Supplementary Information 1

Main input datasets used in PCR-GLOBWB 2 modules are described below:

S.No	Datasets	Source
1.	Weather variables - temperature - precipitation - reference potential evaporation	ERA-Interim (Dee et al., 2011)
2.	Soil parameters (upper and lower layer) - soil thickness - residual soil moisture content - soil moisture at saturation	FAO (2007) soil map; Van Beek and Bierkens (2009)
3.	Land cover fractions Land cover area	MIRCA2000 dataset (Portmann et al., 2010);

For detailed information, refer to Sutanudjaja et al.,(2018).

Supplementary Information II

The newly developed model framework integrates the PCR-GLOBWB 2 hydrological and water resources model with the WOFOST crop model through a one-way and two-way model coupling. Hydrological and crop simulations were conducted for each land-cover class, including maize, soybean, and wheat on a 5 arc-minute spatial resolution grid. To facilitate this integration, we employed a Basic Model Interface (BMI), chosen for its language independence, allowing for the coupling between PCR-GLOBWB 2 and WOFOST regardless of the programming language. This flexibility is exemplified by the WOFOST crop model being written in C language, while the PCR-GLOBWB 2 hydrological and water resources model is written in Python.

BMI functions for the development of coupled PCR-GLOWB 2 - WOFOST model framework

The coupling of the WOFOST and PCRGLOBWB 2 models is achieved through BMI functions. The rationale for selecting BMI over alternative model coupling techniques lies in its non-invasive nature; no modifications are necessitated within the code. This noninvasiveness ensures a flexible coupling framework, allowing for continuous model development without disrupting the coupling. Once BMI functions are incorporated into WOFOST and PCRGLOBWB 2, an ensemble of BMI functions becomes accessible for retrieving or altering (setting) information about model variables.

However, to establish a Python-based coupling framework, an additional wrapper was required. This wrapper serves to translate the model-specific BMI functions into Python-compatible information. The Babelizer wrapper (CSDMS, 2024) is specifically utilized in the WOFOST BMI. Conversely, no supplementary wrapper is needed in the PCRGLOBWB 2 BMI, as the model is inherently Python-compatible due to its programming language.

Babelizer, leveraging information from the babelizer input file, comprehensively details the WOFOST model. This input file contains crucial information such as the model library, entry point, packages, and author details. The necessary dependencies are then constructed to generate Python bindings, facilitated by the babelizer input file. Following the generation of Python bindings, the successful loading of the WOFOST BMI in Python is ensured through the building of the binding.

Workflow of PCR-GLOBWB 2 - WOFOST model framework

In the PCR-GLOBWB 2 - WOFOST coupling framework, the workflow following the implementation of BMI functions is consistent for both one-way and two-way coupling until the initialization of the hydrological and crop models (**Fig. S1**).

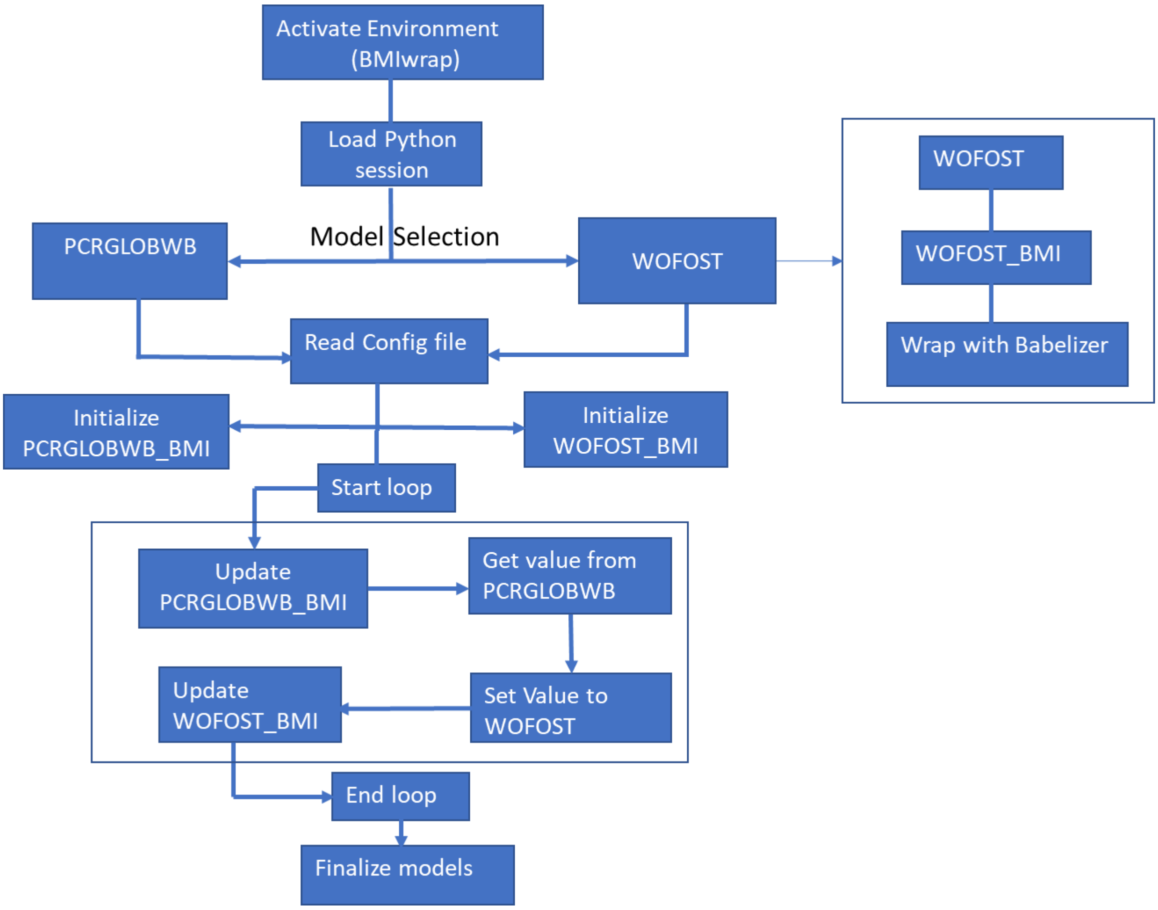


Figure S1: Schematization of workflow of the coupled PCR-GLOBWB 2 - WOFOST model framework

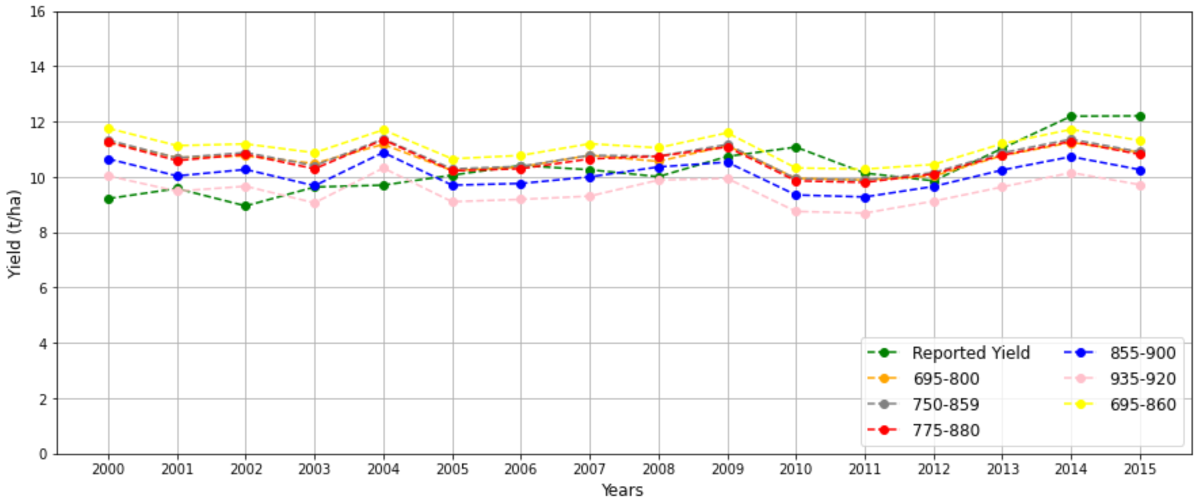
Before initiating the Python session, it is imperative to activate the BMI wrap environment, encompassing essential libraries requisite for both hydrological and crop models. Subsequently, the models PCR-GLOBWB 2 and WOFOST, along with their respective configuration files defining the model coupling settings, are loaded into the Python session. BMIwrap reads the configuration file, initializing the model-specific configuration settings before establishing both models as a coupled entity. Once the coupled models are initialized, a loop is initiated, commencing at the start time and concluding at the end time.

Within this loop, variable exchange occurs between the models based on the one-way or two-way coupling configuration. This iterative process ensures seamless information exchange between the PCR-GLOBWB 2 hydrological and water resources model and WOFOST crop model throughout the simulation period.

Supplementary Information III

Cultivars for each crop, namely maize, soybean, and wheat, were meticulously chosen by analyzing the cultivars present in the WOFOST crop parameter dataset against reported yield statistics. The selection process aimed to identify cultivars that closely matched the reported data, ensuring a representative and reliable set for inclusion in the study as presented for irrigated and rainfed maize (Fig. S2), soybean (Fig. S3) and wheat (Fig S4).

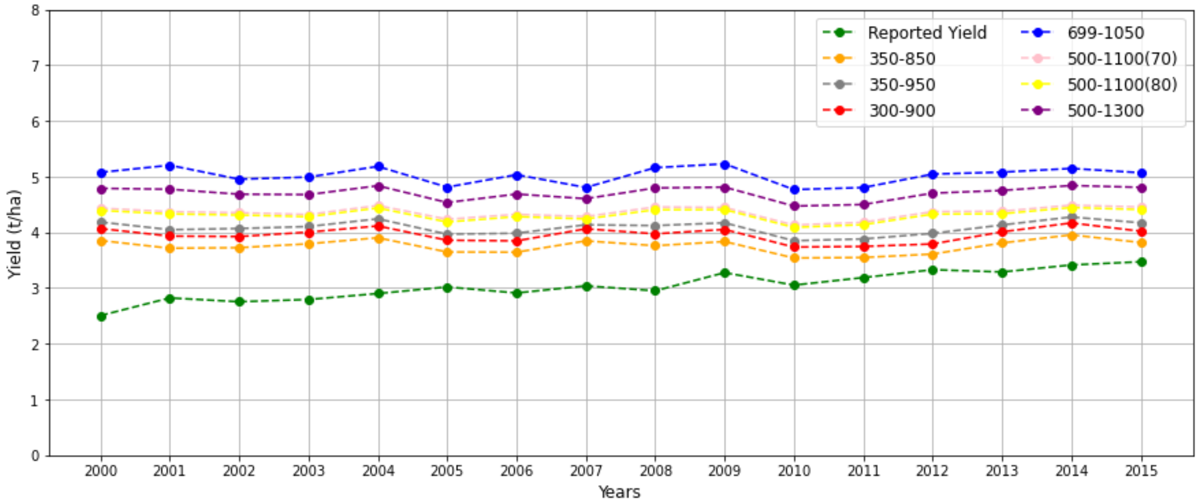
Maize Irrigated



Maize Rained

Figure S2: Reported yield and simulated yield of cultivars for irrigated and rainfed maize.

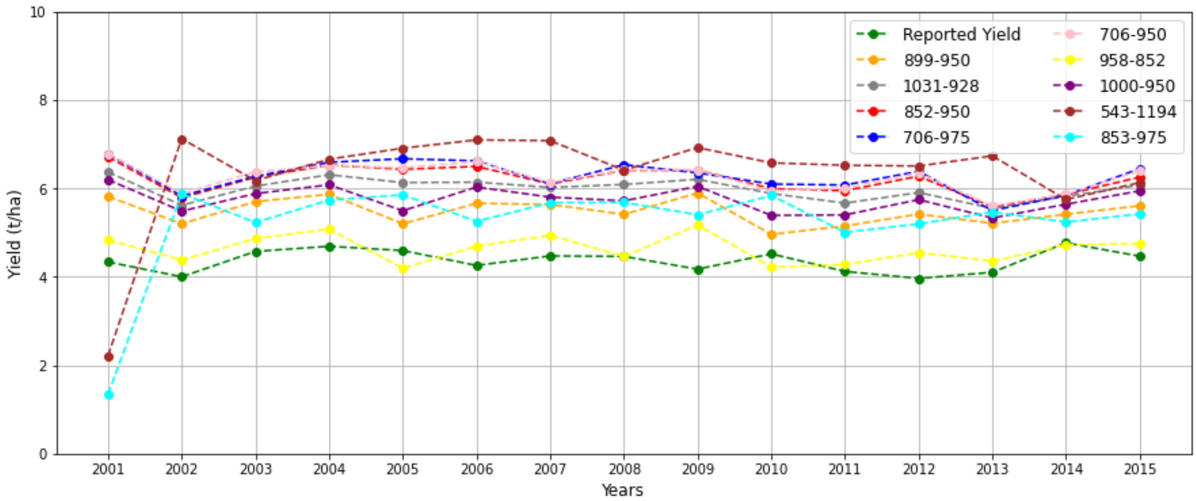
Soybean Irrigated



Soybean Rainfed

Figure S3: Reported yield and simulated yield of cultivars for irrigated and rainfed soybean.

Wheat Irrigated



Wheat Rainfed

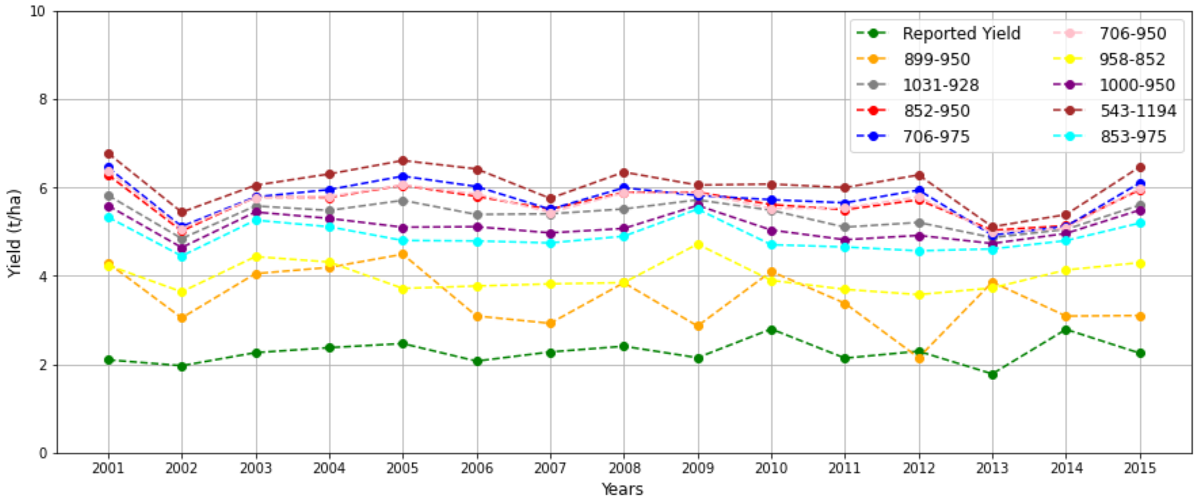
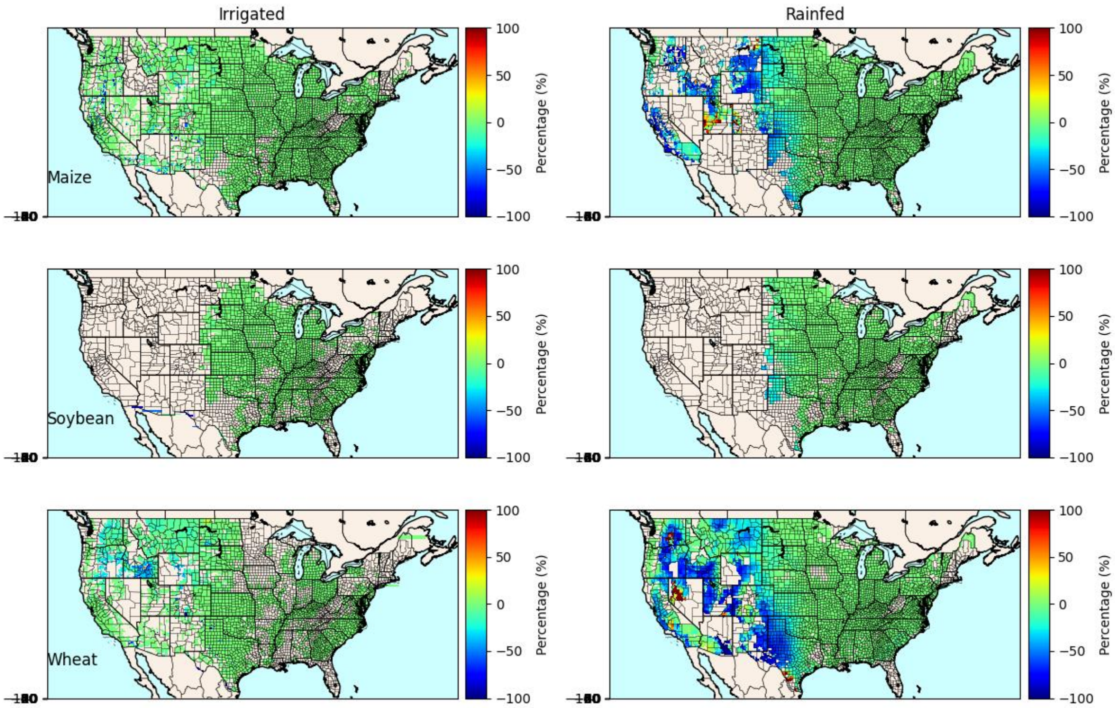
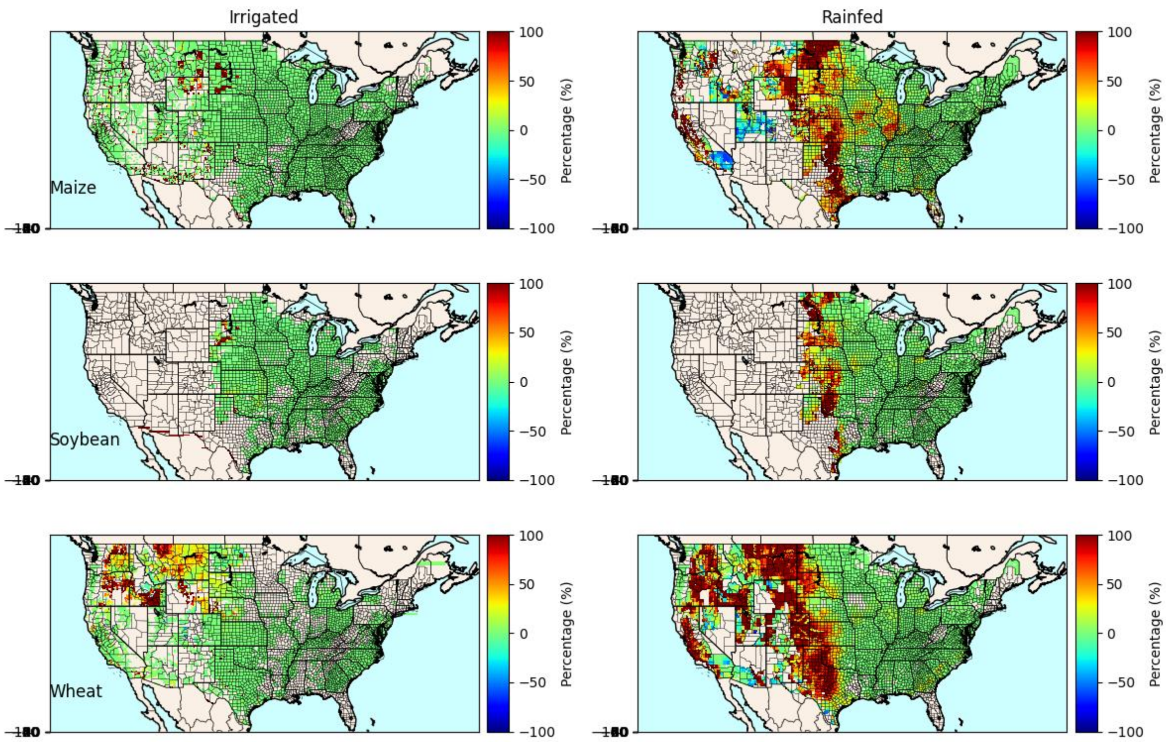


Figure S4: Reported yield and simulated yield of cultivars for irrigated and rainfed wheat.

Supplementary Information IV



Supplementary Figure S5: Relative difference in 1979-2019 mean between two-way and one-way coupling for irrigated and rainfed maize, soybean, and wheat crops.



Supplementary Figure S6: Relative difference in 1979-2019 Coefficient of variance (CV) between two-way and one-way coupling for irrigated and rainfed maize, soybean, and wheat crops.

Supplementary references

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