits fresh (MTFPW) and dry weight (MTDPW) (b) of sweet orange Hamlin.

## Conclusions

The TREEGRO model showed consistent and promising performance, especially following the refinements to the phenological routines and the representation of perennial growth dynamics. It proved effective in simulating key processes related to the growth, development, and yield of sweet orange.

## Acknowledgements

Financial support was provided by the Sao Paulo Research Foundation – Projects 2019/07665-4, 2022/06804-3 and 2023/14692-3.

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## Enhancing soybean phenology in crop models to evaluate its suitability

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**Keywords:** Glycine max, SPA model, STICS model, machine learning, climate change

### Introduction

Soybean is a high-protein, nitrogen-fixing legume with significant potential for sustainable agriculture in Europe (Rotundo et al., 2024). Despite its advantages, the EU27 remains heavily dependent on imports (16.5 Mt/year vs. 2.9 Mt produced locally in 2023; USDA, 2024). In France, soybean production has quadrupled over the past 15 years (0.4 Mt in 2024), and climate change is expected to further expand suitable cultivation areas northward (Nendel et al., 2023). Soybean phenology is primarily driven by photoperiod and temperature, with maturity groups (MGs) ranging from MG0000 to MGIII in Europe (Kurasch et al., 2017). To predict MG suitability under climate change, simple parsimonious model could be used, such as the Simple Phenology Algorithm (SPA), a model simulating key phenological stages based on few climatic data (Schoving et al., 2020a). This kind of model could be easily used on large spatial scale to predict the most adapted MG for a given location. Then to predict agro-environmental impacts of these most adapted MG, more complex models are needed but are less easy to use since they required more data (climate, soil, management), such as the STICS soil-crop model (Brisson et al., 2008). Both models need to predict soybean phenology for several MGs. Before being used at large scale, SPA required to extend the validity of stage-specific parameters across contrasted pedoclimatic conditions. STICS on the other hand underestimated the photoperiod effect beyond the beginning of grain filling (R5), leading to biases in predicting physiological maturity (R7) and yield (Schoving et al., 2020b).

Our final objective is to determine the most suitable MGs for soybean in France in current and future climate and evaluate their agro-environmental impacts. To do so, we aimed at 1-Improving SPA predictions for emergence and phenology stages for multiple MGs using a large dataset from French field trials. 2-Enhancing the STICS phenology formalism to reduce prediction drift for physiological maturity and improve yield simulations and 3- Using both models to predict soybean suitability and performances at high-resolution in France.

### Materials and Methods

We first gathered a database for soybean with 84 sites all over France, 78 with only phenology measurements and 6 with more complete data. For SPA, we developed a new module based on random forest to better predict emergence considering water availability through rainfall. SPA was then calibrated for seven maturity groups (MG0000 to MGII) using a two-stage Monte Carlo optimization (2/3 training, 1/3 validation), adjusting critical photoperiod, photoperiod sensitivity, and thermal time thresholds for flowering (R1) and harvest maturity (R8) stages. We used already known values for cardinal temperatures and optimal photoperiod (Setiyono, 2007; Schoving et al., 2020a; Maury et al., 2023). For STICS, we modified the photoperiod formalism to extend sensitivity until physiological maturity (R7), whereas it was previously limited to the seed-filling stage (R5) and recalibrated thermal time parameters between R5 and R7 on R software using the CROptimizR package (<https://sticsrpacks.github.io>) on a subset of the SPA dataset, which includes initialization, soil and management data required for STICS simulations. SPA simulations were run on 8,602 grid cells of 8x8 km across France for three climate periods (2003–2023, 2024–2044, 2045–2065) under RCP8.5, with optimal sowing dates determined annually based on temperature and water availability to determine the most suitable MG by grid cell





for each period, maximizing the length of R1-R8 phase. Based on these most suitable MGs, STICS will be run to assess their agro-environmental performances.

## Results and Discussion

The random forest model significantly improved emergence prediction accuracy, reducing RMSE from 5.7 to 0.7 days. Calibration of SPA for MGs MG0000 to MGII — using an extensive French field trial dataset — yielded robust predictions for phenological stages: RMSE < 7 days for R1 and 12.7 days for R8. The modified STICS formalism shows better predictions of physiological maturity dates for the different MGs, making it usable to assess soybean performances across France. Simulated sowing date were credible under current climate conditions, and predicted earlier planting (up to 30 days) for future periods (2045–2065). By mid-century, MGII increased by +85% and early MGs (MG0, MG00) by +49% and +31%, respectively (Figure 1). This northward expansion underscores the need for varietal adaptation to earlier flowering and enhanced cold tolerance, offering opportunities for regional self-sufficiency and sustainable cropping system diversification.

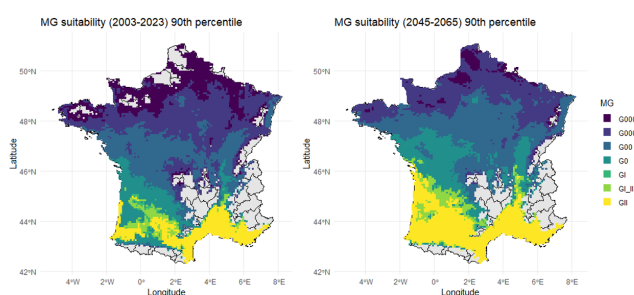


Figure 1. Projected expansion of soybean maturity groups in France between 2003–2023 and 2045–2065 under RCP8.5.

## Conclusions

According to SPA predictions, late MGs will expand northward under climate change, making soybean cultivation feasible across nearly all of France by 2045–2065. These results highlight opportunities for increased self-sufficiency and integration of soybean into new cropping systems. The modification of the STICS photoperiod sensitivity formalism lays the groundwork for further improvements in yield elaboration formalisms and model calibration using a large dataset with contrasted situations. Future work will focus on integrating this process-based model to assess yield potential and environmental impacts of these land-use changes.

## Acknowledgements

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## Adapting the CROPGRO Model for Winter and Spring Field Peas

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### Introduction

Pea (*Pisum sativum* L.) is a C3 legume that is widely grown as a fall-sown crop in areas where winters are sufficiently mild, or as a spring-sown crop in areas with colder winters. Its grain is high in protein and carbohydrate and is used for human consumption and animal feed. The Decision Support System for Agrotechnology Transfer (DSSAT) software (Hoogenboom et al., 2019) has modules for many legume and cereal crops, but it is lacking one for pea. The CROPGRO model within DSSAT is a generic mechanistic process-based model that simulates leaf-level photosynthesis, growth and maintenance respiration, explicit nodule growth and N-fixation, robust phenology, and partitioning. Its FORTRAN source code remains constant for all crops, while species process sensitivities and cultivar traits are read in as external files. With this template approach, DSSAT-CSM-CROPGRO has been successfully adapted for various grain legume species. The objective of this paper is to describe the adaptation of the CROPGRO model for winter pea, based on intensive growth and yield data collected at three sites over two seasons in Eastern OR, USA, with further evaluation of winter pea trials in Pullman, WA, USA, and spring pea trials in Minot, ND, USA.

### Materials and Methods

Experiments were conducted at three rainfed sites in Oregon during two seasons using three cultivars (Granger, an Austrian winter pea, and two food-quality winter pea cultivars Klondike and MiCa). The soils are very deep loess loam, and crops were sown in 25-cm rows with no fertilization in October. Time-series growth, tissue N concentrations, and phenology data were collected and final grain yield was taken in July. At Pullman, WA, phenology and final grain yield were collected from 6 years of rainfed winter pea yield trials. At Minot, ND, phenology and final grain yield were collected from 7 years of rainfed spring pea variety trials.

### Results and Discussion

Adaptation of the model followed the approach described by Boote et al. (2002) for faba bean, where literature information (Adams & Cosner, 2025; Lake et al., 2021) was used to set cardinal temperatures for growth processes (Table 1), followed by calibration against growth analysis data. Tissue compositions were set from literature and from observed tissue N concentrations. The initial template for winter pea was taken from the lentil model (Jing et al., 2024), which showed promise for winter lentil at Pullman, WA. Winter pea is a long-day species with critical long day (CLDL = 17 h) and photoperiod sensitivity (PPSEN = -0.070), along with EM-FL of 29.5 ptd (cv 'Klondike').

Table 1. Cardinal temperatures (°C): base (Tb), first optimum (Topt1), second optimum (Topt2), and ceiling failure (Tceil) for development, photosynthesis, expansive growth, pod addition, single seed growth rate, nodule growth rate, and nitrogenase rate of CROPGRO-Winter Pea

Growth process	Tb	Topt1	Topt2	Tceil
Vegetative development	3.0	25	30	40





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Reprod., Emerg to 1 <sup>st</sup> Seed	2.0	22	26	45
Reprod., 1 <sup>st</sup> Seed to Maturity	2.0	22	35	45
Leaf photosynthesis	2.0	30	31	40
Leaf area & height expansion	-0.8	17	17	---- <sup>1</sup>
Pod and seed addition	6.0	16	24	34
Seed growth rate	3.0	18	21	36
Nodule growth rate	-1.0	13	25	40
Nitrogenase (Nfix) rate	-3.0	11	25	40

<sup>1</sup>no ceiling temperature used, no reduction at high temperature

Parameter modifications included increased rate of rooting depth, lower cardinal temperatures for nodule growth/N-fixation, and modified partitioning among leaf, stem, and root tissues. Cardinal base temperatures were 3, 2, 2, and 3 °C for rate of main stem leaf appearance, reproductive development, leaf photosynthesis, and seed growth rate, respectively (Table 1). Increased rate of rooting depth was needed to reproduce observed deep soil water extraction to 2 m, along with sustained observed plant growth under rainfed conditions. Slow rate of leaf appearance, relatively low partitioning to leaf, and slow hedgerow canopy height-width expansion were needed during winter months to reproduce the slow crop biomass growth during winter months. Model calibrations were successful for three cultivars across two seasons at three sites, with good performance statistics. Growth during the winter was slow but was followed by rapid growth in spring as temperatures warmed up, as shown by leaf mass over time for cv 'MiCa' for five site-years (Figure 1). The total life cycle was more than 250 days, with rapid reproductive growth during the last 30-40 days associated with rapid leaf loss and rapid increase in pod harvest index (Figure 1). Evaluations showed good performance for phenology prediction and yield in rainfed trials of winter pea in Pullman, WA and spring pea in Minot, ND, where careful attention was paid to establishing initial conditions for soil water. This often required running in crop sequence-rotation following a prior wheat crop (typical for these sites) to deplete and set initial soil water. Only minor cultivar phenology parameter modifications were needed for spring pea cultivars, so the CROPGRO-Pea model appears to work well for winter and spring pea. The CSM-CROPGRO-Pea model will be included in a future DSSAT release.

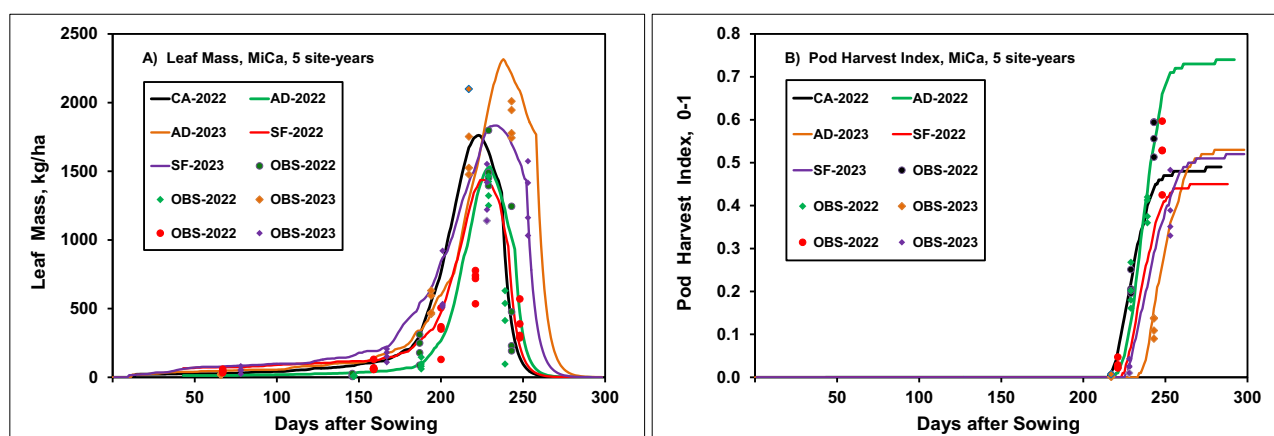




Figure 1. Simulated leaf mass (A) and pod harvest index (B) over time for MiCa winter pea cultivar for 5 site-year treatments.

## Conclusions

CROPGRO was successfully adapted for simulating winter and spring field peas. Relatively low cardinal temperatures for processes were required to simulate growth over winter seasons. Rooting to 2 m was needed to mimic observed deep soil water extraction for rainfed simulations. Evaluations showed good performance against trials of winter pea in Pullman, WA and spring pea in Minot, ND. CROPGRO-Pea will be included in a future release of DSSAT.

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## Towards improved modeling of sugarcane radiation use efficiency: temperature dependence, crop age effects, and model formalisms

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**Keywords Calibri: Saccharum spp.; Cultivar; Cardinal temperatures; Climate change; Crop modelling**

### Introduction

One of the advantages of sugarcane (*Saccharum* spp.) is its exceptional ability to convert sunlight into biomass, with reported radiation use efficiency (RUE) values among the highest of all major crops (Sinclair and Muchow, 1999). RUE is a critical emergent trait in crop physiology and a central parameter in most dynamic sugarcane simulation models. However, debate persists over whether RUE is stable across varieties and growing conditions, particularly when distinguishing between apparent RUE ( $RUE_A$ ) and maximum seasonal RUE ( $RUE_{MAX}$ ) (Jones et al., 2019). C4 species such as sugarcane are well adapted to high temperatures ( $>25^{\circ}\text{C}$ ), but it is also acknowledged that these species are significantly sensitive to variations in air temperature within the  $20\text{--}30^{\circ}\text{C}$  range. This is particularly relevant as climate change may shift growing environments closer to or beyond these thresholds. Current sugarcane models differ substantially in their representation of  $RUE_{MAX}$  temperature response (Jones et al., 2019). Such structural differences can strongly influence biomass predictions under future climate scenarios. In this context, the International Consortium for Sugarcane Modelling undertook a coordinated effort to evaluate temperature response formalisms using a global dataset to refine model calibration and improve varietal sensitivity representation (Christina et al., 2025).

### Materials and Methods

We analyzed an international dataset including field experiments from six countries (Brazil, South Africa, United States, Zimbabwe, Argentina, and La Réunion) covering more than 40 varieties. We estimated apparent RUE ( $RUE_A$ ) and maximum RUE ( $RUE_{MAX}$ ) from observed biomass accumulation and intercepted radiation. We then parameterized different temperature response functions for  $RUE_{MAX}$ , which is currently used in APSIM-Sugar, DSSAT-Canegro, MOSICAS, and other emerging approaches. Model predictions of  $RUE_A$  were evaluated against independent observations in different countries, and the implications of the choice of model formalism or parameterization regarding projection under climate change were assessed.





## Results and Discussion

Our results confirmed that  $RUE_{MAX}$  was stable across varieties (as suggested by Dias et al., 2021), while  $RUE_A$  exhibited significant variation driven by both environmental conditions and genotype (Christina et al., 2025). Across all sites,  $RUE_{MAX}$  showed a consistent temperature optimum between 30–33 °C depending on formalism (Figure 1). Simulations highlighted substantial differences in the ability of existing model formalisms to reproduce observed patterns, with direct consequences for projected biomass accumulation under current and future climates.

Even under apparent optimal growing conditions, our analyses suggested a decline of RUE with crop age, which depends on the variety, a phenomenon insufficiently represented in current models. Several hypotheses may explain this decline as part of the “reduced growth phenomenon” (Park et al., 2005), including reductions in leaf nitrogen content, changes in sugar partitioning, increased maintenance respiration, or structural effects such as lodging. These hypotheses are the focus of ongoing work within the consortium, and the way crop models represent these formalisms will be evaluated against experimental data.

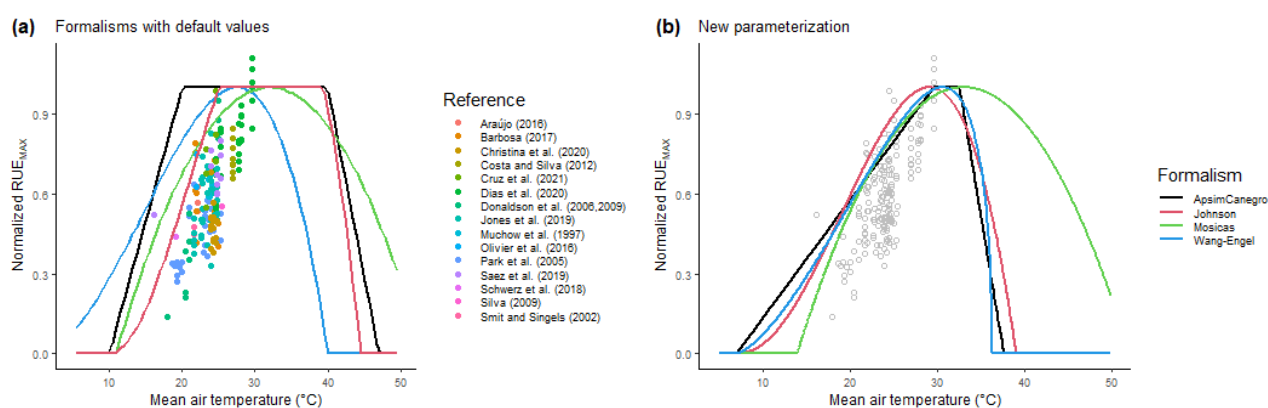


Figure 1. Change in normalized maximum radiation use efficiency ( $RUE_{MAX}$ ) with mean air temperature depending on formalism (ApsimCanegro, Johnson, Mosicas, and Wang-Engel) based on default parameters values (a) and quantile regression (b). Details on methodology is available in Christina et al. (2025).

## Conclusions

Accurate representation of RUE temperature dependence is essential for reliable sugarcane biomass projections under climate change. Current formalisms differ substantially in their ability to capture observed dynamics, emphasizing the need for refined parameterization and structure. Current work is extending this analysis to age-related effects on RUE, which may further improve crop model projections under climate change. Within the international consortium, we have also formulated recommendations for calibration strategy in sugarcane crop models and varietal-sensitivity improvements, to guide future model development and application.

## Acknowledgements

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## Introducing the Radish Crop into the DSSAT-Cropping System Model

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**Keywords:** Digital twins, CROPGRO, Korean radish, model development, *Raphanus sativus*

### Introduction

Radish (*Raphanus sativus* L.) is an edible root and one of the most consumed vegetables in the *Brassicaceae* family worldwide. As an integral part of numerous Korean dishes, its year-round availability is crucial to guarantee a steady supply to domestic consumers (Pusik and Pusik, 2025).

Estimating radish growth and yield helps optimize crop management by testing scenarios for current and new environments, supporting farmers' decisions. A systems approach with dynamic crop models can complement field research, reduce the need for costly new trials, and improve management strategies.

Crop models such as CROPGRO within the Decision Support System for Agrotechnology Transfer - Cropping System Model (DSSAT-CSM) have a mechanistic approach and a generic feature that enables them to be adapted for new species (Hoogenboom et al., 2019). In this context, the main goal of this study was to develop a radish model for DSSAT-CSM by adapting the CROPGRO model using field trial data conducted in the Republic of Korea by the Rural Development Administration.

### Materials and Methods

We used experimental data collected from two seasons (2023-2024). The field trials were carried out at the National Institute of Horticultural and Herbal Science facility in Wanju-gun, Jeonbuk, Republic of Korea, using the Cheongdu-gold variety. The radish plants were distributed in rows and irrigated. Daily weather data were obtained from a nearby automated weather station.

The crop growth data consisted of measurements of root and above-ground biomass dry weight ( $\text{kg ha}^{-1}$ ), Leaf Area Index (LAI), number of leaves, leaf N concentration (%), canopy height and width (m), and rooting depth (m).

The CROPGRO-Soybean model in DSSAT v4.8.5 (Hoogenboom et al., 2024) was used as a template to start the parameterization of key genetic coefficients for radish based on a thorough literature review and field observations. For the model adaptation, we modified the three files related to genotypic features, i.e., cultivar, ecotype, and species files, in DSSAT.

The model's performance was assessed by calculating the root mean square error (RMSE) and the Willmott index of agreement (d-stat).

### Results and Discussion

The CROPGRO model demonstrated satisfactory ability in simulating radish growth and yield under optimal conditions. When analyzing the 2-year observed data, the model provided simulations of above-ground biomass with high accuracy (RMSE =  $108 \text{ kg ha}^{-1}$ ) and precision (d-stat = 0.97). Similar responses were observed for root mass simulations (RMSE:  $362 \text{ kg ha}^{-1}$ , and d-stat = 0.96) (Fig. 1). Also, the model was able to reproduce the radish responses to the environmental variability from year to year.



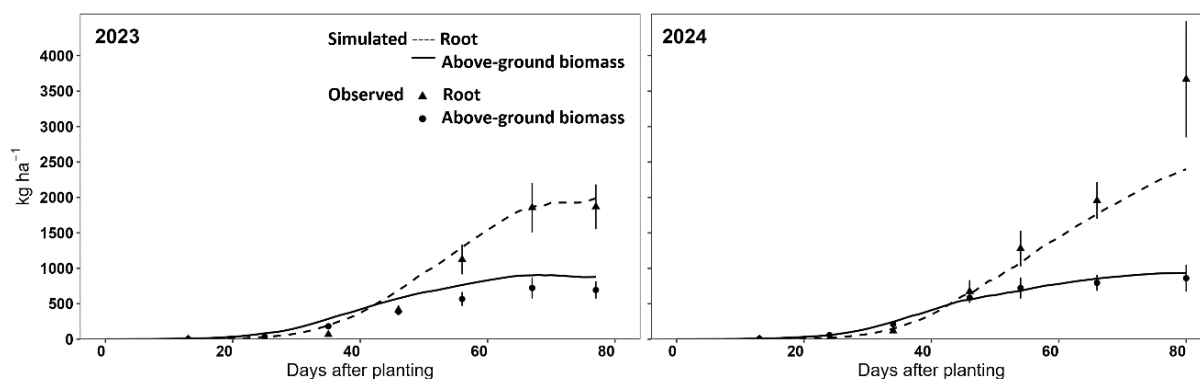


Figure 1. Simulated (lines) and observed (symbols) radish root mass and above-ground biomass (kg ha<sup>-1</sup>) for the 2023 (left panel) and 2024 (right panel) growing seasons. Error bars show the standard deviation across the replicates.

## Conclusions

The parametrization of the CROPGRO model shows promising results in simulating radish growth and yield, which will enable the introduction of this crop to DSSAT. Additionally, further tests will be conducted for evaluating the effect of water and nitrogen on radish.

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## A Process-Based Framework for Simulating Cereal–Grain Legume Intercropping Systems

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**Keywords:** intercrop modeling; competition-facilitation, agroecology.

### Introduction

The growing demand for sustainable agriculture has renewed interest in cereal–grain legume intercropping, thanks to its potential to reduce chemical inputs, enhance land-use efficiency, and deliver multiple ecosystem services (Bedoussac et al., 2015). However, predicting the performance of intercropping systems remains challenging due to complex interactions among plant species, environmental conditions, and management practices. While process-based agroecosystem models are valuable for exploring these interactions throughout the growing season, few existing models are capable of accurately simulating intercropping dynamics (Vezy et al., 2023).

### Materials and Methods

This study presents and evaluates a new modeling framework for bi-specific intercropping systems, adapted from the WeedyCoSMo approach originally developed for simulating crop–weed interactions (Movedi et al., 2022). The proposed formalism is simple, generic, and designed to be easily integrated into existing dynamic crop models. We demonstrate its implementation in a modified version of the MONICA crop model (Nendel et al., 2011), in which two crop modules interact dynamically through a shared soil module. The framework simulates key physiological and ecological processes—including phenology, biomass accumulation, yield formation, light interception, and carbon and nutrient cycling—while accounting for interspecific competition for light, water, and nitrogen. It dynamically predicts both species-specific and community-level state and rate variables and quantifies each species' suitability under competitive conditions via their relative abundance (Figure 1). Data for calibration and evaluation were collected from literature and dedicated intercropping field trials conducted in Italy and Germany. These datasets included various cereal–grain legume combinations (durum wheat, common wheat and oat intercropped with lentil and chickpea), spanning a wide range of pedo-climatic conditions, experimental designs, and both spring and winter cropping seasons. Variables measured included above- and below-ground biomass, grain yield, plant tissue nitrogen content, plant height, leaf area index, and soil nitrogen and moisture. The MONICA model had already been parameterized for most of the crops involved; however, sole crop data from the dataset were used to refine these parameters and to calibrate the few additional ones required for WeedyCoSMo. Data from intercropped plots were exclusively used to evaluate the model framework.

### Results and Discussion

Preliminary results suggest that the model performs robustly across a diversity of environments and cropping systems. The model reproduced biomass-related and other intercrop variables from field experiments, achieving nRMSE values of 15–60% and a Willmott index of agreement between 0.29 and 0.85. Despite requiring relatively few additional parameters, its predictive accuracy is comparable to that of more complex models. The framework effectively captures key species differences and crop combinations, and is capable of reproducing both competitive (one species dominating over the other) and facilitative interactions (e.g., nitrogen fixation) between intercropped species.



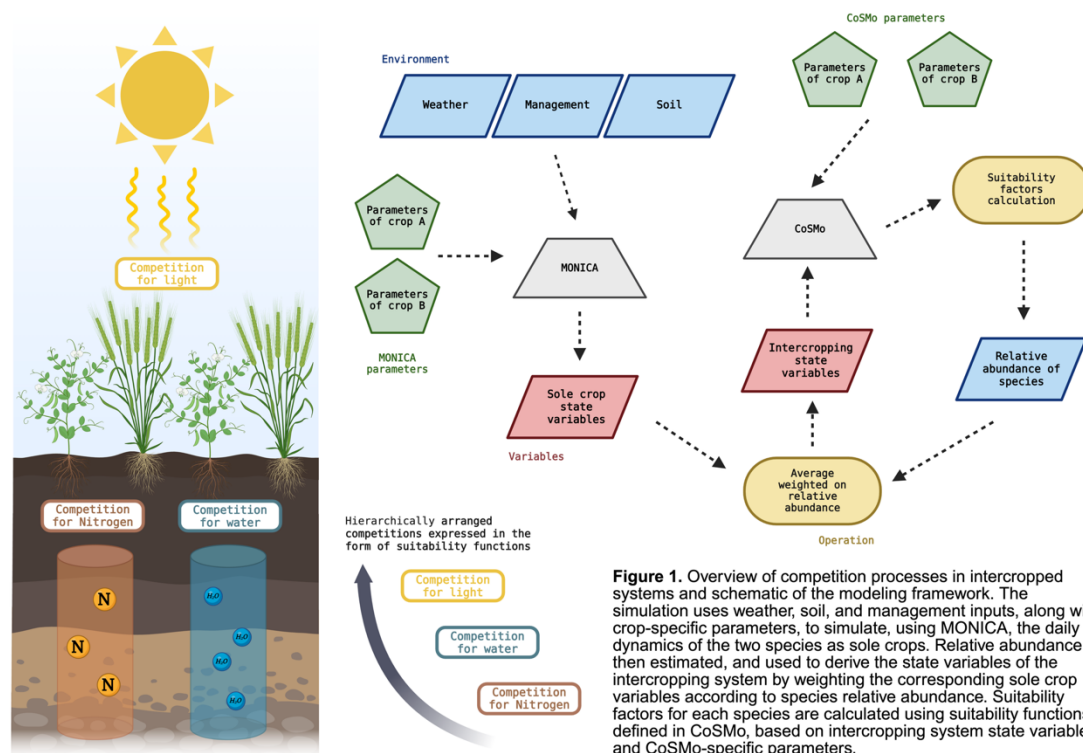


Figure 1. General concept and functioning of the modeling framework

## Conclusions

In summary, this modeling framework provides a promising tool for the design and virtual pre-evaluation of sustainable, locally adapted intercropping strategies. By enabling in silico experimentation, it contributes to agroecological transition efforts and enhances the capacity to develop more resilient farming systems.

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## DeepCGM-generic: A Deep Learning Based Crop Growth Model for Multi-Varieties

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**Keywords:** crop growth model, hybrid model, deep learning

### Introduction

Traditional crop models are based on fixed mathematical equations and require manual modification, which leads to inefficient data use and slow improvement. The rise of data science and AI is shifting mechanism-centric scientific fields toward data-centric approaches. Our previously developed Deep Learning Crop Growth Model (DeepCGM) is a hybrid model that leverages both process-based and data-driven approaches (Han et al. 2025). However, its architecture prevents it from being adapted to other cultivars. This study proposed DeepCGM-generic, which introduces a module for learning crop attributes and the a phenology module. The model is evaluated on a synthetic dataset.

### Materials and Methods

**The synthetic dataset** containing 900 cultivars  $\times$  10 seasons data was generated by PCSE model. The inputs are cultivar parameters, weather data, and management data. The output is the time-series crop states. Cultivars are defined by using different values of eight cultivar parameters.

**DeepCGM** features a Recurrent Neural Network architecture, controlling information flow with a mass-conserving gated unit. It overcomes the overfitting problem caused by sparse observation data by leveraging an architecture and training strategies informed by principles of plant physiology and physics.

**DeepCGM-generic** aims to overcome cultivar-adaptation limitations. Our approach integrates a Hypernet (David et al. 2016) with Low-Rank Adaptation (Hu et al. 2021) modules to learn and represent cultivar parameters (Figure 1a). Another advancement is the new phenology module that replaces the Growing Degree Day method with an effective time calculation. A gating unit processes various factors into a daily effectiveness coefficient to determine phenology increment.

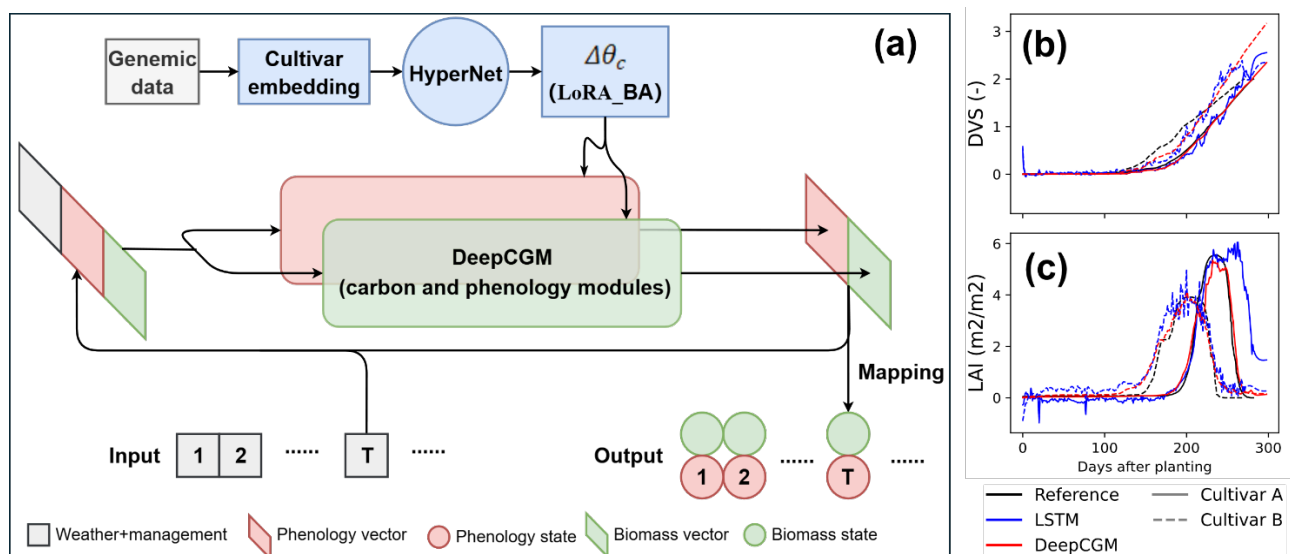


Figure 1. (a) The framework of DeepCGM-generic. (b) and (c) are the simulations of two new cultivars by different models





## Results and Discussion

A experiment was designed with 36 scenarios by varying the number of cultivars (4 levels), observation interval (3 levels), and observation noise (3 levels) (Table1). A same test set was used across all scenarios. A weighted normalized mean square error loss is used as evaluation metrics. The different time-series prediction pattern shows that DeepCGM can identify different cultivars (Figure 1b, c). In addition to overcoming the overfitting caused by data sparsity, DeepCGM also achieves higher simulation accuracy in new cultivar, as shown in the LAI simulation results for cultivar A. Compared to the LSTM model, DeepCGM requires less data and achieves superior performance in most scenarios (Table 1).

Table 1. Test set loss (values  $\times 10^4$ ). Interval, cultivar, and noise denote the pretraining configurations.

Interval		40				20				10				
Cultivar		10	50	200	800	10	50	200	800	10	50	200	800	
Observation (10 <sup>3</sup> )		0.5	2.4	9.6	38.4	1	4.8	19.2	76.8	1.9	9.6	38.4	153.6	
LSTM	Noise	0.05	358	201	89	93	311	184	<b>68</b>	60	216	136	<b>61</b>	71
		0.1	375	220	100	71	328	200	<b>76</b>	68	234	164	<b>61</b>	62
		0.2	370	242	134	80	326	219	101	78	283	187	<b>85</b>	63
0.05		<b>171</b>	<b>112</b>	<b>81</b>	<b>57</b>	<b>154</b>	<b>106</b>	76	<b>57</b>	<b>149</b>	<b>96</b>	77	<b>60</b>	
0.1		<b>188</b>	<b>141</b>	<b>88</b>	<b>62</b>	<b>172</b>	<b>108</b>	81	<b>60</b>	<b>165</b>	<b>107</b>	82	<b>57</b>	
0.2		<b>247</b>	<b>143</b>	<b>99</b>	<b>67</b>	<b>202</b>	<b>115</b>	<b>83</b>	<b>65</b>	<b>196</b>	<b>109</b>	88	<b>61</b>	

## Conclusions

This work introduces DeepCGM-generic, an enhanced DeepCGM model equipped with an architecture for cultivar adaptation and a phenology simulation module, which outperforms purely data-driven models and requires less data when adapting to new cultivars.

## Acknowledgements

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## Bridging literature and models: a workflow for creating agricultural datasets for model applications using AI

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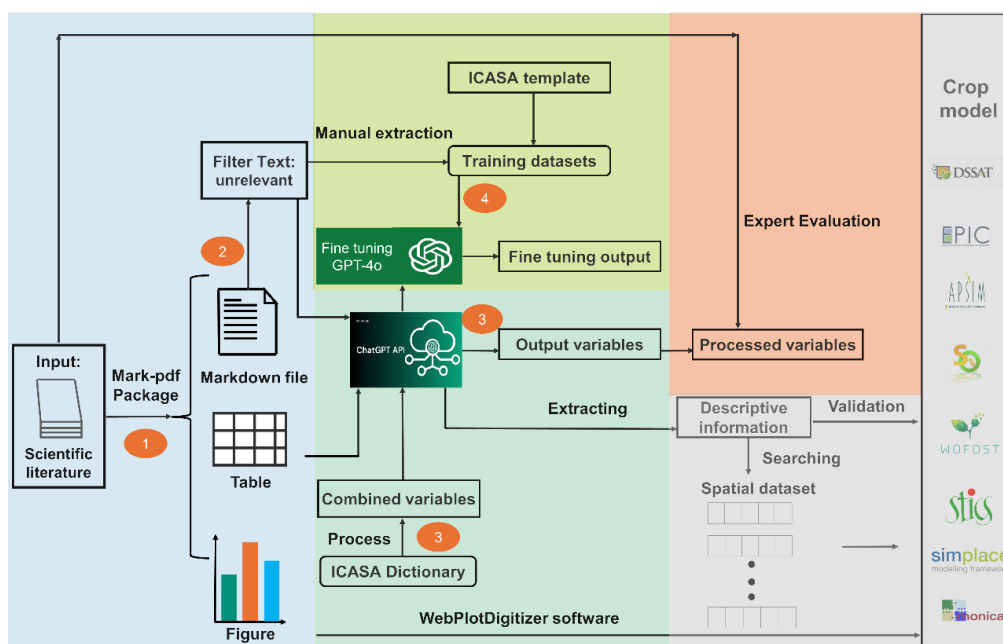
**Key words:** Simulation models, agricultural data extraction, ICASA variables, large language Model

### Introduction

Simulation models were tools for agricultural research, providing critical insights into complex crop-soil interactions and informing data-driven decisions around sustainable cropping system management. However, models remained underutilized due to the limited availability of standardized and comprehensive experimental datasets suitable for model development, parameterization and evaluation. In crop research papers, authors typically included content to describe how experiments were conducted as well as results. However, it largely existed in unstructured prose, summary tables and figures. Development of Large Language Models enabled efficient extraction of structured, actionable data from unstructured text by non-experts (Gartlehner et al., 2024; Polak and Morgan, 2024).

### Materials and Methods

In this study, we introduce a novel automated workflow to address data limitations by systematically extracting and harmonizing data from published literature (Fig. 1). Our approach comprises five key steps: (1) converting PDF documents to Markdown files to enable efficient text parsing and tabular data extraction, (2) isolating the materials and methods sections to capture essential experimental context, (3) mapping text and table outputs to International Consortium for Agricultural Systems Applications (ICASA) variables using a large language model, (4) fine-tuning the large language model based on training datasets extracted manually, and (5) establishing connections between related publications to enhance data completeness and contextual understanding.



# Crop Modelling for Agriculture and Food Security under Global Change



**Figure 1.** An automated workflow that processes data, incorporates a fine-tuned model, and enables seamless integration for agricultural model applications.

## Results and Discussion

The workflow is both fast and accurate, effectively extracting ICASA variables from various publications. Achieving a balance between consistency and accuracy remains a major challenge. To address incomplete datasets issues, we plan to link the extracted experimental data with spatial soil, weather, crop and crop management datasets, based on the geographical information inside the PDFs.

## Conclusions

By improving the findability and interoperability of model inputs, this research demonstrates the feasibility of using AI-driven tools for extracting structured data from unstructured scientific literature.

## Acknowledgements

This work was financially supported by FAIRagro project.

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## Improving phenology and yield predictions in APSIMx using exclusively public data: a reproducible calibration workflow

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**Keywords:** modelling, wheat, barley, maize, oilseed rape.

### Introduction

Regional modeling depends on robust calibration, yet it is often limited by inconsistent, inaccessible, or sparse datasets. The increasing availability of public agronomic data offers new opportunities for model calibration, especially for resource-limited or regional-scale projects. While manual trial-and-error calibration remains common, recent research has advanced harmonized workflows, particularly through the Agricultural Modeling Intercomparison Project (AgMIP). The *croptimizR* R package (Buis et al., 2024) has standardized calibration by providing an accessible workflow for parameter estimation, automatically optimizing results based on observational data and user-defined parameters.

Process-based models like APSIM (Agricultural Production Systems sIMulator) are widely used for agricultural impact assessments, with APSIM Next Generation (APSIMx) offering improved computational performance and flexibility. However, validated crop parameters for Central European conditions are lacking in APSIMx, and previous calibrations—primarily with APSIM classic—have often been site-specific and manual, limiting reproducibility. The resulting APSIM classic parameters may be overly tailored to local conditions and cannot be directly transferred to APSIMx due to structural model changes.

To avoid overfitting, calibration should incorporate data from multiple sites with contrasting conditions. The increasing availability of public German agricultural datasets offers opportunities for standardized, transparent model calibration. While workflows for APSIM classic are well documented, a workflow for APSIMx using public datasets has not been previously described. This study addresses these limitations by presenting a reproducible calibration workflow using the *croptimizR* for German key crops - winter wheat, silage maize, winter oilseed rape and spring barley - in APSIMx, leveraging only public datasets. It demonstrates the usefulness of public data for modeling and supports transparent, policy-relevant agricultural research.

### Materials and Methods

To ensure not only reproducibility but also spatial transferability, we relied exclusively on publicly available datasets that cover all of Germany for model input, calibration, and validation. Using the *croptimizR* (Buis et al., 2024), we first calibrated phenology and then yields at two contrasting locations in Schleswig-Holstein, Northern Germany, and Saxony, Central Germany for the years 2010-2023. As observational input we used phenological observation data (DWD, 2024) and average district-level dry matter yields (Duden et al., 2023), which were complemented by 2023 yield data from the federal statistics office (Statistische Ämter des Bundes und der Länder, 2024). Then, we validated the crop parameters to evaluate the robustness of the parameters at two additional locations in the same states, but with differing pedoclimatic conditions. Weather data was extracted from gridded weather files for the phenological observation station





locations (DWD, upon request). As soil input we used chemical and physical soil profile core data of soil types typically under crop production in the regions from the national German soil inventory (Poeplau et al., 2020). Regionally typical management assumptions were made for each crop in consultation with experts and federal state recommendations. For the parameter ranges used in the calibration, i.a. regional temperature sum quantiles for crop-specific phenological phases were used from Möller and Gerstmann (2023) and Möller et al. (2020).

## Results and Discussion

Both phenology and yield predictions were improved for the four crops compared to initial cultivars, using the calibrated parameters at the calibration sites and at validation sites. The RMSE and nRMSE of all phenological phases at the two calibration sites ranged from 7.7 days and 13 % for silage maize to 18.8 days and 21 % for spring barley after calibration, respectively (Heiß et al., submitted). Yield predictions for all crops could be improved overall, but sometimes at the cost of one prediction accuracy at one of the calibration or validation sites due to the strong pedoclimatic differences between the sites. Compared to other calibration studies with either very detailed field experiments over often shorter time periods or large-scale calibration studies the yield prediction performed well with the calibrated parameters, especially considering the uncertainties related to the data sets used. This could also explain why interannual yield variability is captured rather poorly. Nevertheless, for regional modelling studies the performance may still be sufficient, as often average yields are used for certain periods. (e.g. Bonato et al., 2025).

## Conclusion

This study demonstrated successful calibration of four key crops, winter wheat, silage maize, winter oilseed rape and spring barley, in APSIMx using exclusively public datasets, despite inherent data uncertainties. The calibrated parameters improved both phenology and yield predictions across contrasting pedoclimatic conditions, achieving accuracy levels comparable to experimental calibration studies. While interannual yield variability was not fully captured, the achieved accuracy may be sufficient for many regional modeling objectives. The automated calibration workflow using *croptimizR*, combined with public data, effectively lowered barriers for crop model adoption, particularly for resource-limited projects. By making all workflows and parameters publicly available, this study promotes FAIR (Findable, Accessible, Interoperable and Reproducible) modeling practices. Future work could build on these generic crop parameters through sensitivity analyses and richer observational datasets. Overall, this workflow demonstrates the potential of public data for robust APSIMx calibration, advancing model reliability for sustainable agricultural management in Central Europe and beyond.

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## Uncertainties among soybean models in simulating N balance

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**Keywords:** Nitrogen fixation, Partial nitrogen balance, crop models, soybean, climate change

### Introduction

Soybean is a major leguminous crop with unique biological nitrogen (N) fixation capabilities through symbiosis with rhizobia. Because it usually requires little or no nitrogen fertilizer, it is a beneficial component of crop rotations aimed at reducing dependence on synthetic nitrogen fertilizers. Understanding the net N contributions from soybean to the system or partial N balance is vital for optimizing grain crop rotations and minimizing environmental losses such as nitrate leaching and nitrous oxide emissions. Process-based crop models help simulate these dynamics under varying environments and management, but simulations differ due to input, parameter, and structural uncertainties. Multi-model sensitivity analyses can be helpful to improve accuracy, capture climate change effects, and inform sustainable nitrogen management. The objective of this study is to investigate the uncertainties of commonly used soybean simulation models in estimating partial nitrogen balance, including the impacts of climate change factors such as elevated CO<sub>2</sub> and temperature on N balance components.

### Materials and Methods

A group of nine process-based crop models were calibrated using multi-year experimental data from five locations (Azul, Argentina; Brasilia, Brazil; Auzeville, France; and Ames, Iowa and Fayetteville, AR in the U.S.) (Kothari et al., 2022). All locations included detailed in-season growth data, in addition to detailed crop N data from two of the locations (France and Iowa). The calibration was performed in two stages: Blind (phenology only) and Full (crop growth and N, yield, and soil moisture data). Following calibration, 30-year sensitivity analyses (1980–2009) tested responses to five temperature scenarios (–3 to +9 °C), five [CO<sub>2</sub>] levels (360–720 ppm), and to irrigated vs. rainfed conditions. Partial nitrogen balance was calculated as: Fixed N - Grain N - Leached N - Volatilized N - Denitrified N and nitrogen harvest index (NHI) as: GrainN / ShootN. Model outputs for different components of the N balance, partial N balance, and NHI were analyzed across sites and climate change scenarios.

### Results and Discussion

Soybean models showed large variability in simulated partial N balance, ranging from strongly positive to negative (Figure 1), associated to major uncertainties in biological nitrogen fixation (BNF) and N loss processes (not shown). Most models simulated negative partial N balance due to high grain N export, highlighting risks of soil N depletion, except for LINTUL and DSSAT-EBL. The variation among the soybean models simulating N balance components and the derived partial N balance can be attributed to structural differences among models, such as how models handled leaf senescence and N mobilization from vegetative N pools. Results indicate that while current soybean models provide reasonable estimates of NHI, substantial uncertainty persists in the simulation of partial N balance, particularly under variable water regimes. Results evaluating the multiple soybean models under variable temperature and [CO<sub>2</sub>] scenarios will be also presented.





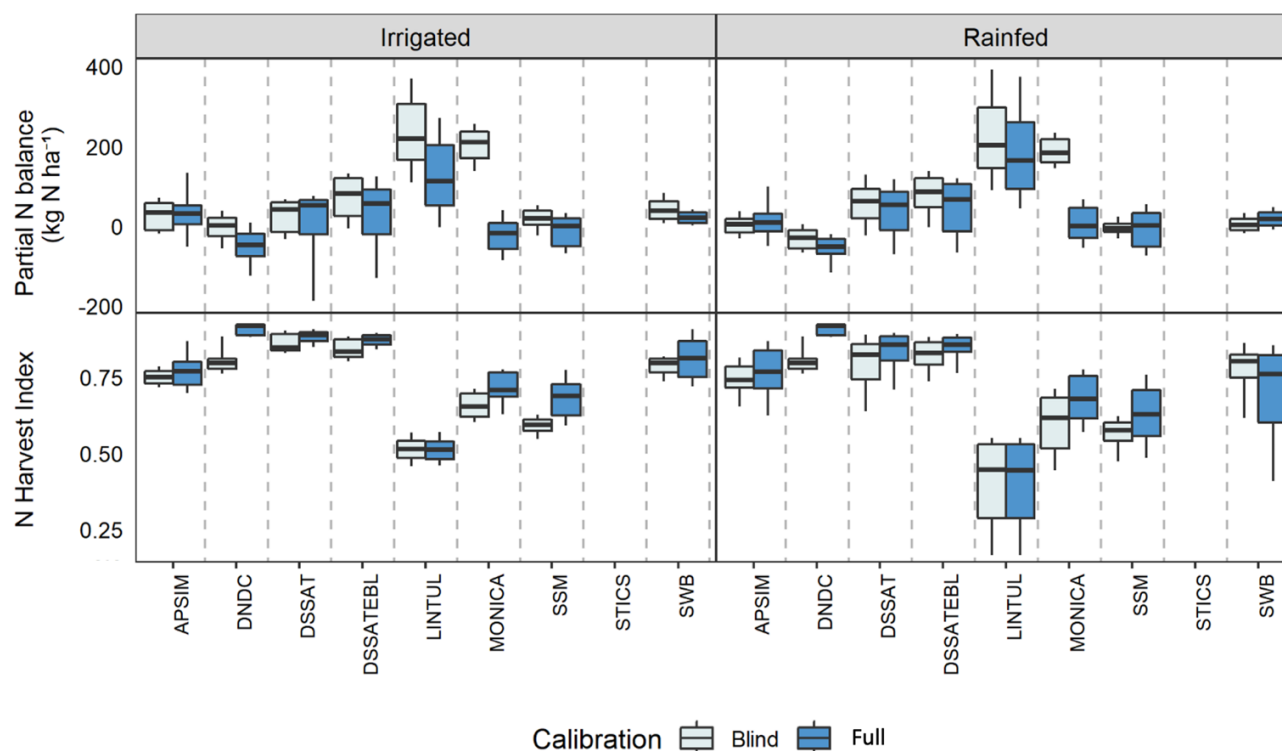


Figure 1: Partial nitrogen balance (top row) and nitrogen harvest index (bottom row) simulated by nine soybean models under irrigated (left panels) and rainfed (right panels) conditions. Each boxplot represents the distribution of model outputs across experimental sites and treatments. Gray and blue bars depict the two calibration strategies: Blind and Full. Positive partial N balance values indicate greater N inputs via biological fixation relative to losses and grain export, while negative values suggest potential soil N depletion. Differences among models reflect variation in their representation of biological nitrogen fixation, N allocation, and loss pathways.

## Conclusions

Soybean models reliably predict nitrogen harvest index, but estimates of soil nitrogen balance vary widely irrespective of the water conditions. Improving how models handle nitrogen fixation and losses is important for sustainable farming.

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## Integrating molecular and physiological models improves genotype–phenotype prediction of wheat flowering time

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**Keywords:** Phenology, anthesis time, cereals, gene-based modelling, APSIM Next Generation

### Introduction

Genotype-to-phenotype prediction in crops requires quantifying both physiological responses to environmental drivers and their underlying genetic controls. Flowering time is a critical trait for aligning cereal genotypes with target environments, yet current molecular models insufficiently incorporate environmental signals, while physiological models struggle to capture the interactions among vernalization, photoperiod, and temperature across contrasting environments. We address this challenge by integrating molecular insights into physiology models through a redesigned phenology module in the APSIM Next Generation Wheat model.

### Materials and Methods

We developed the Cereal Anthesis Molecular Phenology (CAMP) model (Wang et al., 2025), building on a previous hypothetical prototype (Brown et al., 2013), to incorporate the regulatory roles of three major virtual genes—*Vrn1*, *Vrn2*, and *Vrn3*—in flowering physiology of cereal crops (e.g. wheat and barley). It simulates phenological development based on the expression of these genes in response to temperature and photoperiod (Fig. 1a). The enhanced molecular–physiology linkage enables a simplified phenotyping approach, using mainstem final leaf numbers of wheat and barley grown under controlled conditions, to characterize new genotypes and define model parameters for the earliness per se (MinLN), photoperiod sensitivity (PpLN), vernalization sensitivity (CvLN), and photoperiod x vernalization interaction (PvLN) (Fig. 1b). The controlled environments consist of four treatments: cold-vernalized plants growing under warm temperature (>20°C) with 16hr (CL) or 8hr photoperiod (CS), non-vernalized plants growing under warm temperature (>20°C) with 16hr (WL) or 8hr photoperiod (WS) (Fig. 1b). The new model was implemented in the APSIM Next Generation (APSIM NG) framework (Holzworth et al, 2014), parameterized for wheat and tested against field data across diverse environments, covering four sites in Australia and across two years (2020–2021), each year with 8 times of sowing ranged from 2 March to 16 July (Fig. 1c).

### Results and Discussion

The new phenology model (CAMP) was able to capture 88% of the variations in observed flowering dates, predicted flowering time within 4–7 days across 64 genetically diverse wheat cultivars grown under contrasting environments (Fig. 1c). There were large differences between replicates of the observed flowering dates at early times of sowing, indicating significant spatial variation, which accounted for about half of the prediction errors (RMSE in Fig. 1c). The largest errors are with the early sowing dates. Considering the ‘commercially relevant’ sowing dates from mid-April onwards, the





prediction errors are reduced by nearly half to around 4 days. The leaf-number phenotyping method reduced phenotyping time by more than 80%, offering a practical alternative to resource-intensive field trials. These results demonstrate the model's performance to predict flowering time of diverse wheat genotypes across contrasting environments.

The CAMP model enables simplified phenotyping for cultivar characterization and model parameterization, which involves simply measuring the final leaf number (FLN) and anthesis date on the mainstem of wheat grown in controlled environments that are designed to ensure complete saturation or deprivation of photoperiod and vernalization effects using factorial combinations of short or long photoperiod together with cold or warm temperature treatments during emergence. These data allow the simulation of expression rates of *Vrn1*, *Vrn2* and *Vrn3* and other parameters in the model. This simplifies field observations and has potential to reduce the substantial costs of field experiments used to derive cultivar parameters.

The enhanced molecular–physiology linkage makes it possible to more accurately predict flowering time directly from genotypic data (e.g., SNPs), potentially eliminating the need for costly field experiments. The new model is currently being used to combine genotypic and phenotypic data from wheat for the development of a genomic prediction model that predicts CAMP model parameters using SNPs. This will enable flowering time predictions directly using genotypic data (SNPs), representing a step change in molecular-physiological modeling, supporting faster deployment of new cultivars and more effective design of wheat for future climates. The CAMP model is now being used to develop a prototype Flowering Calculator to optimize sowing programs for wheat and barley across Australia so that crops flower at optimal time to minimize water, frost and heat stresses (<https://www.cropflowering.com.au/>).

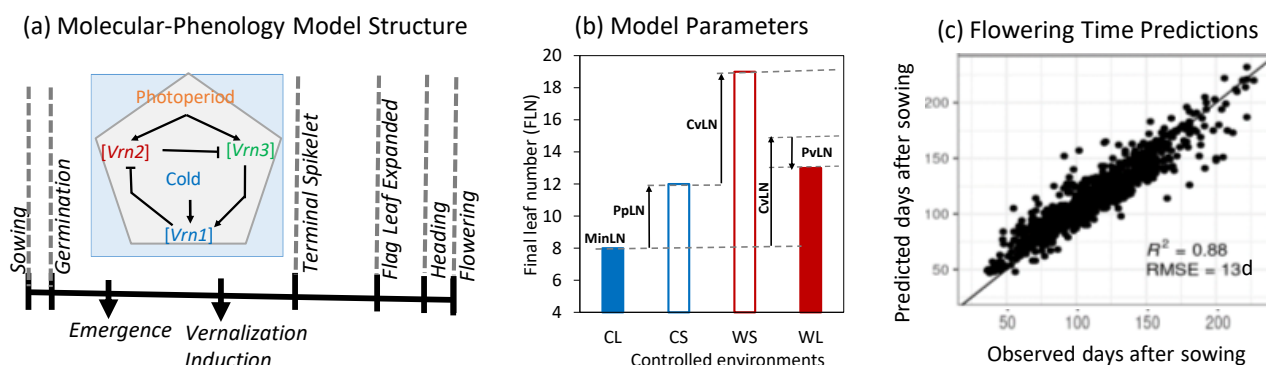


Figure 1. The simplified diagram of the CAMP model in APSIM Next Generation, showing the stages where it incorporates the regulatory roles of three virtual genes—*Vrn1*, *Vrn2*, and *Vrn3* (a), the new model parameters derived based on final leaf number on main stem using data from the controlled environment experiments (b), and the model performance for simulating flowering time of wheat across environments in Australia (c). In (b): MinLN - the earliness per se, PpLN - photoperiod sensitivity, CvLN - vernalization sensitivity, PvLN - photoperiod x vernalization interaction.

## Conclusions

Integration of molecular understanding into a physiologically based crop model helps to disentangle the complex interactions of temperature and photoperiod as they impact on phenological development of cereal crops towards flowering. The enhanced molecular–physiology linkage enables simplified and better phenotyping strategies, reduces the experimental costs, and increases the prediction accuracy, facilitating the prediction of flowering time directly from genotypic data.



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## Advances in CROptimizR and CroPlotR R packages for crop model parameter estimation and evaluation

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**Keywords:** R package, calibration, AgMIP protocol, parameter selection.

### Introduction

Effective parameter estimation and model evaluation remain major challenges in the crop modeling community. Until recently, there has been neither consensus on standardized methods or protocols, nor widely available software tools to facilitate their implementation and testing across different crop models. In response, the AgMIP Calibration activity was launched to test and compare calibration procedures across a broad range of crop models with the ultimate goal of establishing shared guidelines and protocols, fostering consensus on model calibration and evaluation practices. To support this effort, the CROptimizR (Buis et al., 2024) and CroPlotR (Vezy et al., 2024) R packages provide dedicated software solutions for efficient implementation, comparison, and automation of parameter estimation and evaluation workflows for crop models (Figure 1).

### Key features of CROptimizR and CroPlotRw

CROptimizR provides frequentist (e.g., Nelder-Mead simplex) and Bayesian (e.g., DREAM-zs) algorithms for parameter estimation via external packages like nloptr and BayesianTools. Key features include the ability to select among various goodness-of-fit criteria, fine-tune algorithm options, define parameter constraints (equality or inequality), apply transformations to variables, and automate selection of parameters to estimate. CroPlotR complements CROptimizR by offering tools for analyzing and visualizing model outputs, producing dynamics and scatter plots to compare simulations and observations, computing 32 statistical indicators, and supporting group comparisons (e.g. model versions or parameterizations).

Recent developments currently available in a beta version under testing have further expanded these capabilities with the addition of a flexible multi-step parameter estimation feature. This allows automation of successive estimation steps, with full control over the specification of observations, parameters, methods, and options used at each stage. They also include a full integration of the AgMIP calibration protocol (Wallach et al., 2024, 2025) through a dedicated function that automates the entire protocol workflow and generates the associated diagnostics.

### Connection with crop models

Both packages rely on a generic interface that connects crop models to estimation and evaluation workflows through model wrappers (Figure 1). These R functions enable simulations to be run by passing parameter values to crop models and returning model results in a standardized format. A wrapper must be specifically developed for each model. These





wrappers can interface models written in most programming languages (e.g., Fortran, C++, C#) through direct calls, shared libraries, or system calls (using e.g. `system2`). This flexibility has allowed CroptimizR and CroPlotR to be applied to over 15 crop models or platforms, including STICS, APSIM Next Gen. and DSSAT.

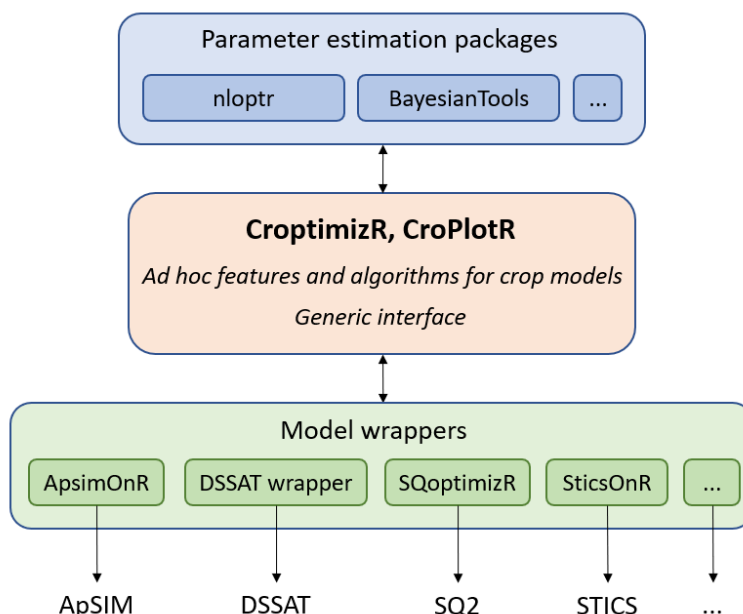


Figure 1. A flexible interface for crop model calibration and evaluation: the CroptimizR and CroPlotR approach. CroptimizR connects crop models or platforms (e.g., STICS, DSSAT, Apsim, SQ2) with parameter estimation packages (BayesianTools, nloptr) through the development of wrappers, while providing specific functionalities tailored to crop modeling. CroPlotR complements it by offering visualization, diagnostics, and statistical analysis of model performance.

## Availability and use in the community

These open-source packages are freely available on GitHub. Their versatility and performance have been demonstrated in several studies (e.g. Wang et al, 2025). Within the AgMIP Calibration project, they helped implement calibration protocols, facilitating their application by modeling groups and enabling rigorous comparisons across a large ensemble of models (Wallach et al., 2024, 2025).

## Acknowledgements

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## On the interest of using high-throughput field phenotyping and satellite data for crop model calibration

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**Keywords:** AgMIP calibration protocol, bread wheat, inverse modeling, SiriusQuality

### Introduction

Crop model parameters are often not directly measurable and must be estimated through calibration procedures. A wide range of strategies is used in practice, and calibration choices strongly affect model results (Wallach et al., 2021). The dataset used is particularly critical: using contrasting environments and frequent observations tends to improve calibration results (Coudron et al., 2021). In this context, high-throughput field phenotyping (HTFP) and satellite observations offer promising opportunities. HTFP provides frequent, accurate, automated measurements of variables, while satellite provides data across diverse environments. This study evaluates the value of integrating HTFP data from experimental plots and satellite data from farmers' fields for crop model calibration.

### Materials and Methods

The dataset combined observations from two INRAE platforms in France (Auzeville and Mauguio), where ten contrasting bread wheat varieties were grown over four growing seasons with different sowing dates, densities, and water regimes. Measured variables included phenology (heading date), total above ground biomass and its partitioning into leaf, stem, and grains, main stem leaf surface area, green area index (GAI), grain yield, and yield. These traits were measured through destructive samplings around growth stage ear at 1 cm, flag ligule just visible, anthesis, and ripeness maturity. The fraction of intercepted PAR (fiPAR), the average leaf angle, heading date, and GAI were estimated using a phenomobile device every 100 °Cdays. In addition, GAI estimated from PlanetScope satellite observations and yield were collected on 17 farmers' fields across France for four of the same varieties.

The crop growth model SiriusQuality2 (SQ2, version 3.1) was used. It simulates wheat development, canopy dynamics, biomass, nitrogen fluxes, and soil processes (Liu et al., 2021). Eighteen genotypic parameters related to phenology, canopy expansion, light interception and use, and yield formation were estimated.

Calibration followed the AgMIP protocol (Wallach et al., 2024), implemented with the CROptimizR R package (Buis et al., 2024) coupled to SQ2. Several scenarios were compared: (i) destructive data only, (ii) HTFP data with a minimal set of destructive measurements (e.g. grain yield), (iii) combined destructive and HTFP data, and (iv) HTFP data with a minimal set of destructive measurements complemented with satellite observations from farmers' fields.

To evaluate these calibration scenarios, a leave-one-out approach was used to assess model predictive performance and parameter stability, and some estimated parameters were compared with HTFP measurements.

### Results and Discussion

First tests showed that the AgMIP calibration protocol outperformed the systematic simultaneous calibration of all initially considered parameters, as its automatic parameter selection and stepwise assimilation approach made better use of multiple observed variables, improved convergence, and reduced overfitting.

Whether measured parameters were fixed to their estimated values and the remaining ones were calibrated, or the AgMIP protocol was applied to scenario iii, both approaches led to poor results, especially for integrative outputs such as grain yield. This suggests that imposing too many constraints on intermediate processes during calibration may reduce





predictive performance for these variables, likely due to model approximations and inconsistencies among simulated processes.

By contrast, using HTFP data combined with a minimal set of destructive measurements (total above ground biomass, grain yield) proved valuable. This scenario produced predictions in new environments that were as good as, or better than, those obtained without HTFP data. The high temporal resolution and precision of HTFP measurements better constrained canopy dynamics and enabled more relevant estimation of parameters related to plant development and growth. Including satellite observations from farmers' fields across diverse environments, in addition to experimental site data, improved the prediction of grain yield and GAI but resulted in poorer simulations of biomass.

Finally, estimated parameter values were not consistently comparable to measured ones across scenarios, raising questions about the ability of calibration procedures to retrieve biologically realistic parameter values and about the assumption that genotypic parameters remain constant across environments.

## Acknowledgements

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## The quest for balance between accuracy and robustness in crop model-aided genomic prediction

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**Keywords:** Equifinality; heading date; number of parameters; spring barley.

### Introduction

Crop simulation models (CSM) are increasingly used to extend the potential of genomic prediction (GP) as they limit the role of statistics to the development of relationships between genomic information and functional traits, the latter being only slightly affected by G×E×M interaction. The influence of environmental and management factors is dynamically simulated by crop models on an ecophysiological basis, under the assumption of a close relationship between model parameters and plant functional traits (Hammer et al., 2002). This allows crop model-aided GP (CSM-GP) to be extended outside the conditions for which genotype-to-phenotype relationships are derived (Messina et al., 2018). However, the number of parameters can expose CSM-GP to a non-negligible risk of equifinality, which can undermine its biological meaningfulness and robustness (Yang et al., 2022). The aim of this study was to analyse the impact on prediction accuracy of increasing number of parameters for a 2-step CSM-GP approach. To account for model structure, two models (WOFOST and Sirius) largely differing in complexity were considered. The case study was on heading date (HD) of spring barley.

### Materials and Methods

The dataset consisted of genomic information (50K SNP array) and HD observations for 151 2-row spring barley genotypes grown in 17 environments from Northern Africa to Northern Europe. The steps of the study were: (i) selection of two models and sensitivity analysis (SA); (ii) generation of four configurations for each model based on SA results, i.e., configuration 1: the two most relevant parameters, configuration 2: the two + n most relevant parameters, etc.; (iii) 2-step CSM-GP for all models and configurations: step 1, decomposition of HD into functional traits and genotype-specific calibration, step 2, GP of model parameters (RR-BLUP approach); (iv) analysis of prediction accuracy using GP parameters for all models and configurations.

### Results and Discussion

SA revealed that the most complex model (Sirius) presented large interactions (difference between 1st and total order effects) between parameters, and that interactions increased with the number of parameters, reaching 29% for the configuration with eight parameters, whereas it never exceeded 5% for WOFOST.

Prediction accuracy of genotype-specific parameter values drastically decreased from the training to the test dataset, where a significant linear decrease in the mean correlation between decomposed and GP parameters was observed while increasing the number of parameters, to the point of becoming negative (Fig. 1). This pattern, which was more pronounced for Sirius, is due to the increased risk of equifinality during parameter optimization.

Despite the loss of biological meaningfulness of CSM-GP for increasing number of parameters, satisfying prediction accuracy was obtained when data from all genotypes and environments were analysed ( $r \geq 0.98$ ) due to the large





variability among environments. However, when prediction accuracy was evaluated within environment, the risk of equifinality reflected in a clear worsening while moving from training ( $r \sim 0.70$ ) to test ( $r \sim 0.25$ ) dataset.

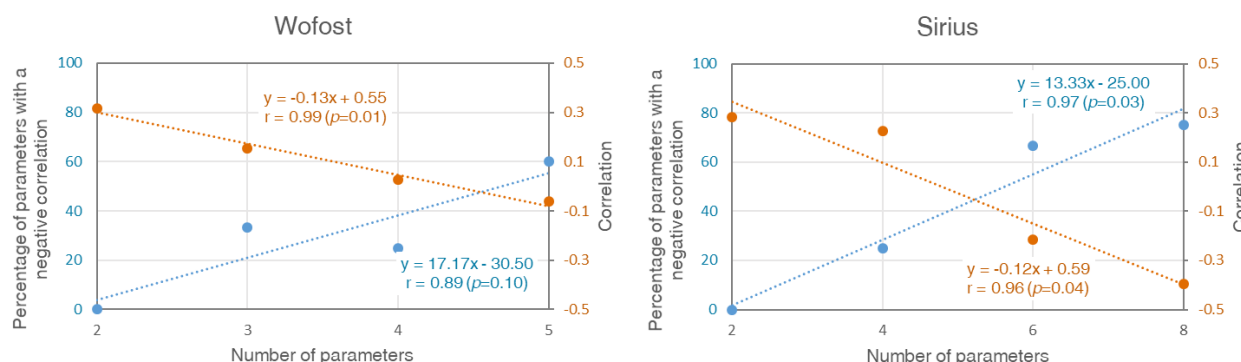


Figure 1. Pearson's correlation (red series) between decomposed and genomic-predicted parameter values for model configuration with increasing number of parameters for the test dataset, and percentage of parameters with a negative correlation (blue series) between decomposed and genomic-predicted values (test dataset). Dotted lines are the corresponding linear regressions.

## Conclusions

The biological meaningfulness of CSM-GP may be strongly undermined when the number of parameters is not kept to the minimum (two for both models in our study), in turn affecting CSM-GP robustness when, e.g., a new environment is explored. This is true especially in case of many interactions among parameters.

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## Using the ICASA Data Dictionary to Increase the “FAIRness” of Datasets for Crop Model Improvement and Applications

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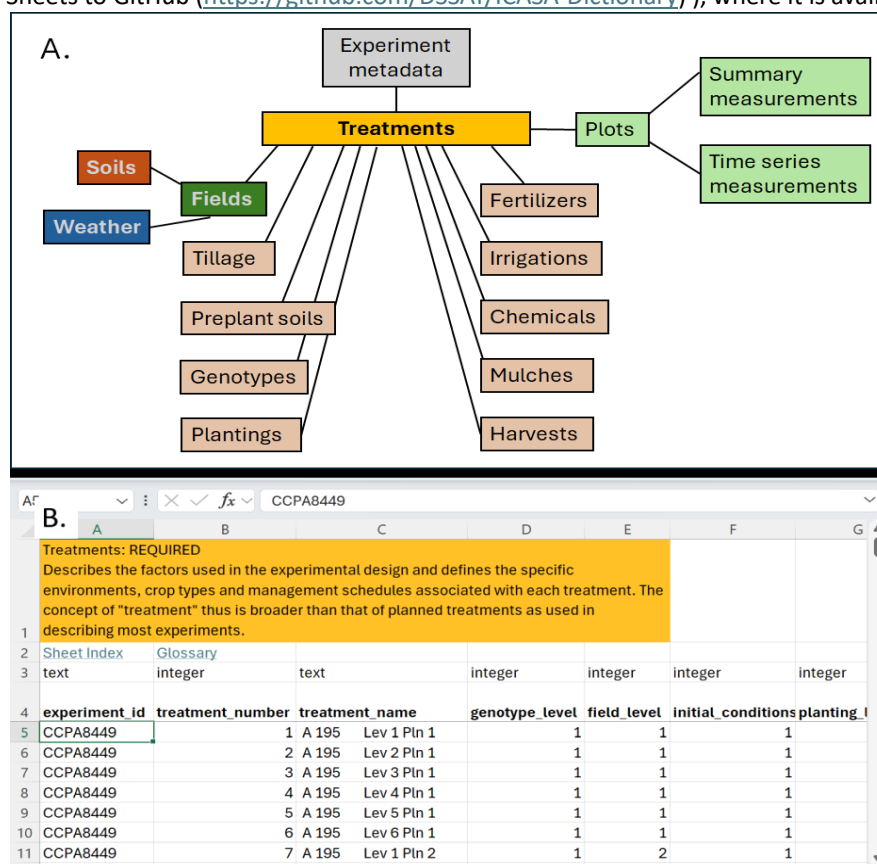
**Keywords:** data management, datasets, FAIR principles, evaluation

### Introduction

Crop modeling depends on well-documented field data, yet shared datasets often lack detail or standardization (Top et al., 2022). The FAIR principles, whereby datasets are Findable, Accessible, Interoperable, Reusable (Wilkinson et al., 2016), highlight these needs. ICASA standards were created to promote reproducibility of experiments (White et al., 2013, 2025) but have seen limited uptake due to complexity and lack of software tools. We present advances linking the ICASA Data Dictionary with spreadsheets and R scripts to generate more datasets for crop modeling that better satisfy FAIR criteria, especially interoperability and reusability.

### Materials and Methods

The ICASA Data Dictionary (IDD) retains its core structure, listing terms for experiment metadata, management, soils, weather, and crop traits, along with names, definitions, units, and codes (Fig. 1A). The IDD has moved from Google Sheets to GitHub (<https://github.com/DSSAT/ICASA-Dictionary>), where it is available as CSV files and a workbook with



issue tracking. A new dataset template mirrors the ICASA structure: sheets for metadata, treatments, management, measurements, soils, and weather, with standardized rows for instructions, examples, and formats (Fig. 1B). Datasets typically include 20 to 30 sheets that are linked by an index and Glossary. The standardized design enables R-based support, including QA tools that flag errors, cross-check identifiers, and verify variables against definitions and units.

### Results and Discussion

The IDD, templates, and R tools have been used for field experiments, including cultivar trials, physiology, and irrigation management. A major effort in

Figure 1. Diagram of the architecture for datasets under the ICASA standards (A) and an example worksheet describing treatments using the workbook template (B).



Florida applies discipline-specific templates to help standardize metadata and measurements for nutrient management, enabling the use of models and AI to improve recommendations (White et al., in review). Challenges include missing management records and soil profiles. The QA tool has proven invaluable for detecting data-entry errors and undefined terms. Areas highlighted for further development include:

- Terminology matching: The 1300+ IDD terms are challenging to align with local or non-English usage; automated translation and AI may help.
- Replicates vs. means: We distinguish replicate data from treatment means by using “\_MEANS” for worksheets where means are reported.
- Multiple measures of a variable: Traits such as leaf area or canopy height may have several measures, especially with sensor data. We propose integer suffixes (e.g., SLAD\_1, SLAD\_2) with definitions for each.

Other challenges include handling time series with varying intervals, geospatially organized data, and sub-daily measurements. R scripts also support data entry and analysis; prototypes show that template-based datasets can directly generate DSSAT model input files for immediate use.

## Conclusions

The IDD, dataset templates, and R scripts provide a flexible, practical way to document field experiments. Experience from AgMIP and recent template advances confirm that interoperability and reusability can be enhanced without the need for complex databases or software. We encourage the crop modeling community to adopt the IDD and templates to promote FAIR datasets and advance model development.

## Acknowledgements

The authors acknowledge Tony Hunt, Jim Jones, and Ken Boote's contributions in developing the ICASA standards. We also thank the Florida Department of Agriculture and Consumer Services (FDACS) and its collaborators for supporting their variant of the ICASA template for nutrient management research.

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## An integrated energy balance framework for wheat leaf and spike under compound heat–drought stress

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**Keywords:** energy balance model; evapotranspiration; heat–drought interaction; organ temperature; stomatal conductance.

### Introduction

Compound heat and drought (H×D) extremes are intensifying under climate change, yet their interactive effects have not been well quantified in crop models (Rosenzweig et al., 2016). Most current approaches treat the canopy as a single homogeneous unit, overlooking organ-specific responses of leaves and spikes to environmental drivers such as temperature, water status or radiation (Allen et al., 1998; Lawson & Milliken, 2023). To address this limitation, we developed an organ-resolved framework that incorporates a newly constructed heat–drought interaction factor with cumulative effects ( $f(HD)$ ) into a Jarvis–Penman–Monteith scheme and explicitly simulates leaf temperatures ( $T_{leaf}$ ) and spike temperature ( $T_{spike}$ ) within an energy-balance structure, with  $T_{leaf}$  and  $T_{spike}$  subsequently replacing air temperature as drivers for simulating crop development and yield formation under H×D conditions.

### Materials and Methods

We conducted a two-year glasshouse experiment with factorial H×D treatments during post-anthesis period on two wheat cultivars, continuously measuring leaf stomatal conductance ( $g_{s,leaf}$ ), spike conductance ( $g_{spike}$ ), whole-plant ET,  $T_{leaf}$  and  $T_{spike}$ . The framework was further evaluated against the INRAE H×D dataset for ET and validated for organ temperatures using an infrared-warming field experiment. The model structure includes: (i) a Jarvis-type module for  $g_{s,leaf}$  and  $g_{spike}$ , integrated with  $f(HD)$ ; (ii) a Penman–Monteith ET module coupled with the  $g_s$  model; and (iii) an energy-balance solver computing  $T_{leaf}$  and  $T_{spike}$ , which feed back into  $g_{s,leaf}$ ,  $g_{spike}$ ,  $r_{a,leaf}$ , and  $r_{a,spike}$ , forming a closed-loop system (Figure 1).

### Results and Discussion

Incorporating  $f(HD)$  improved simulations of  $g_{s,leaf}$  under H×D stress, reducing bias and better capturing its continuous dynamics throughout treatment and recovery periods. When coupled with the Penman–Monteith scheme, accounting for spike transpiration yielded more accurate canopy-level ET under H×D, with the largest gains at night where conventional frameworks tended to underestimate nocturnal ET. Further integration into the energy balance model improved the accuracy of simulated  $T_{leaf}$  and  $T_{spike}$  and better captured the diurnal differences between  $T_{leaf}$  and  $T_{spike}$ . Substituting these organ temperatures for air temperature further improved predictions of grain-filling duration and fertility, linking environment  $\rightarrow g_s \rightarrow ET \rightarrow T_c \rightarrow$  development/yield in a mechanistically consistent pathway.

### Conclusions

The main conclusions of our work are:

- (1) Introducing the cumulative heat–drought interaction factor  $f(HD)$  substantially improves  $g_{s,leaf}$  simulation;





- (2) Coupling the  $g_s$  module and explicitly representing  $g_{spike}$  delivers the best ET prediction performance under HxD, especially at night;
- (3) The energy-balance module realistically simulates  $T_{leaf}$  and  $T_{spike}$  under HxD and provides more informative temperature drivers for downstream processes. The framework is modular and can be coupled with crop growth models for climate-impact assessments.

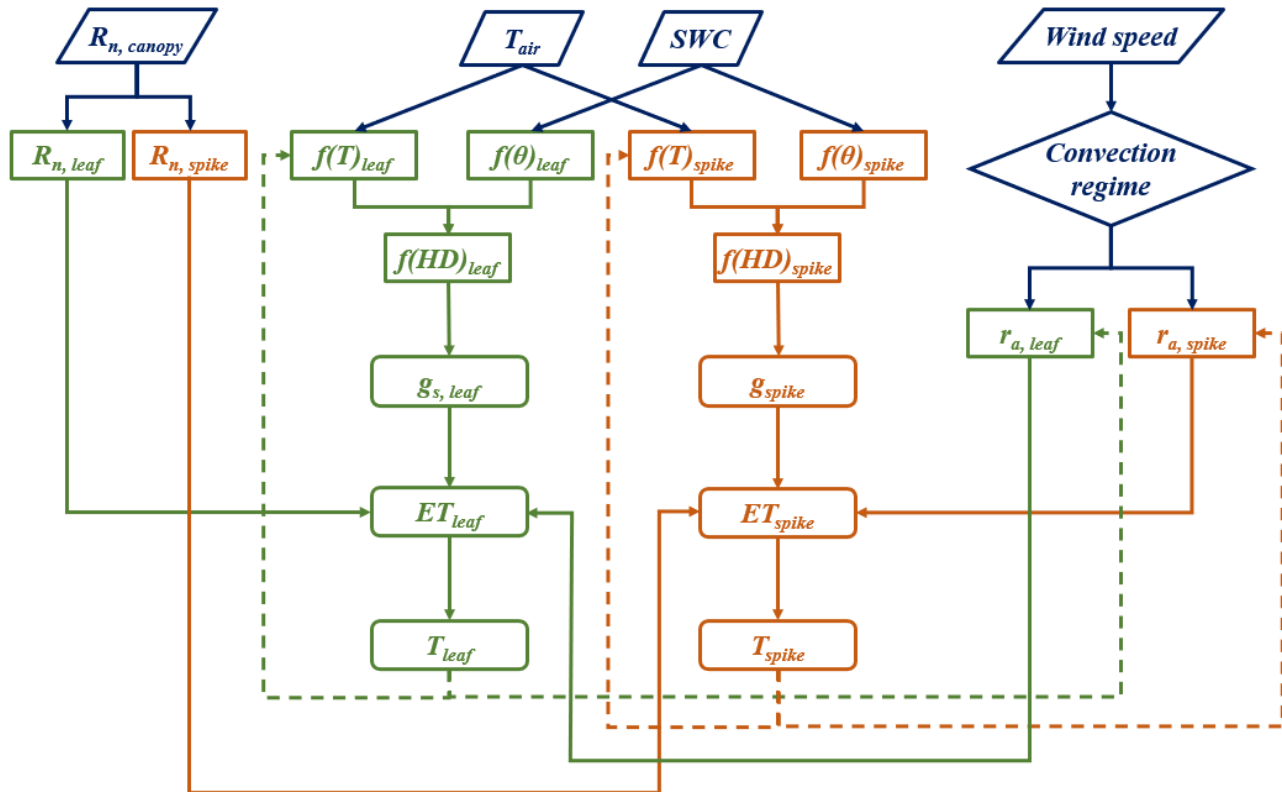


Figure 1. Flowchart of the organ-resolved energy balance framework under compound heat-drought stress. The dashed line indicate convergence loops on organ temperature and aerodynamic conductance. Key parameters are defined as follows:  $R_{n, canopy}$ : net radiation at the canopy surface;  $R_{n, leaf}$ : net radiation intercepted by leaves;  $R_{n, spike}$ : net radiation intercepted by spikes;  $T_{air}$ : air temperature;  $SWC$ : soil water content.  $f(T)_{leaf}$ : temperature factor for leaf stomatal conductance;  $f(\theta)_{leaf}$ : drought factor for leaf stomatal conductance;  $f(T)_{spike}$ : temperature factor for spike conductance;  $f(\theta)_{spike}$ : drought factor for spike conductance;  $f(HD)_{leaf}$ : heat - drought interaction factor for leaf stomatal conductance;  $f(HD)_{spike}$ : heat-drought interaction factor for spike conductance;  $r_{a, leaf}$ : aerodynamic resistance of leaves;  $r_{a, spike}$ : aerodynamic resistance of spikes



## Acknowledgements

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## Simulating seasonal dynamics of P and N concentrations in maize aboveground biomass using DSSAT CSM-CERES and CSM-IXIM

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**Keywords:** crop model; P fertilizer; P and N uptake

### Introduction

Within the Decision Support System for Agrotechnology Transfer (DSSAT), two maize (*Zea mays* L.) crop simulation models—CSM-CERES and CSM-IXIM—have been widely applied to simulate maize yields (Jones & Kiniry, 1986; Lizaso et al., 2011; Yakoub et al., 2017; Hoogenboom et al., 2021). While their nitrogen (N) uptake simulations were tested under different N fertilizer levels (Yakoub et al., 2017), their phosphorus (P) and N uptake simulations have not been intensively tested particularly using multiple in-season observations under varying P fertilizer levels in P-deficient soils (Dzotsi et al., 2010; Lizaso et al., 2022). In this study, the seasonal dynamics of P and N concentrations in aboveground biomass, as simulated by CERES and IXIM, were evaluated against field observations from southern Germany based on experiment with one level of N and four levels of P applied.

### Materials and Methods

DSSAT CERES and IXIM (with minor code modifications to root P intake coefficient (ROOTRAD)) (v. 4.8.5) were evaluated based on data from a field experiment conducted in 2022 and 2023 in Southern Germany on P-deficient soils (8.9 mg P kg<sup>-1</sup> soil), with P fertilizer (di-ammonium phosphate) treatments of 0, 25, 50, and 75 kg P ha<sup>-1</sup> and N fertilizer (stabilized urea) of 120 kg N ha<sup>-1</sup>. Maize cultivar *Stabil* (FAO220, KWS Germany) was planted on 19 May 2022 and 25 May 2023. Cultivar coefficients were estimated using the Time-Series-based cultivar coefficient Estimator (TSE, Memic et al., 2021). Target variables for calibration included leaf area index, leaf, stem, and grain dry weight aiming at the lowest error between simulated and observed values based on the 75 kg P ha<sup>-1</sup> treatment data from the 2022 experiment. For species coefficients calibration, P concentration in each plant organ and root radius for P uptake, data of 0, 25, 50, and 75 kg P ha<sup>-1</sup> in 2023 were utilized. Since P and N concentrations in total aboveground biomass are not directly reported in DSSAT output files, they were calculated as the ratio of cumulative P or N uptake (shoot, grain, and shell) to total aboveground dry weight (leaf+stem+tassel+shell).

### Results and Discussion

Figure 1 presents the simulated P and N concentration of aboveground biomass by CERES and IXIM with their observed values in the field (2022). Overall, CERES showed slightly better performance, with higher d-stat values and lower nRMSE compared to IXIM, although the differences in accuracy between the two models were small. For P concentration, CERES achieved an average d-stat of 0.839 and an nRMSE of 23.3%, while for N concentration it achieved an average d-stat of 0.968 and an nRMSE of 16.2% across all fertilizer treatments (0, 25, 50, and 75 kg P ha<sup>-1</sup>). Similarly, IXIM performed well, with average d-stat values of 0.818 and 0.960, and nRMSE values of 24.4% and 17.2% for P and N concentrations, respectively, across all treatments.

In CERES, simulated P concentration in aboveground biomass tended to be overestimated throughout the growing season. In contrast, IXIM underestimated P concentration in the beginning but overestimated it at the end of the season (Figure 1). Both models captured the increase in P concentration observed after 100 days after sowing (DAS) (Figure 1a, b). Differences among P fertilizer rates were more pronounced in IXIM simulations than in CERES between the 0 and 75 kg P ha<sup>-1</sup> treatments.







The initial P concentration in aboveground biomass (0.271%) was well reflected in both models. However, despite using the same maize cultivar (*Stabil*) in both years, observed P concentrations at emergence differed between 2022 (0.414%) and 2023 (0.271%). These differences likely reflect soil and weather conditions, which should be considered in model calibration, as initial P concentration is sensitive to species coefficient values. In contrast, the default N concentration values in the species files aligned closely with the observed data, and no adjustment was made. The minimum N concentration in aboveground biomass at emergence was 4.4% in the default setting and changed to 4.2% in this study. For more accurate simulations of plant N concentration, future work should consider refining N-related coefficients based on observed data.

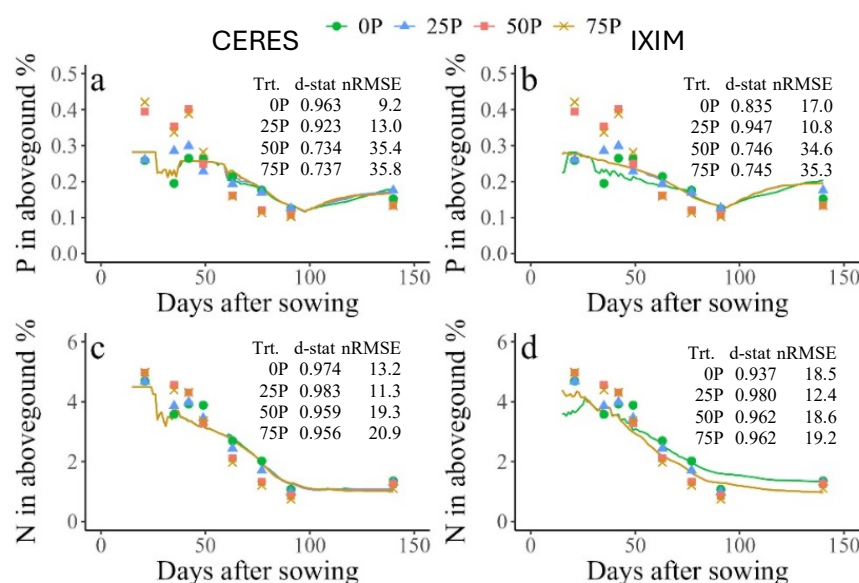


Figure 1. Simulated (lines) aboveground biomass P concentration (a: CERES, b: IXIM) and N concentration (c: CERES, d: IXIM) for 0, 25, 50, and 75P in 2022 with measured field data (dots). Model performance statistics (d-stat and nRMSE %) are shown in each panel.

## Conclusions

This study compared simulations of P and N concentrations in aboveground biomass between the CERES and IXIM models. Both models performed satisfactorily, with high d-stat values (CERES: 0.839; IXIM: 0.818). While CERES showed slightly better overall accuracy, the IXIM simulations provided better reflections of the effects of different P fertilizer levels on plant P and N concentrations. Further evaluation under diverse conditions, including varying weather, soil, genetic backgrounds, and crop management practices, is required to more comprehensively test the ability of DSSAT models to simulate P and N concentrations. Additionally, sufficient data on initial nutrient concentrations should be collected to refine genetic coefficients, as the starting values of shoot P concentration significantly influence simulated seasonal P dynamics.



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## Operational parameterization of 800 soft wheat varieties: reconciling decision support with unequal levels of knowledge

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**Keywords:** calibration ; *Triticum aestivum* ; expertise ; methods comparison ; decision-making

### Introduction

Many studies have highlighted the importance of improving crop phenology prediction by accounting for varietal behavioral differences. Arvalis provides stage prediction models for decision support systems, available through commercial tools. Phenological models rely on vernalization–photoperiod–thermal time sums were built using *Soissons* as a reference variety. The aim for Arvalis is to deliver reliable predictions for an ever-growing number of varieties while saving time and resources.

### Materials and Methods

In this study, we compare different calibration methodologies, taking into account the level of knowledge available for each variety. We assembled a dataset of 800 varieties, spanning 1979–2023, across 374 locations in France, for the stages 1cm-ear (Z30) and heading (Z55) on Zadoks scale (Zadoks *et al.*, 1974).

Besides *Soissons*, we distinguish three varietal lists with decreasing levels of knowledge (P, N, I). The P list is composed of well characterized varieties, with their own parameters. N cultivars are less known and are associated with P varieties using relative proximity indicators based on an earliness score. Varieties into I category are not characterized yet and are predicted like *Soissons* by default. The dataset is composed of 105 P-list varieties, 525 from N-list and 172 belonging to I-list. The reference method (Method1) relies on Nelder-Mead optimization (for *Soissons*) ; association methods for P and N varieties require considerable time, with strong expertise before and after calibration.

Therefore, we propose four others methods of calibration: AgMIP-based protocol (Method2 ) (Wallach *et al.*, 2021, 2023), mixed-effects model (Method3), L-BFGS-B (Method4), and marker-based approach (Method5 ; (Bogard *et al.*, 2021b, 2021a)). Due to the time simulation AgMIP-based method was tested on *Soissons* only. L-BFGS-B method also permitted to include expertise by adjusting parameters bounds. Marker-based method was evaluated on less situations (and varieties) because the genetic parameters were not available for some recently registered varieties at the time of the study. We could compare methods from computing indicators of performance after cross-validation.

### Results and Discussion

Results confirm the importance of expert knowledge. For well-known varieties, the historical method is as efficient as L-BFGS-B (RMSEP  $\approx$  6.3 and 3 days; EF = 0.78 and 0.91 at Z30 and Z55). L-BFGS-B performs best for N- and I-lists, while the marker-based approach outperforms others for heading in I-list and enables prediction of new varieties without trials (Table 1).

Regarding time, mixed-effects calibration took 1 day for 800 varieties, vs 9 days for L-BFGS-B and 20–30 for the historical method.



### Conclusions

Considering both the performance and computational time of each approach, L-BFGS-B method and marker-based approach appear the most promising candidates for further development, with the latter to be reassessed with new varieties. AgMIP-based method requires long runtimes relative to its performance, while mixed-effect model does not achieve the expected accuracy compared with (1) L-BFGS-B method under similar data volume and execution time, (2) marker-based one, which does not rely on experimental data. Ultimately, regardless of the chosen method, a layer of expert judgment will remain essential to ensure consistency with biological reality.



		1 cm ear (Z30)					Heading (Z55)				
		Method 1	Method 2	Method 3	Method 4	Method 5	Method 1	Method 2	Method 3	Method 4	Method 5
Global	EF	0.76		0.67	0.79	0.72	0.9		0.88	0.90	0.9
	Bias	-0.73		-2.75	-0.03	0.43	0.06		-1.17	-0.02	-0.61
	RMSEP	6.96		8.20	6.45	7.32	3.24		3.49	3.12	3.25
	RRMSEP	8.41		9.91	7.80	8.74	2.37		2.55	2.28	2.37
	n	11672		11672	11672	10440	11672		11672	11672	10440
Soissons	EF	0.86	0.8	0.85	0.86	0.77	0.89	0.86	0.89	0.89	0.89
	Bias	-0.36	0.42	-0.77	-0.13	4.17	0.26	-1.40	-0.58	0.2	0.26
	RMSEP	5.48	6.48	5.52	5.47	6.98	2.88	3.21	2.93	2.85	2.88
	RRMSEP	6.57	3.21	6.62	6.56	8.36	2.12	2.36	2.15	2.09	2.12
	n	1208	1208	1208	1208	1208	1208	1208	1208	1208	1208
P	EF	0.78		0.67	0.79	0.74	0.91		0.88	0.91	0.9
	Bias	-0.52		-3.00	0.03	0.6	0.2		-1.16	0.06	-0.56
	RMSEP	6.37		7.9	6.21	7.02	2.99		3.39	2.97	3.16
	RRMSEP	7.62		9.45	7.43	8.35	2.17		2.47	2.16	2.30
	n	8693		8693	8693	7978	8693		8693	8693	7978
N	EF	0.69		0.63	0.78	0.68	0.87		0.87	0.88	0.89
	Bias	-1.34		-2.28	-0.16	-0.16	-0.53		-1.27	-0.34	-0.84
	RMSEP	8.19		9.00	6.99	8.05	3.83		3.78	3.57	3.55
	RRMSEP	10.2		11.3	8.74	9.71	2.86		2.82	2.66	2.62
	n	2761		2761	2761	2286	2761		2761	2761	2286
I	EF	0.73		0.82	0.85	0.79	0.86		0.92	0.92	0.95
	Bias	-1.54		1.34	-1.01	0.68	1.88		-0.19	0.81	0.14
	RMSEP	11.3		9.1	8.4	10.0	4.37		3.30	3.29	2.88
	RRMSEP	13.2		10.7	9.87	12.0	3.18		2.4	2.39	2.07
	n	218		218	218	176	218		218	218	176

**Table 1:** Summary table comparing performances results based on different calibration methods for predicting 1cm-ear (Z30) and heading (Z55) in soft winter wheat. Calibration methods were : reference (Method1), AGMIP (Method2), mixed-effects model (Method3), L-BFGS-B (Method4) and marker-based model (Method5), respectively. Indicators are : Nash-Sutcliffe efficiency (EF), Bias, Predicted root mean squared error (RMSEP), Relative RMSEP (RRMSEP) and number of situations (n), respectively.

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## Integrating measurable-pool soil organic carbon and nitrogen into cropping system models

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**Keywords:** Particulate organic matter, mineral-associated organic matter, modelling, cropping systems

### Introduction

In cropping systems, soil organic matter (SOM) affects crop productivity, greenhouse gas emissions and soil structure, but it is strongly influenced by soil characteristics, weather and management. Through cropping system modeling, these complex interactions can be better understood. Most cropping system models represent SOM as conceptual pools (active, passive, and slow) that are not directly measurable (Campbell & Paustian, 2015). As a result, these models can be calibrated only against total soil organic matter rather than individual pool sizes. In contrast, SOM can be characterized through measurable fractions of particulate organic matter (POM) and mineral-associated organic matter (MAOM), which differ in their physical and chemical properties and respond distinctly to management and climate (Lavalée et al., 2020). Only a limited number of models using this framework have been developed specifically for arable soils.

Against this background, the AMPSOM model was developed to simulate soil carbon and nitrogen dynamics in POM and MAOM in response to crop development, management practices, soil texture, water, nitrogen availability and temperature (Tougma et al., 2024).

### Materials and Methods

AMPSOM is a depth-explicit process-based SOM model, with each layer having one mineral N pool and five soil organic carbon (SOC) and N pools. To better constrain the turnover time of slowly cycling SOC pools, the model also incorporates radiocarbon isotope (<sup>14</sup>C) of SOC. In AMPSOM, decomposed aboveground litter enters in the soil through the POM pool, which is defined as the sum of fresh root litter, the non-water soluble part of decomposed aboveground litter and crop residues. Through microbial activity influenced by soil temperature and moisture, POM undergoes depolymerization and goes to the dissolved organic matter (DOM) pool. The water-soluble part of decomposed aboveground litter contributes directly to the DOM pool of the first soil layer, while root exudates of each layer are added to the DOM pool of the respective layer. Competition for the DOM pool occurs between microbes and mineral protection, the latter pathway contributing to MAOM accumulation. At every time step, a part of the microbes dies and moves into the necromass pool, where it can either be decomposed into DOM or stabilized as part of the MAOM pool.

AMPSOM was first developed in R and then integrated within the cropping system modeling framework SIMPLACE (Enders et al., 2023). Here it was integrated to other modules simulating crop (Lintul5) and root (SlimRoots) growth and development, water dynamics in the soil and in the plants, litter decomposition and soil and canopy temperature. It was then calibrated and evaluated using size-fractionated (Cambardella & Elliott, 1992) soil data in thirty-six sandy and loamy arable soils in Brandenburg, Germany. The objective function used for calibration was the average relative root mean square error (RRMSE), across all sites and profile depths for simulated and measured 1) POM C and N content, 2) MAOM C and N content, 3) microbial C and N content, and 4) total soil  $\Delta^{14}\text{C}$ .





## Results and Discussion

The AMPSOM model evaluation showed it was able to capture observed SOC and N stocks in POM and MAOM along depth gradients, with mean RRMSE values of 33% in sandy soils and 29% in loamy soils. Performance of POM-C was good in the top 0–20 cm where the RRMSE averaged 27%, but accuracy declined in deeper layers. The model overestimated MAOM-N concentrations in the upper 0–30 cm but underestimated them at depth. Predictions of microbial C and N were too high, with average overestimation around 60%. The  $^{14}\text{C}$  profile was reproduced between 30 and 90 cm, and subsoil  $^{14}\text{C}$  showed greater variability than in surface layers.

The simulated depth profile of  $\Delta^{14}\text{C}$  was consistent with the commonly observed pattern of younger carbon in the topsoil compared to the subsoil. While only a few studies have explored the simulation of measurable pool-based SOM models in croplands, many have applied them in grasslands and reported comparable performance. Similarly, agroecosystem models based on a conceptual pool-based approach were able to simulate total soil carbon stocks, with RRMSE values comparable to those of AMPSOM.

## Conclusions

This study represents a scientific and methodological advance in cropping system modelling by explicitly simulating measurable SOM pools, including  $^{14}\text{C}$  dynamics and calibrating the soil-crop model with size-fractionated data. This approach is not widely used in arable-land model development, constituting an opportunity to improve understanding of soil carbon and nitrogen dynamics in response to crop and soil management. Future work should focus on improving N dynamics and root exudates simulation, as well as including tillage. Additional studies are needed to extend model evaluation across broader agro ecological environments and applying the framework to assess long-term sustainability of cropping systems.

## Acknowledgements

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## AgriScale: A distributed framework for gridded crop model ensemble applications

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**Keywords:** ensemble modeling, crop simulation models, spatial modeling, climate change, software framework

### Introduction

Recent advances in high-performance computing (HPC) and cloud infrastructures are transforming agricultural research by enabling large-scale simulations of cropping systems to explore climate change adaptation strategies. Gridded crop modeling platforms provide valuable tools for this purpose (Franke et al., 2020), but they are often restricted to a single Process-based crop model (PBM), tied to specific applications or computing environments (CE), and limited in computational efficiency. This raises key questions: how can we foster the integration and comparison of multiple models within a unified framework, improve the scalability and efficiency of spatially explicit multi-model simulations across heterogeneous CE, and reduce barriers to deploy these large-scale simulations across diverse CE?

### Methods and Use Cases

AgriScale is a distributed framework that integrates multiple PBM to enable simulations across various spatial scales, resolutions, management practices, and simulation configurations. It provides a formal description of gridded input datasets, and standardizes data flows via database schemas (Giner et al., 2024; Affholder et al., 2012). It encapsulates PBM engines, ensuring portability across heterogeneous CE. To improve efficiency, a caching system minimizes redundant input file generation, while distributed computation scheduling leverages both intra- and inter-task parallelism without communication (Figure 1). An adaptive subdomain decomposition further balances workloads, and dynamically optimizes data storage.

We evaluated AgriScale with three models—DSSAT, STICS, and CELSIUS—driven by gridded datasets from multiple sources. Benchmark experiments were run across 3 CE (2 HPC clusters and 1 cloud) configured with different file systems - WekaFS, ZFS, and EXT4 - each influencing performances in data-intensive application. Two case studies assessed performance and scalability: (i) 66,480 maize growth simulations in Senegal, and (ii) 3,830,650 simulations across Sub-Saharan Africa. The second case study was completed on each HPC in less than 4 hours using 120 cores for this ensemble of 3 models.

### Results and Discussion

AgriScale consistently achieved high computational efficiency (>70%) across all file systems at various simulation scales. On ZFS, typically constrained by intensive I/O, the use of large RAM disks for intermediate results enabled performance comparable to WekaFS with SSD storage. Among models, CELSIUS was the fastest, averaging 0.04 s per one-year simulation per core, whereas DSSAT and STICS each required 0.1-0.2s. Although EXT4 shows a longer wall-clock time with few cores, it achieves a near-superlinear speedup at higher core counts, which may be attributed to







memory hierarchy effects. AgriScale successfully produced NetCDF outputs for each model and scenario, including yearly time series of crop phenology, biomass, yield, soil water and nitrogen content, and other key soil–crop variables (Figure 2).

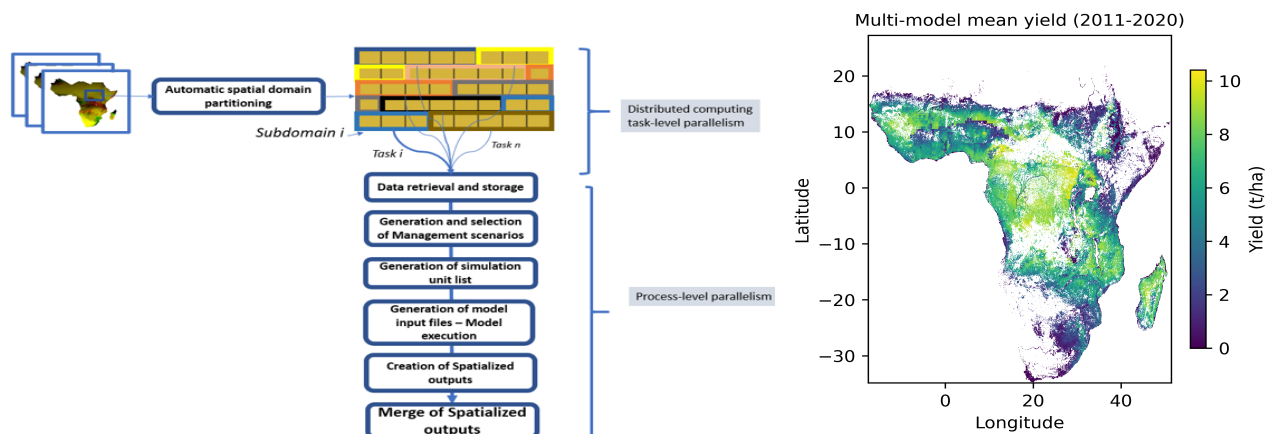


Figure 2: AgriScale functional workflow

Figure 2: Spatial distribution of 10-year multi-model mean maize yield simulated by DSSAT, STICS, and CELSIUS

## Conclusions

AgriScale efficiently runs large-scale crop simulations on HPC and cloud platforms without requiring modifications to existing PBMs. It allows to evaluate cropping systems through model ensemble analyses under climate variability and change, with applications ranging from optimizing sowing dates and cultivar choice, to designing sustainable intensification options. Ongoing developments are extending its multi-model capacity with other PBMs, positioning AgriScale to serve as a reference framework for the GGCM project (Franke et al., 2020).

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## The AgMIP calibration protocol

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**Keywords :** Crop model, Parameter selection, Weighted least squares, Diagnostic tools, Akaike information criterion

### Introduction

Calibration of crop models melds the theory embodied in the model with the ground truth embodied in the data. It is probably the most important aspect of applying a crop model to a new problem. Making effective use of the available data is essential for minimizing prediction error. Furthermore, if one wants to compare process equations, or whole models, or the usefulness of different data sets, it is important not to complicate the comparison with differences in calibration approach. Thus, one needs a reliable, widely applicable calibration approach. Since 2018, the AgMIP calibration group has pursued three objectives: Documenting and comparing current calibration practices, proposing a widely applicable standard calibration protocol and developing tools for applying that protocol. In an initial phase, a calibration protocol for phenology data was proposed. This was then extended to a calibration protocol applicable to essentially any data set and crop models.

### Calibration Protocol

The heart of the protocol is the treatment of two particularly difficult aspects of crop model calibration, namely the choice of which parameters to estimate from the data and the way to handle multiple observed variables. For the choice of parameters to estimate, the protocol considers one variable group at a time. All phenology variables are in one group. Measurements over time of the same variable, e.g. biomass, are together in one group. All other variables are in a group by themselves. For each group, one identifies one parameter per variable (two if there are multiple measurements over time) that is likely to strongly reduce bias. These parameters are automatically chosen to be estimated. One also identifies a list of “candidate” parameters, which might explain a substantial part of the variability between environments or treatments. The candidate parameters are tested as in forward regression, using the corrected Akaike Information Criterion (AICc), which is designed to avoid over-fitting, to test whether the parameter should be estimated or fixed at its default value. This is very closely based on standard practice of parameter estimation in regression. The protocol includes a simple diagnostic which shows to what extent bias is in fact reduced by estimating the supposed bias reducing parameters.

Treating one variable group at a time greatly simplifies the numerical problem, but may lead to a poor final fit to some variables, if the simulated values of those variables are affected by fitting subsequent variable groups. Therefore, the protocol includes a final, weighted least squares (WLS) step, where all parameters are estimated together. This again is closely analogous to standard statistical procedure. One first obtains an estimate to the parameter values, here by treating one variable group at a time, and then uses that estimate to obtain weights for a WLS step. The protocol includes a simple graphical diagnostic that shows visually the extent of feedbacks.

### Application of the Protocol

The protocol was tested using artificial data (Wallach et al., 2024), then for a single model using real data (Wallach et al., 2025), and recently in a multi-model simulation experiment. This multi-model study shows that the protocol is easily





applied to a wide range of model structures. The data set used included multiple variables (phenology, biomass, ear and grain number, biomass N, yield, seed protein). In fact, the protocol is designed to handle essentially any data set. The protocol recommends using all observed variables with simulated equivalents, because fitting as many processes as possible should maximize the overall realism of the simulations.

Over-fitting is a major danger in calibration, because of the very large number of model parameters. In the tests of the protocol, it was systematically found that prediction error was similar to fitting error, i.e. there was no indication of over-fitting (Buis et al. 2024).

In the multi-model study, all modeling teams obtained very good results for phenology and biomass, but much worse results for other variables. Average final relative root mean squared error for the calibration data ranged from 0.02 for time to stem elongation, 0.35 for biomass N, with yield second worst at 0.29. There was of course variability between modeling teams, but the same trend was observed for all teams. This may be the best crop models can do, with this data set.

## Conclusions

The AgMIP calibration protocol is applicable to essentially all crop models and data sets. It is closely based on statistical parameter estimation, which increases confidence in the procedure. It includes diagnostics to better understand the calibration results. Software to automate application of the protocol is under development. We suggest that the AgMIP calibration protocol is a very promising candidate for a standardized calibration procedure for crop models.

## Acknowledgements

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## Integrating crop models with deep learning: from synthetic datasets to tunable algorithms

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**Keywords:** machine learning, phenotyping, remote sensing

### Introduction

Crop models became well established in the periods from the 1960s into the 1980s capturing most of the major crop processes. From the 1990s to 2010s, model developments captured increasingly complex processes based on more detailed experimentation and at the same time, the use of models greatly broadened from decision making and risk analysis in the agronomy of cropping systems through to applications in plant breeding and in the use of ensemble models to analyse global impacts of climate change. However, throughout these periods, crop models have been still largely ‘hand-crafted’ and require explicit parameterization especially for genotype characteristics (phenological and physiological responses to environment) and for soil parameters and their initial conditions. One departure from this constraint of parameterization is where crop models have been interfaced with quantitative genetics models. In CGM-WGP (Crop Growth Model – Whole Genome Prediction) strategies, crop parameters are effectively estimated as functions of genomic markers, i.e. enabling incorporation of ‘physiological trait effects’ into modern genomic prediction-based breeding programs (Cooper et al 2021).

With the increased capability of deep learning methods, it is appropriate to consider ways in which such methods might be utilized to continue the advancement and application of crop models. While crop models may retain an advantage in prediction and forecasting roles (e.g. climate change analysis), deep learning models have been promoted for use in situations where real-time information about crop growth is available, for example via satellite sensing or phenotyping.

In these situations, it may be possible to ‘replace’ a crop model with a deep learner (sometimes called an emulator) to describe biomass accumulation as a function of remote sensing indices and weather.

### Materials and Methods

This paper provides examples of how we are utilizing crop models to

- Train deep learning models to address ‘inversion problems’ for prediction of model parameters or estimation of growth traits
- Integrate with deep learning models through PIML (physics informed machine learning) approaches

### Results and Discussion

In decision support research to manage climate risk, cropping system models were historically used to create massive synthetic databases of crop management interventions (e.g. WhopperCropper, Nelson et al 2002) and to provide ‘real-time’ simulations of in-crop decision making (e.g. YieldProphet Hochman et al 2009). Research in plant breeding further motivated the use of crop models to create ‘synthetic datasets’ and initiated various research efforts to improve statistical methodologies used in ‘real-world datasets’; for example (Bustos-Korts et al., 2019) demonstrated how synthetic datasets could be used for evaluation of alternative phenotyping strategies.





Bustos Korts et al. (2019) used synthetic datasets to validate precision of statistical methods to interpret phenotypic data, e.g. time series of biomass. Building from this concept, we used crop models to generate massive synthetic datasets for a range of soil plant available water content (PAWC) conditions (Nguyen et al 2025). We demonstrated that a deep learning (DL) model (multi-modal sequential cross-model transformer) could be trained using synthetic time-series data of biomass, leaf area index NDVI and weather variables such that it could estimate the PAWC classes used to initialize the synthetic datasets with some reasonable precision. With sufficient diversity of time-series data, DL could discriminate among lower PAWCs (via impact on time-series of growth variables) although it was challenging in discriminating among higher PAWCs as there was little signal in the contrasting time series when PAWC was high.

In other research, we have used deep learning to address a related issue in remote sensing. We linked a radiative transfer model (PROSAIL) to the APSIM crop model to generate spectral information from these large synthetic datasets of LAI, chlorophyll (N) content (Chen et al., 2022). We then used a DL model to invert this synthetic dataset in order to estimate the APSIM daily outputs. This DL model could then be applied to real-world datasets in order to demonstrate its utility in estimation of remote sensing targets like LAI and chlorophyll content. Chen et al. (2022) showed that by using APSIM to create synthetic training datasets for PROSAIL, the DL model was able to 'learn' from a 'biologically constrained' training set and perform better than if all possible PROSAIL parameter combinations were used to create the training set, e.g. the crop model permitted only 'sensible' combinations of LAI and chlorophyll to be used by the DL.

In our most recent research, we aim to develop physics-informed machine learning (PIML) techniques for crop trait prediction that effectively integrate empirical data with established physical and physiological knowledge. By combining the strengths of both data-driven and physics-informed approaches, this activity seeks to deliver accurate and robust crop trait predictions across diverse environmental conditions and management practices, using readily available data sources such as reflectance indices from multispectral imagery. Rather than relying solely on data, as in standard machine learning, the models will be guided by physical principles during training. In particular, the PIML framework will utilize simulations and low-cost sensor data to train models for predicting key crop traits such as biomass, water use efficiency (WUE), and nitrogen use efficiency (NUE).

### Conclusions

The next generation of crop models will utilize deep learning methods in parameterization of both environmental and crop/genetic parameters and progress development of hybrid methods which combine crop and deep learning models including for biological processes which are challenging to parameterise.



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## Does model formalization impact its ability to simulate high yielding situations : Lessons learned from a multi-model ensemble

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**Keywords :** AgMIP-Wheat, High yield, Multi-model ensemble, Model formalization, ROTS dataset.

### Introduction

Wheat is the most traded crop commodity at the global scale and provides more than 20% of calories and protein in human diets (Shiferaw et al., 2013). However, cropping systems' ability to produce food in quantity and quality is impacted among others by climate change through increased temperatures, changing precipitation patterns, and greater frequency of extreme events (drought, waterlogging, etc.). Identifying Genotype (G) traits and adapted Management







(M) practices allowing to maintain high and stable yielding situations across various Environment (E) remains a challenge in face of the GxExM interactions complexity (Dueri et al., 2022, Stella et al., 2023).

Process-based crop models have been used from local to global scales to investigate the effects of management and climate change on crop growth, including grain yield and nutritional quality (Gurain et al., 2022), and environmental impacts, such as SOC and GHG emissions (Basso et al., 2025). Research over the last several decades has shown that there is no silver-bullet soil-crop model and that multi-model ensembles (MMEs) have quite high skill and are better than most, if not all, individual models to capture and simulate the diversity of broader sets of environmental conditions and management practices (Wallach et al., 2018). Crop models remain simplified representations of complex agro-ecosystem functioning. Each model incorporates varying theoretical assumptions, leading to conceptualization ranging from (semi-)empirical to accurate formalization of physically-based process or mechanism. As one moves away from the conditions under which they were developed, calibrated and validated, other mechanisms may come into play that the model would not represent (Basso et al., 2025).

Wheat yield elaboration is the result of complex dynamic and interacting processes. Understanding drivers and limits in high yielding situation – i.e. when yield gets closer to its biophysical limits - requires more insight into the deterministic pathways of yields elaboration. To help visualize and analyse the interrelationships within the ecophysiology of wheat grain yield setting, the concept of wiring diagram has recently been proposed (Reynolds et al., 2022). It offers insights into the dynamic switch between source- and sink-force that underlines grain yield elaboration and has been linked to the harvest index (HI) concept, i.e. the ratio between aboveground source and sink organs at harvest.

We propose to use the wiring diagram framework to investigate how formalization within a MME can impact MME's ability to simulate high yielding situations.

## Materials and Methods

Wheat growth and yield were monitored at Rots, in France, between 2002-04, 2008-10 and 2012-16. Data collected included dynamic records of phenology, total biomass, plant N uptake, grain yield components (final yield, ear number, thousand kernel weight) and grain N content, as well as meteorological conditions.

The MME was constituted of 27 models. Simulations of the 11 years were performed under 4 modes, namely i) actual soil water and N supply (LO), ii) unlimited N supply (UN), iii) unlimited water supply (UW) and iv) unlimited water and N (UL). As it seemed that a problem with soil water holding capacity existed, UW mode was retained for this study.

Model were clustered on two main criteria regarding their formalization :

- Light utilization : do model rely on RUE approach or another one (e.g. photosynthesis/respiration) ;
- Yield elaboration : do model rely on explicit simulation of grain number or on HI approach.

## Results and Discussion

The e.Median of models' cluster simulating light use using RUE concept showed slightly better performances in simulating biomass and yield, but tended to compensate by simulating a longer grain filling period, by anticipating anthesis date.

The e.Median of models' simulating explicitly sink strength (grain number) tended to perform slightly worst in predicting yield and biomass, due to a systematic underestimation (Fig.1). This was particularly true for low yielding situations.

Important differences in phenology simulation performances were reported for the different clusters, as well as in *ex post* HI.





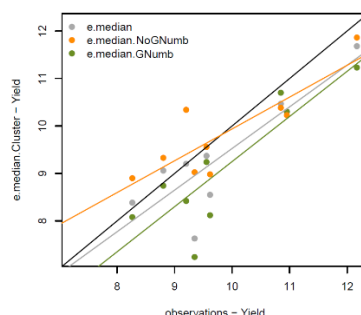


Figure 1. Global and clustered e.Median - by yield elaboration formalisms - against observations.

## Conclusions

We showed that model formalization, especially formalisms related to the simulation of sink and source strengths might have an important impact on model's ability to reflect contrasts between high yielding and low yielding situations.

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## Simulating the Impact of Biotic Stresses on Wheat through Disease-coupled Multi-Model Ensembles

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**Keywords:** Disease modeling, crop growth models, DSSAT, D-MME, fusarium head blight

### Introduction

Pests and diseases (P&D) pose a significant threat to wheat production and, thus, global food security. By 2050, wheat output must increase 35–56% to feed the world population (Van Dijk et al., 2021). However, shifts of global temperature and precipitation patterns under a changing climate add uncertainty for agricultural systems to meet such expectations. The effects of a more humid and warmer climate with an increased occurrence of extreme weather events can further exacerbate wheat production loss due to biotic stress (Pequeno et al., 2024).

Modeling P&D impacts has been limited due to the complexity of the system, knowledge gaps, and the difficulty in making reliable predictions. So far only a few studies have integrated agrophysiological and epidemiological processes, and disease-coupled crop models remain scarce, often relying on a single wheat model. Meanwhile, Multi-Model Ensembles (MME) have shown that ensemble mean (E-mean) and median (E-median) can reduce uncertainty and better match observations than individual models (Martre et al., 2015). However, most crop models cannot simulate P&D interactions, leaving biotic stress as a major source of uncertainty of crop model projections. The goal of this study is to introduce a Disease-coupled Multi-Model Ensemble (D-MME) approach within the Cropping System Model (CSM) of the Decision Support System for Agrotechnology Transfer (DSSAT; Hoogenboom et al., 2019), enabling simultaneous simulation of abiotic and biotic stresses on wheat development and yield.

### Materials and Methods

Pest coupling points were implemented in CSM-CROPSIM-Wheat and CSM-CROPSIM-CERES-Wheat and used with the disease-coupled CSM-NWheat model (Ferreira et al., 2021) to simulate the effect of *Fusarium head blight* (FHB; *Fusarium graminearum*) on wheat. These coupling points are linked to model rate and state variables, enabling integration with P&D damage modules. Field data from six locations over six years (2017–2022) were used for calibration and evaluation of the disease-coupled models. At one site, a two-year dataset captured natural FHB infections under four fungicide regimes: 7-day, 14-day, 21-day, and a control with no fungicide application. The 7-day treatment showed little to no visible symptoms of infection and was considered disease-free, providing a basis for evaluating the individual models and ensemble performance.

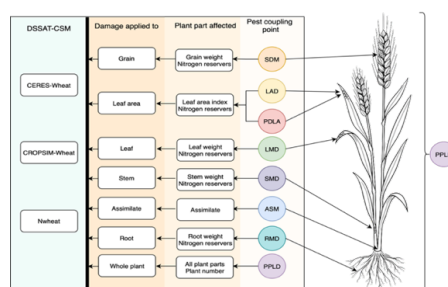


Figure 1. Graphical representation of the coupling method between pest and disease models and wheat growth modules within the DSSAT-CSM.



## Results and Discussion

The three wheat models showed different responses when simulating the daily grain development under disease pressure. The D-MME approach showed a greater statistical significance in simulating yield under the effect of disease damage for both the E-mean and E-median (Table 1). A comparison between disease-coupled and uncoupled approach was conducted to highlight how crop models that do not account for biotic stress pressure would perform.

*Table 1.* Grain yield of wheat under fungicide treatments at Coxilha, RS, Brazil, in 2018 and 2019. Model results and statistical evaluation compare yields simulated by disease-coupled models and the ensemble approach against end-of-season observations.

Treatment	Field observations	CSM-CERES-Wheat	CSM-CROPSIM-Wheat	CSM-NWheat	E-mean	E-median
<b>2018</b>						
7-day interval	3832	3760	3920	3798	3826	3798
14-day interval	3593	3449	3616	3598	3554	3598
21-day interval	3367	3365	3532	3554	3484	3554
No Fungicide	2852	2825	2973	3269	3022	2983
<b>2019</b>						
7-day interval	4468	5452	4726	3919	4699	4744
14-day interval	4138	4648	4072	3476	4065	4088
21-day interval	3985	4240	3737	3247	3741	3751
No Fungicide	3073	3925	3474	3073	3491	3487
<b>Statistical analysis</b>						
Disease-coupled approach	<i>RMSE (kg ha<sup>-1</sup>)</i>	406.6	207.6	517.3	<b>197.3</b>	<b>205.5</b>
	<i>NSE</i>	0.23	0.79	-0.24	<b>0.83</b>	<b>0.80</b>
	<i>R<sup>2</sup></i>	0.90	0.81	0.14	<b>0.82</b>	<b>0.82</b>
Uncoupled approach	<i>RMSE (kg ha<sup>-1</sup>)</i>	1007.9	636.71	430	584.8	592.2
	<i>NSE</i>	-3.72	-0.88	0.14	-0.59	-0.63
	<i>R<sup>2</sup></i>	0.57	0.57	0.57	0.57	0.57

Variability among individual model simulations emphasizes the importance of using MMEs rather than relying on individual model outputs for decision-making. The D-MME results demonstrated improved agreement with the observations across all treatments when simulating crop growth under both abiotic and biotic pressures. Both E-mean and E-median outperformed the statistical metrics of the individual wheat models.

## Conclusions

As most crop simulation models fail to account for the impacts of P&D on crop growth and yield losses, the use of diseased-coupled crop models capable of simulating biotic and abiotic dynamics can address this critical gap in current crop modelling studies. The novel D-MME enables a more accurate representation of agrosystems and an initial step for more accurate predictions of crop production projections under a changing climate.



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## The FraNchEstYN modelling framework for the synchronous estimates of yield losses due to plant diseases

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**Keywords:** Crop modeling, Epidemiology, Yield loss, R-package, SEIR.

### Introduction

Operational tools that quantitatively link plant-disease epidemics to crop production remain scarce (de Angelo Luca et al., 2024), even as losses stay substantial and uneven across regions and climate change reshapes pathosystem dynamics. In response, we present FraNchEstYN, an open-source R package delivering an interoperable crop-disease framework that runs stand-alone or couples at run time to external crop models. This framework aims to provide synchronous estimates of yield losses due to plant diseases.

### Materials and Methods

The FraNchEstYN framework provides a modular environment to quantify disease-induced yield losses under contrasting environments and management (Figure 1). Temperature- and moisture-driven suitability, adapted from Magarey et al. (2005) feeds a Susceptible-Exposed-Infected-Removed (SEIR) epidemiological core, and simulated disease severity (DS) is translated into yield loss via four damage mechanisms, i.e., light stealers, assimilate sappers, senescence accelerators, and radiation use efficiency (RUE) reducers. The crop component operates either as a simplified RUE-based internal engine computing phenology, and attainable intercepted light, biomass, and yield, or by ingesting attainable trajectories from external models and applying the damage mechanisms. FraNchEstYN also provides a fungicide module simulating time-varying efficacy, automatic crop and disease model calibration with diagnostics and uncertainty, and an output layer that harmonizes time series and seasonal summaries, computes metrics, and optionally generates decision-support messages with a large language model, all backed by reproducible vignettes. We clarified model behavior through a global sensitivity analyses, performed using the Morris method (Morris, 1991) extended by Campolongo et al. (2007). The analysis focused on parameters within the Suitability, Disease, and Damage modules across six AgMIP-wheat study locations that span contrasting environments (Asseng et al., 2019). The study specifically compared two pathogen "archetypes" with discordant ecophysiology: a rust-like, non-splashborne pathogen with short wetness requirements and high sensitivity to dry interruptions, and a blast-like, splashborne pathogen with longer wetness requirements and weak dry-interruption sensitivity. The performance of the framework were tested in four case studies with open data: yellow rust (*Puccinia striiformis*) in Egypt; Septoria (*Septoria tritici blotch*) in Indiana and Ethiopia; wheat blast (*Magnaporthe oryzae* pathotype triticum ) in Brazil.

### Results and Discussion

The global sensitivity analysis, performed across the six contrasting locations, demonstrated the plasticity of the FraNchEstYN framework in reproducing discordant epidemic development across pathogen types and environments. Simulated DS trajectories and yield losses varied widely across sites. In arid environments, pathogen suitability was modest and disease severity remained low for both archetypes. At temperate sites, the rust-like archetype exhibited high severity and yield loss, consistent with its adaptation to humid conditions. In contrast, the blast-like archetype showed delayed suitability and lower severity in cooler environments, while reaching high severity in some temperate sites after prolonged favorable conditions (precipitations).



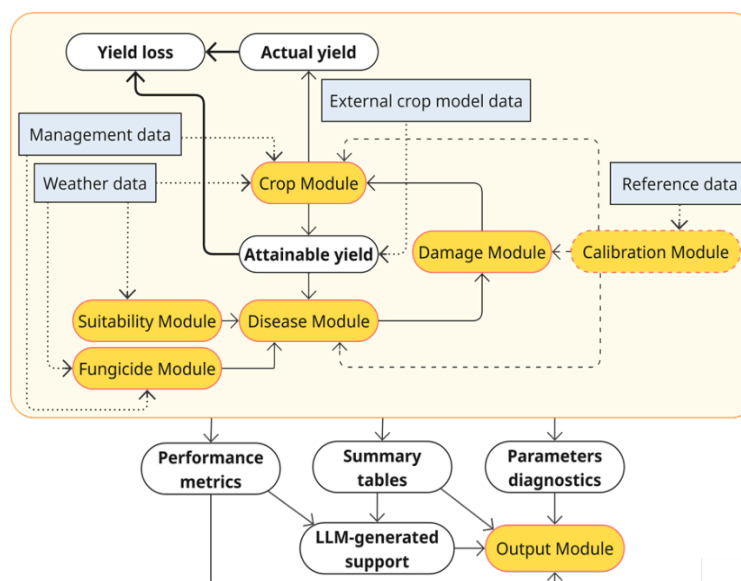


Figure 1. The framework's structure comprises external inputs (cyan boxes), core process modules (yellow boxes), and main outputs (white ellipses). Solid arrows indicate the main flow of information between modules (e.g., Crop, Disease, Damage), while dotted arrows highlight external inputs necessary for driving epidemiological and yield loss estimates

Simulated DS, for both pathogen archetypes, was found to be highly sensitive to the parameters of the Suitability module, particularly those describing temperature responses, leaf wetness, and relative humidity thresholds. This indicates that epidemic trajectories are strongly affected even by small variations in these ecophysiological factors. Furthermore, DS simulation showed a consistently high sensitivity to the parameters controlling primary inoculum, especially for the rust-like pathogen, underlining the critical importance of external infection sources. Conversely, the influence of parameters associated with secondary inoculum and epidemic clocks on variance was limited.

For yield loss, the ranking of influential parameters was partly reshuffled, and parameters of the Damage module, which had no effect on simulated disease severity, gained prominence. In the blast-like archetype, yield loss remained most sensitive to temperature response parameters, followed by humidity and wetness thresholds. In contrast, for the rust-like archetype, damage parameters acquired relatively higher influence, sometimes reaching importance comparable to suitability parameters. This shift reflects the closer coupling between epidemic development and yield reduction in rust epidemics, whereas blast-type epidemics were primarily constrained by environmental suitability.

The model's ability to operate in diverse, real-world scenarios was confirmed by its evaluation against the four distinct crop-disease case studies. The framework successfully simulated disease severity and corresponding yield loss under varied local conditions and crop managements, including crop resistance and fungicide applications, and provides a strong proof-of-concept for the framework's robust predictive capacity.

## Acknowledgements

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## Algorithm-driven root optimization for maize water uptake and yield in the Midwest

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Effective soil root exploration is central to improving water uptake and yield, yet root system distribution remains a lesser explored dimension of crop improvement. This study integrates the Cycles agroecosystem model (Kemanian et al., 2024) with an evolutionary algorithm to identify optimal maize root distributions across the U.S. Midwest, offering a novel framework for algorithm-driven trait design. We evaluated how root architecture expressed the root functional distribution with depth influences water uptake dynamics and grain yield under climatic conditions spanning historical (1980–2020) and future (2051–2075, 2076–2099) scenarios across the Midwest.

The results reveal distinct spatial patterns driven by climatic gradients. Optimization for 1980–2020 yielded four dominant phenotypes from top-heavy to balanced root distribution (Fig. 1). Precipitation, subsoil plant-available water, and vapor pressure deficit (VPD) strongly influencing optimal strategies. In wetter regions, the depth at which 50% of roots are located (D50) was  $\approx 0.8$  m, enabling access to water throughout the profile and increasing transpiration by up to 33% and yield by 26% compared to non-optimized phenotypes. In drier western zones, bimodal distributions prevailed in the current climate, balancing access to surface summer precipitation and subsoil water. These phenotypes limited transpiration in wet years but preserved water for reproductive stages, stabilizing yield across seasons.

Under future climate scenarios, maize yields declined if hybrid phenology remained static, despite increased precipitation in some areas. Increased VPD was a key driver of yield loss, alongside shortened growing seasons and accelerated early-season water demand. Optimization could only partially offset these losses. Future optimal phenotypes clustered similarly to historical ones, though bimodal distributions declined in favor of shallower or balanced architectures.

This work highlights the potential of algorithm-based phenotype design tailored to regional hydric regimes to enhance water-use efficiency and resilience to climate variability. It illustrates the broader utility of optimization algorithms in discovering site-specific adaptive traits that can synergistically complement field experimentation and genomic selection in accelerating the development of site-specific and climate-resilient cultivars.





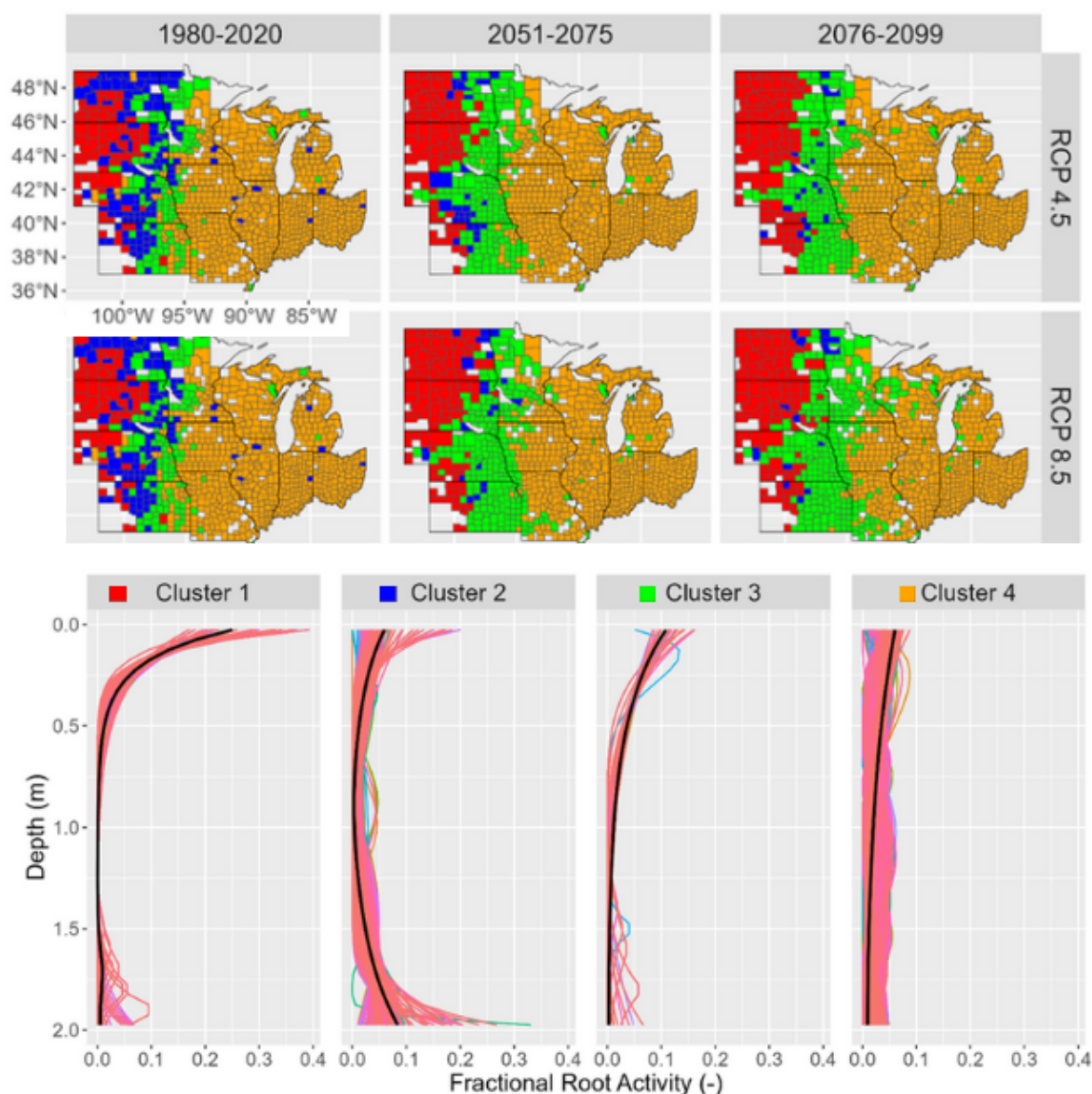


Fig. 1. Optimized root phenotype clusters and their geographic distribution for distinct climatic scenarios. Cluster 1 = top-heavy, cluster 2 = bimodal, cluster 3 = mildly top-heavy, cluster 4 = balanced.



## Estimating spatial and temporal variability of crop growth by radiation-driven models based on satellite data assimilation

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**Keywords:** precision agriculture; production efficiency models; LAI; earth observation; sensitivity analysis

### Introduction

Precision agriculture aims to improve field management by accounting for spatial variability in dynamic cropping systems (CS). To support farmers in optimizing crop management, it has become important to develop tools that capture both spatial and temporal heterogeneity within crop production. Mechanistic crop models simulate aboveground biomass (AGB) accumulation by explicitly representing physiological and environmental processes linking absorbed solar radiation, transpiration, and nutrient uptake. However, these process-based models typically require site- and cultivar-specific calibration and often fail to capture fine-scale variability. Assimilating remote sensing (RS) data into radiation-driven Production Efficiency Models (PEM; Monteith, 1977; McCallum et al., 2009), offers a promising solution by providing spatio-temporal explicit predictions of biomass growth, and thus crop requirements or responses.

### Materials and Methods

A PEM was developed and implemented in a PostGIS database to run at a daily time steps and with Sentinel-2 (S2) resolution (10 x 10 m). Leaf Area Index (LAI), derived from the S2 biophysical processor (Weiss et al., 2020), was assimilated daily to estimate the fraction of intercepted solar radiation by crops at pixel level via the Lambert–Beer law.

The PEM was calibrated and evaluated for wheat and maize grown in the Po Valley (northern Italy) using two independent datasets. Calibration relied on 120 AGB observations (2022-2023) from five different sites with different management practices, while evaluation was carried out on 312 observations (2025) from four additional sites.

Although the temporal and spatial dynamics of LAI should implicitly reflect the effects of limiting factors, a development stage-dependent Morris sensitivity analysis (SA) was conducted to assess how variations in LAI dynamics, air temperature, and senescence affect simulated AGB.

### Results and Discussion

The simulations performed for each S2 pixel provide reliable estimates of AGB. On evaluation, the model achieved a relative Root Mean Square Error of 0.23 and a model efficiency of 0.92, effectively capturing temporal and spatial variability across and within the different CS (Figure 1). Assimilating LAI enabled the model to overcome common limits of process-based models that require site- and crop-specific tuning. SA highlighted that LAI accuracy during early growth stages strongly affects AGB predictions and in-season decisions. From stem elongation onward, radiation use efficiency (RUE) and temperature responses became dominant drivers, with senescence adjustment from milk ripening stage preventing overestimation at harvest.



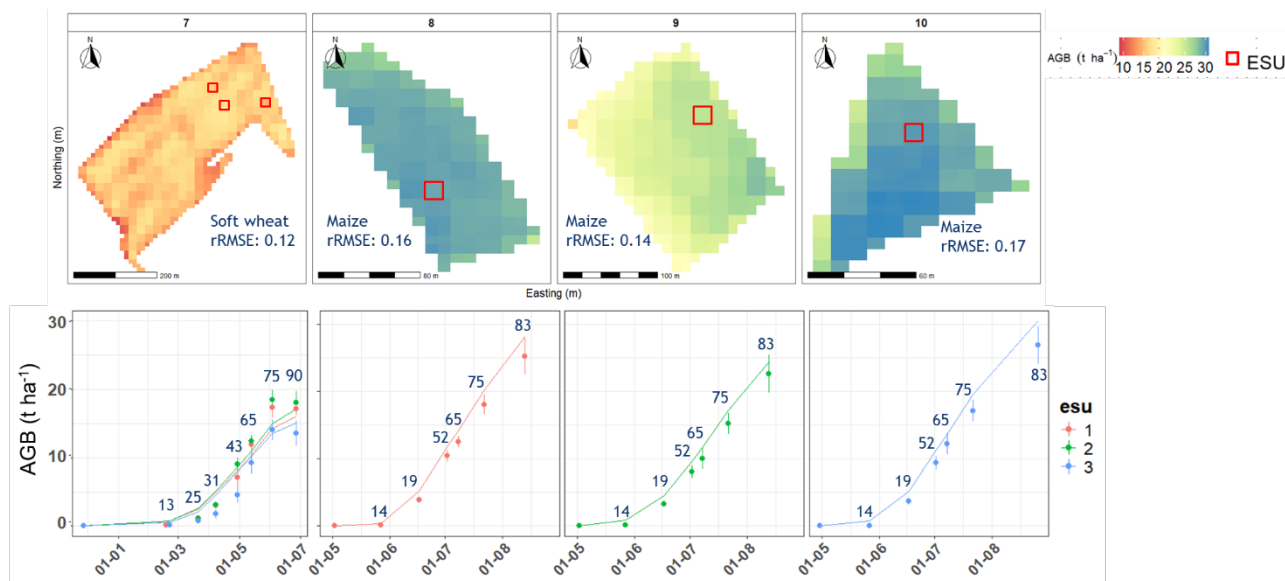


Figure 1. Top: maps of evaluation sites at harvest, showing the relative Root Mean Square Error (rRMSE) for each elementary sampling unit (ESU). Bottom: simulated crop growth over time (solid line) compared with observed data (points), with phenological stages indicated using the BBCH scale.

## Conclusions

Integrating daily LAI assimilation into a simplified radiation-driven framework captured spatial and temporal variability across crops, sites, management systems and seasons. Accurate early-season LAI estimates are critical, while RUE, temperature, and senescence primarily drive AGB growth in later stages. By assimilating RS data, the model overcomes common limitations of process-based approaches and provides a robust tool for monitoring crop productivity across heterogeneous CS.

## Acknowledgements

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## Integrating Process-Based and Data-Driven Models for Wheat Yield Prediction Under Variable Meteorological Conditions

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**Keywords:** Crop modelling, Random forests, Hybrid modelling, Climate variability, Model evaluation

### Introduction

Understanding spatial and interannual variation in crop yield is crucial for effective crop management under climate change. Quantitative models are widely used to evaluate climate-related impacts on food security (Jägermeyr et al., 2021). To this end, diverse modeling approaches are applied, compared and sometimes combined (Leng & Hall, 2020). Process-based crop models capture underlying biophysical mechanisms – such as phenology, water balance and temperature response - and provide interpretable diagnostics, but they often exhibit systematic biases and limited local calibration. Statistical models, such as linear models (LM) or random forests (RF) can outperform process-based models in interpolation tasks; however, they lack mechanistic interpretability and may perform poorly when extrapolating beyond observed conditions. Pragmatic approaches integrate different modeling methods to correct residual biases or combine predictions.

### Materials and Methods

For 212 observations of winter wheat (*Triticum aestivum* ‘Capo’) yield, collected from field trials across Austria between 2004 and 2024, corresponding gridded meteorological data (INCA; Haiden et al., 2011) were obtained. Each trial site was assigned to soil class of the Soil Map of the European Communities (Reinds et al., 1992). Yields were estimated with two reference models, and six hybrid models created from combinations of the reference models with statistical models. Model performance was compared overall and for different combinations of yearly temperature and precipitation sum levels. The **crop model** WOFOST (van Diepen et al., 1989) was calibrated to observed phenology and yield data with 5-fold cross validation (reference model 1). In addition, we estimated yield with a **random effects (RE) model** using soil characteristics, weather covariates (growing degree days, precipitation, frost days, heat days, global radiation by phenological phase), their interactions, and a random effect for variety, as predictors (reference model 2).

Subsequently, two classes of hybrid models explained yield with soil class, yearly precipitation and temperature sums. For the augmented models, a RF model was complemented with the estimated yields of the reference models as additional explanatory variables (**crop model RF augmented** and **RE-model RF augmented**). For the residual correction models, the residuals of each reference model were fitted with the LM and RF model, respectively, and predicted values of these models were added to the estimates of the reference model (**crop model LM-residual-corrected**, **crop model RF-residual-corrected**, **RE-model LM-residual-corrected**, **RE-model RF-residual-corrected**). All models were trained and tested using 5-fold cross validation.

As metrics for model performance, Root Mean Square Error (RMSE), Pearson’s correlation ( $R^2$ ), Bias, Absolute Bias and the Willmott’s index as overall performance score were calculated. Performance was calculated for the whole dataset as well as within nine meteorological categories defined by the combination of low, medium and high levels of yearly precipitation and temperature sums. Additionally, a category-averaged score was calculated as mean value of the metrics over the categories. To evaluate the effect of binning, three methods were used to define category breaks: quantile-based, standard deviation-based, and equal-width approaches.





## Results and Discussion

Overall, model performance according to Willmott's index was similar among the reference models (Figure 1A). The RE-model achieved a higher  $R^2$ , whereas the crop model showed slightly lower bias. Hybrid modelling further improved the crop model, with the best results obtained from residual correction using a linear model (LM). RMSE varied little across models.

Model performance across meteorological categories, as measured by the average Willmott's index, is shown in Figure 1B. Averaged across categories (column 1), the RE-model outperformed the crop model, although the crop model achieved higher performance in 5 of 9 categories and was further improved through LM and RF residual correction. Models generally performed better in categories with medium to high precipitation and temperature levels. Results shown in Figure 1 are based on the quantile binning approach. Absolute values of model performance metrics were influenced by the chosen binning approach. However, for all approaches, the LM-residual corrected crop model performed.

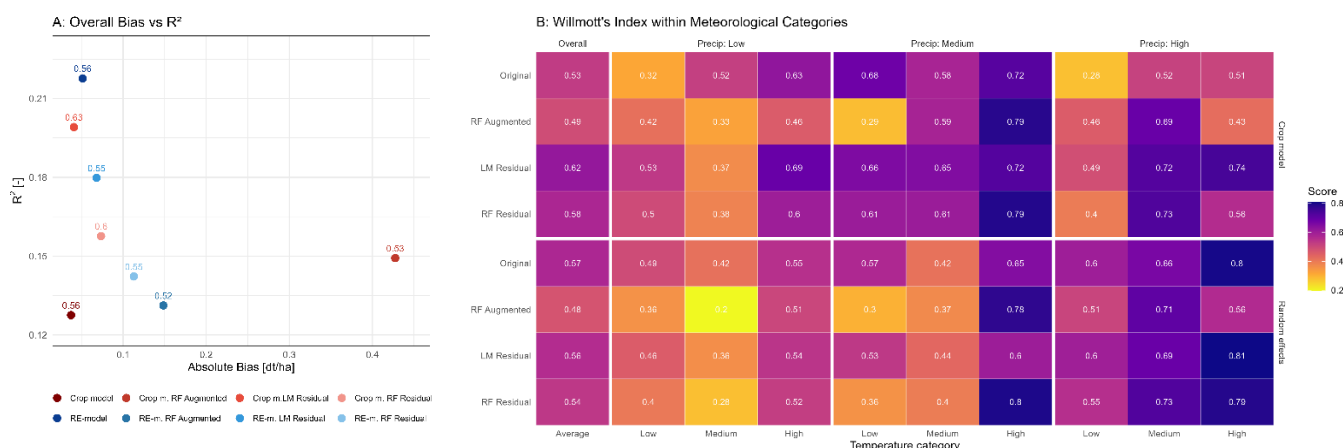


Figure 1. A: Model performance metrics for the whole dataset with Willmott's index as labels. B: Willmott's index averaged over meteorological categories and within each quantile-defined category

## Conclusions

While data-driven statistical models achieve high overall accuracy in predicting wheat yields for a given dataset, process-based crop models can outperform them under diverse meteorological conditions, such as certain temperature and precipitation regimes represented in the data. Hybrid approaches retain the mechanistic interpretability of crop models while improving predictive performance. The results further highlight conditions, such as cool and dry periods, where model performance could be improved.

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## From theory to gradients: crop growth models for the AI era

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**Keywords:** crop modeling, machine learning, differentiable programming

### Introduction

Crop Growth Simulation Models (CGSMs) are versatile tools for forecasting yields, assessing climate impacts, and supporting resource management. Rooted in decades of agricultural knowledge, they provide explainable, theory-based predictions. Nevertheless, traditional CGSMs often face challenges related to parameterization, incomplete representation of complex processes, and limited ability to fully leverage large-scale datasets. Data-driven models have emerged as alternatives but face limitations in interpretability and data demands. In geosciences, differentiable programming, embedding gradient-based optimization into scientific models, has successfully bridged data-driven and process-based approaches, enabling large-scale data assimilation and hybrid modelling (Gelbrecht et al., 2023; Shen et al., 2023; Tsai et al., 2021). Yet, such approaches remain largely unexplored in agriculture due to the legacy implementation of CGSMs.

### Materials and Methods

We aim to advance crop growth modelling by re-implementing WOFOST, a widely used process-based crop growth model (de Wit et al., 2019), as a differentiable model. This enables gradient-based parameter estimation, scalable data assimilation, and replacement of ill-posed modules with AI components, while ensuring compatibility with existing WOFOST workflows. The implementation is based on PyTorch, supporting automatic differentiation, GPU/TPU acceleration, and HPC deployment. The framework is openly available at <https://github.com/WUR-AI/diffWOFOST>.

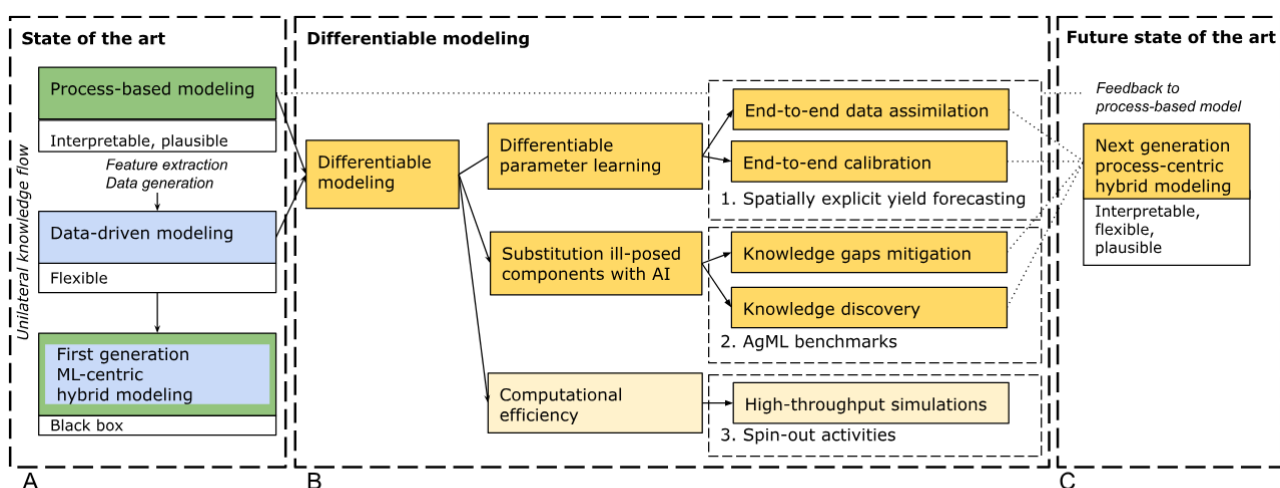


Figure 1 (A) Process-based modeling and data-driven modeling are treated as separate entities with no integration. Knowledge flow is unidirectional. (B) Differentiable modeling allows for the full integration of process-based and data-driven approaches. Advantages are illustrated through three distinct use cases. (C) Differentiable modeling will pave the way for creating of next generation hybrid crop growth models.





## Results and Discussion

The differentiable WOFOST framework is currently under development and will be demonstrated through three distinct use cases. The first use case focuses on spatially explicit yield forecasting across all arable parcels in the Netherlands (2017–2024), integrating satellite-derived leaf area index data to evaluate the capacity of differentiable parameter learning for large-scale calibration. The second use case applies our framework in AgML benchmarks, focusing on yield prediction under climate change scenarios and subnational yield forecasting (Paudel et al., 2025), thereby situating our approach within state-of-the-art machine learning competitions. Our third use case explores computationally intensive applications such as reinforcement learning for crop management and agricultural digital twins, where the efficiency gains of vectorization and hardware acceleration allow more extensive experimentation than current implementations permit. Collectively, these demonstrations aim to illustrate how differentiable programming can overcome long-standing calibration bottlenecks, enhance integration with remote sensing, and facilitate process-centric hybrid modelling.

## Conclusions

Differentiable programming provides a promising approach to combining established process-based knowledge with AI-driven flexibility. The differentiable WOFOST model is designed to offer interpretable, generalizable, and computationally efficient simulations, and may serve as a foundation for further research in precision agriculture, food security, and crop breeding.

## Acknowledgements

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## LLM-assisted workflow for crop model components generation towards interoperable agricultural platforms

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**Keywords : Code Analysis; Crop2ML; Large language models; Model reuse**

### Introduction

Process-based crop models encapsulate agronomic knowledge in modular components, yet structural heterogeneity across modelling platforms constrains component reuse (Donatelli et al., 2014). Decoupling the scientific logic of the model from platform architecture is a prerequisite for reusability (Holzworth et al., 2010). In response, the framework Crop2ML serves this purpose by representing components through a set of semantic metadata and by implementing a bidirectional transpilation process between platform and CyML languages (Midingoyi et al., 2023). Crop2ML relies on manual curation of semantic metadata, which is prone to errors and time consuming. Recent advances in large language models (LLMs) have shown their ability to extract meaningful content from source code using semantic context (Jelodar et al., 2025). Here we aim to facilitate the curation of semantic metadata by integrating LLM into the Crop2ML framework.

### Materials and Methods

We designed a reproducible LLM-assisted Python workflow to semi-automatically generate Crop2ML components from legacy crop model code, by extracting and generating structured semantic metadata, and by transpiling code into CyML (Figure 1).



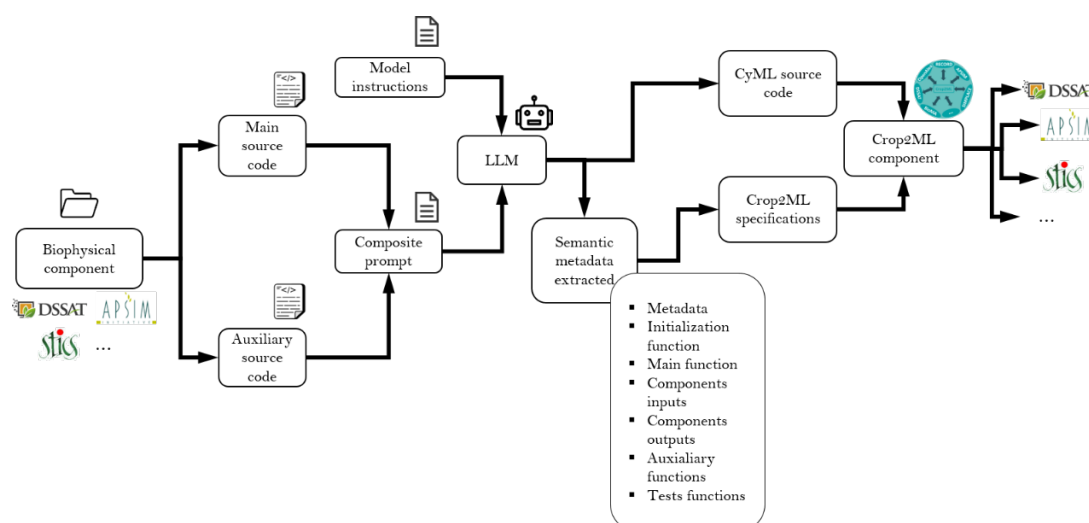


Figure 1. Schema of the LLM-assisted workflow transforming a crop model component into a Crop2ML component.

Our workflow has been evaluated on two use cases: (UC1) 8 soil temperature components drawn from 6 widely used crop modelling platforms (from the Agricultural Model Exchange Initiative; Martre et al., 2018) to represent a range of programming languages and code architecture; and (UC2) 12 subcomponents (simple strategies) from an energy balance model component implemented in the modeling framework BioMA. The evaluation of the workflow was based on ground-truth Crop2ML components created by experts of each platform. Retrieval metrics and classification checks were used to identify input/output variables and the consistency of their specifications. Recognizing the non-deterministic outputs of LLMs, the workflow was executed in 10 independent runs to report variability.

## Results and Discussion

Evaluation across UC1 components demonstrated over 75% accuracy in input extraction, and over 90% accuracy in output extraction (for 6 out of 8 components). Evaluation on UC2 showed over 80% for both precision and recall. Classification of data type highlighted a near perfect score for each component and the workflow successfully inferred plausible metadata when documentation was ambiguous or incomplete.

Good results are contingent on explicit code structure, well-encapsulated components and rich contextual documentation, whereas components with numerous variables produced higher false positives. Practically, the workflow reduces manual annotation time (around two minutes per component) but still requires human verification to correct errors and to validate classifications. The adoption of transparent coding standards and thorough documentation, alongside a human-in-the-loop process, contributes substantially to improved reliability.

## Conclusions

This study demonstrates that a LLM-driven workflow can semi-automatize the transformation of crop model components from heterogeneous platforms into a shared interoperable representation (e.g. Crop2ML). The approach should be understood as an accelerator for the generation of interoperable components that can require manual correction, but enable broader interoperability across the crop modelling community. To maximize accuracy and reproducibility, best practices include supplying comprehensive source code and documentation.



## Acknowledgements

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## Data-driven and interpretable crop growth modeling using sparse identification of nonlinear dynamics (SINDy)

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**Keywords:** sparse regression, reduced-order modeling, high-throughput phenotyping

### Introduction

Crop growth models (CGMs) are important tools for understanding genotype-by-environment-by-management (G×E×M) interactions. Process-based CGMs such as WOFOST (Van Diepen et al., 1989) build on decades of physiological research, but their many parameters and calibration requirements limit large-scale use, e.g., in plant breeding. To address this issue, we apply the Sparse Identification of Nonlinear Dynamics (SINDy) (Brunton et al., 2016), which combines data-driven model discovery with expert knowledge. In this framework, the user guides model identification by specifying relevant environmental drivers and choosing the set of candidate functions. This combination of data-driven flexibility and physiological insight enables compact models that are both accurate and interpretable.

### Materials and Methods

SINDy extracts compact systems of ordinary differential equations (ODEs) from time series of crop and environment data. Candidate basis functions are selected by the user, and sparse regression is employed to select the minimal set needed to describe the dynamics. As a proof of concept, we used *in silico* WOFOST simulations (De Wit, 2018) of potato (five cultivars across multiple years). Our analyses focused on the simulated leaf area index (LAI) and dry weight of storage organs (WSO), although the approach is readily applicable to UAV- and sensor-based traits as well. Robustness and generalization were assessed with leave-one-year-out cross-validation (LOYOCV).

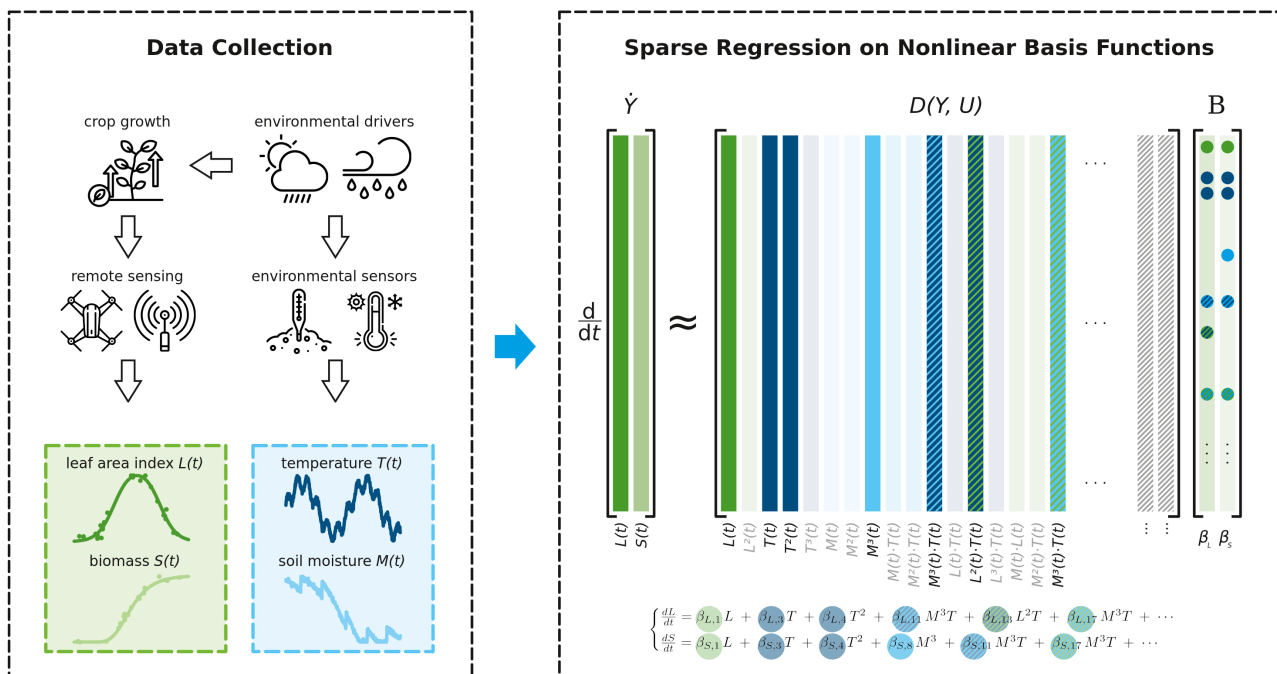


Figure 1. Workflow of the proposed SINDy-based approach. Data sources (e.g., remote sensing and environmental sensors) provide time series of crop traits (e.g., leaf area index  $L(t)$ , storage organ weight  $S(t)$ ) and environmental drivers (e.g., temperature  $T(t)$ , soil moisture  $M(t)$ ). Sparse regression on nonlinear, user-selected basis functions (collected in the matrix  $D$ ) identifies compact ordinary differential equations that together



form a reduced-order, data-driven crop growth model. This reduced-order CGM captures crop growth dynamics directly from data while retaining interpretability through explicit physiological terms and coefficients.

## Results and Discussion

The compact models (10–30 terms) identified by SINDy reproduced WOFOST-simulated growth with  $R^2 > 0.9$  and RMSE within 2–4% of simulated dry weight of storage organs. This highlights the method's strength: governing equations were learned directly from data, while user knowledge guided the selection of environmental drivers. The resulting models produced physiologically meaningful terms, such as soil moisture  $\times$  temperature effects, that remained largely consistent across environments and cultivars, suggesting that the coefficients could serve as quantitative descriptors of genotype-specific dynamics. Current limitations are weaker performance for LAI dynamics, especially during senescence, and the fact that results are based on *in silico* data; validation with empirical phenotyping datasets will be essential for real-world applications.

## Conclusions

SINDy provides a framework for identifying compact, interpretable crop growth equations directly from data. By combining physiological insights with data-driven flexibility, it supports integration of novel data streams such as high-throughput phenotyping and remote sensing, while retaining interpretability. This suggests a pathway toward hybrid crop models that are interpretable and scalable across many genotypes, enabling approximation of crop growth dynamics for entire breeding populations rather than single cultivars.

## Acknowledgements

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## From measured traits to genotype-specific parameters: a modeling approach applied to maize phenology and development components

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**Keywords:** Genotypic variability, maize, phenology, phenotyping.

### Introduction

Crop Models (CMs) are used to understand, analyze and predict crop responses to environments. There has been an increased effort for CMs to better capture the genotype x environment interactions (GxE) especially with the rising risk of water shortage and other extreme climatic scenarios due to climate change. One of the targeted goals being to define realistic and achievable ideotypes for tomorrow based on the genetic diversity available today.

Although CMs are becoming increasingly mechanistic, with explicit integration of genetic variability, important limitations remain. First, genotype-specific parameters (GSPs) often mix species-level constants and genotype-level variability, making it difficult to disentangle the genetic basis of crop performance (Boote et al., 2021). Second, many widely used parameters are emergent outcomes of multiple processes rather than direct genetic traits, which limits their physiological interpretability for geneticists and breeders (Parent & Tardieu, 2014). Finally, current CMs often require a process of estimation of the GSPs, leading to possible equifinality and other limitations, which complicates its combination with genetics (Lamsal et al., 2018).

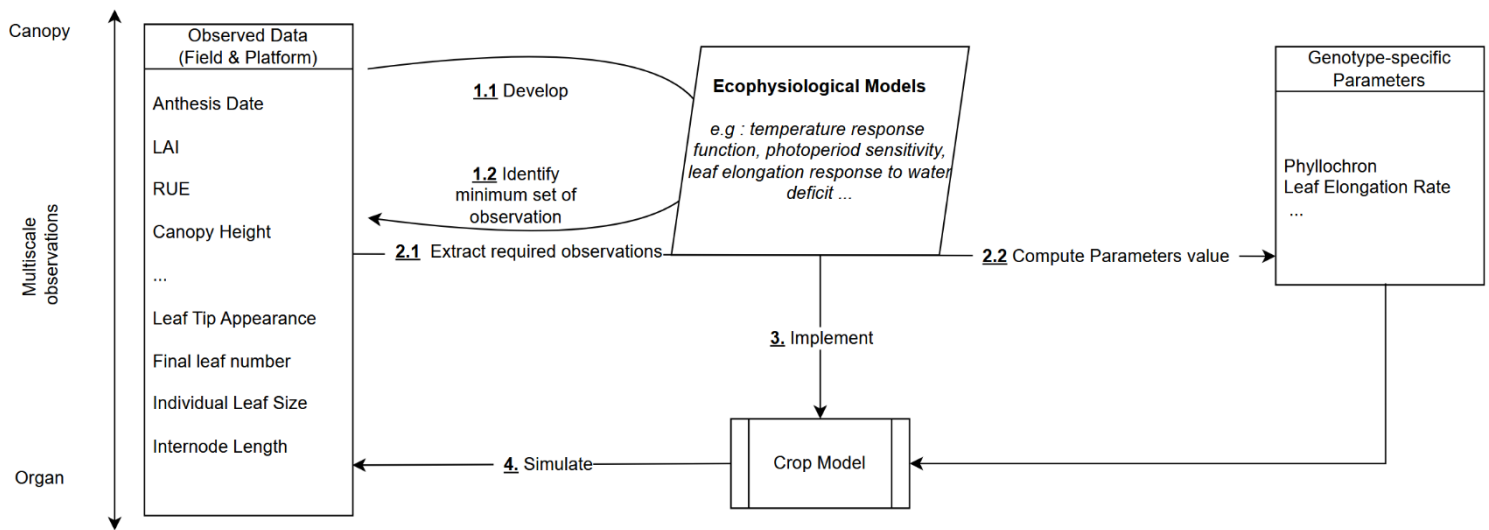
The ultimate goal of this work is to develop a generic sorghum - maize crop model, expliciting the genotypic variability of both species with a common set of GSPs. Here, we present the methodology we developed to build the maize components of phenology and development based on the SiriusQuality modeling framework (Martre et al., 2006). We developed independent components using the Crop2ML formalism (Midingoyi et al., 2021), grounded in a robust parameter set derived directly from measurements and supported by ecophysiological formalisms that represent the observed genotypic variability within a panel of maize hybrids.

### Materials and Methods

Our approach relies on the multi-scale integration of traits measured under complementary experimental conditions. Traits were collected both in controlled phenotyping platforms and in field experiments (Fig. 1). These observations were then linked through ecophysiological formalisms describing the underlying processes. The formalisms are designed to allow the genotypic parameters to be directly measured, or calibrated using observation of traits related to the subprocess they represent. (i.e. Final leaf number measured directly, leaf elongation rate parameters optimized using the observed dimension of an individual leaf)



Figure 1. Schematic representation of the modelling approach using this work.



The resulting model components were evaluated with independent field datasets. Evaluation emphasized not only final outputs such as LAI or anthesis date, but also dynamic variables and intermediate states (e.g., leaf tip appearance, leaf ligulation, individual leaf size). All developments were implemented within the Crop2ML framework, ensuring modularity and reusability.

## Results and Discussion

The developed Crop2ML components representing maize phenology and development allowed a good representation of the observed diversity of output variables such as anthesis date and LAI, as well as dynamic observations of intermediate states. The described methodology permitted the development of a model defined with GSPs, computed from observed data, that have a clear physiological meaning and are representative of the genetic variability observed in the different simulated processes. Importantly, we identified a minimum set of observable traits required to compute GSP values that capture genotype-specific variability for phenology and development. By formalizing the link between measured traits and process-based model parameters, the approach advances toward disentangling genetic effects from environmental influences in crop modeling.

## Conclusions

By integrating phenotyping and field data through ecophysiological knowledge, and by grounding parameterization in measurable and stable traits, this work ultimately supports the definition of ideotypes for future climates as it facilitates the dialogue between modelers, geneticists, and breeders by providing a transparent and physiologically meaningful link between genetic variability and crop model parameters.

## Acknowledgements

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## Enhancing predictions through model component exchange: A case study on soil temperature models using Crop2ML

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**Keywords Calibri pt 10 : provide a maximum of 5 keywords different from the title.**

### Introduction

Agricultural models have to offer the scientist the possibility to create highly diverse models (modelling solutions) combining model components from different domains seamlessly. As we look to develop more general digital workflows and processing pipelines, the ability to ‘stitch’ together useful features existing in disparate tools could be very useful. To support exchange of models for streamlined model component intercomparison and improvement between research groups and modelling platforms, the Agricultural Model Exchange Initiative (AMEI; <http://crop2ml.org>) has recently developed an open-source modeling framework (named Crop2ML) for exchanging and reusing crop model components between modeling platforms (Midingoyi et al., 2023). Crop2ML facilitates porting from one modeling environment to another of code representing a specific biophysical process thanks to bi-directional code transformation, alleviating the need to program a new process into a model from scratch.

In this study, we focused on the modeling of soil temperature. Soil temperature determines the rate of key plant (e.g. germination, emergence timing, and root growth) and soil (e.g. N mineralization, greenhouse gas emissions, and carbon sequestration) processes that are essential to predict the adaptation to and impact of climate change, extreme weather events, and new agronomic practices (e.g. intercropping, mulch, direct sowing, or sowing arrangement). However, a recent maize models intercomparison study (Kimball et al., 2024) has revealed large intermodel variability in simulated soil temperature. In that study, the authors could not separate the uncertainty of the soil temperature models from the errors in soil temperature model inputs simulated by the maize models in which they were integrated. Here, we used the capability offered by Crop2ML to separate the two sources of uncertainty and to intercompare different soil temperature models across crop models. This work provides deeper experience in applying Crop2ML to crop models and is a runway for more general outcome.

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## Materials and Methods

We exchanged nine soil temperature models (APEX, Campbell, DSSAT ST, EPIC, MONICA, Parton-SWAT, SWAT, SiriusQuality, and STICS) across six modeling platforms (APSIM, BioMA, DSSAT-CSM, MONICA, SIMPLACE, and SiriusQuality). Initially, the models were implemented as standalone drivers within each platform to verify consistent results with the original code and perform a global sensitivity analysis to their drivers (inputs). We then integrated all soil temperature models into wheat crop models within each modeling platform and evaluated them over a nine-year fallow period in Ames, USA.





## Results and Discussion

We demonstrated Crop2ML's practical application with a use case focused on soil temperature models, a critical driver of cropping system responses to climate. The sensitivity analysis revealed significant discrepancies in simulated soil temperature among the models and their sensitivity weather conditions and climate, to soil type, soil water content, and ground cover (Fig. 1).

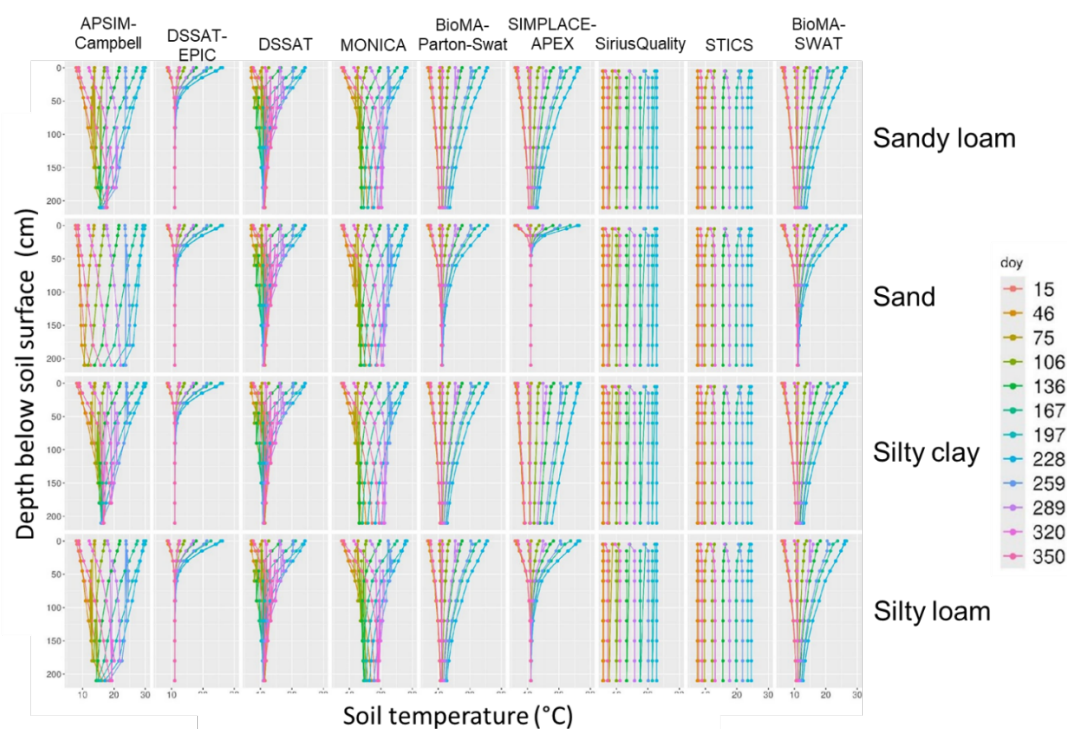


Figure 1. Soil depth versus soil temperature for different days of the years (doy) at Montpellier, France, in sandy loam, sand, silty clay, and silty loam soils simulated with nine soil temperature models. Data are 30 years averages for dry bare soils.

The simulation results from the Ames bare soil experiments demonstrated that errors in simulated soil temperature model drivers can be a major source of soil temperature uncertainty. As a result, the performance of the soil temperature models strongly depended on the crop model in which they were integrated, illustrating the importance of calibrating and evaluating model components in standalone drivers independently of larger modeling solutions.

## Conclusions

Our findings demonstrate Crop2ML's usefulness and potential to support and accelerate crop models' improvement through model component exchanges, addressing stakeholders' evolving needs.

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## Acknowledgements

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