



Supplement of

Relevance of feedbacks between water availability and crop systems using a coupled hydrological–crop growth model

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S1. Main input datasets used in PCR-GLOBWB 2

Table S1. Main input datasets used in PCR-GLOBWB 2 modules are described below:

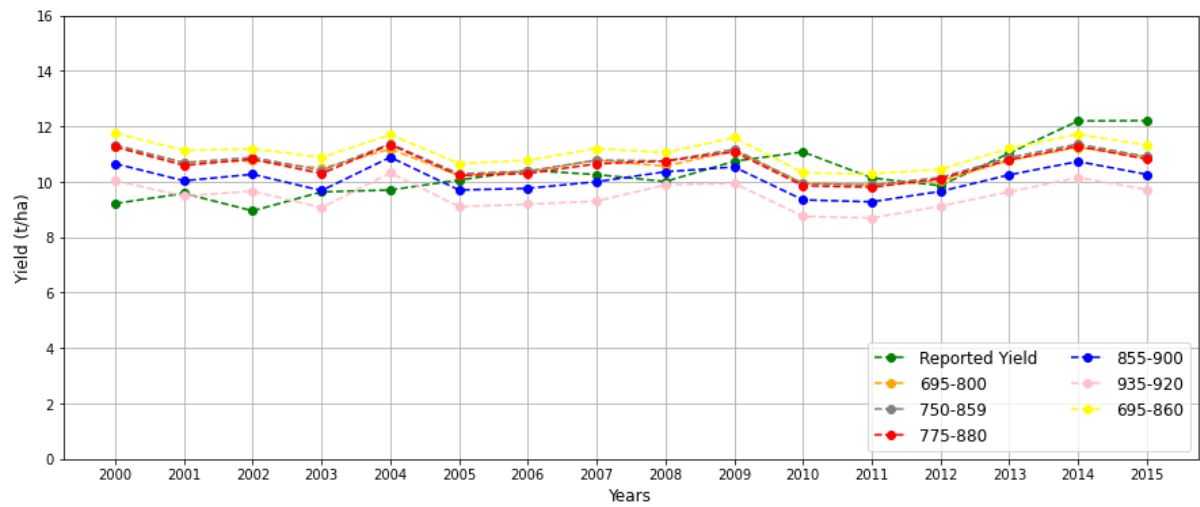
S.No	Datasets	Source
1.	Weather variables - temperature - precipitation - reference potential evaporation	ERA-Interim (Dee et al., 2011)
2.	Soil parameters (upper and lower layer) - soil thickness - residual soil moisture content - soil moisture at saturation	FAO (2007) soil map; Van Beek and Bierkens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

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

S2. Cultivars calibration

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. S1), soybean (Fig. S2) and wheat (Fig. S3).

Maize Irrigated



Maize Rained

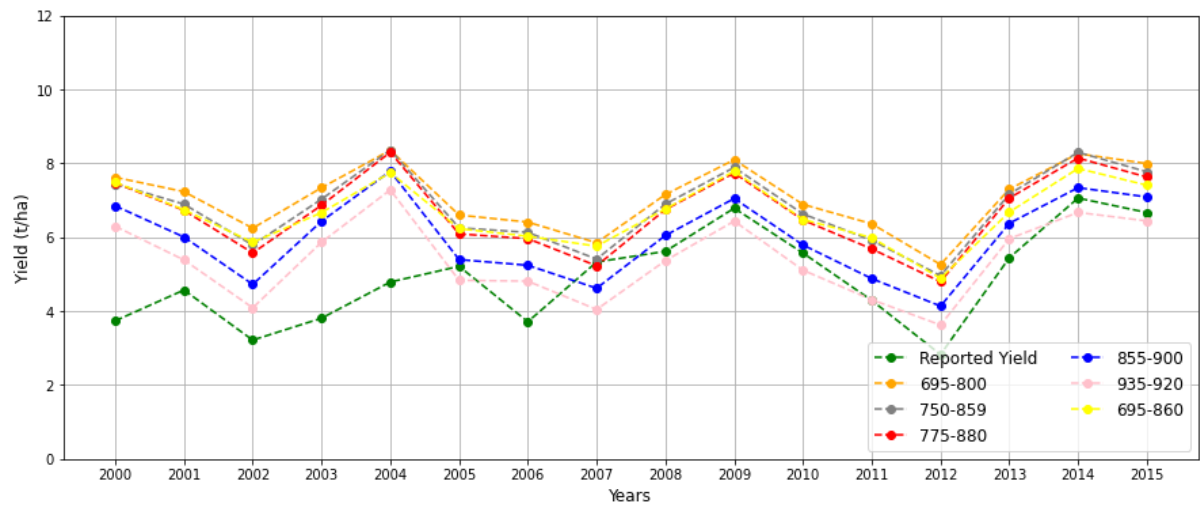
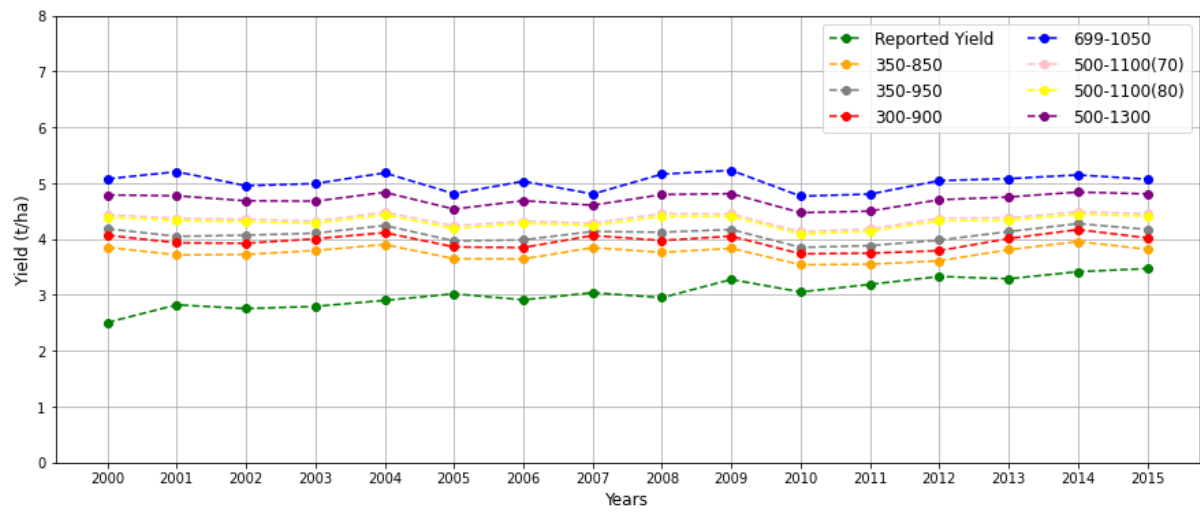


Figure S1: Reported yield and simulated yield of cultivars for irrigated and rainfed maize.

Soybean Irrigated



Soybean Rainfed

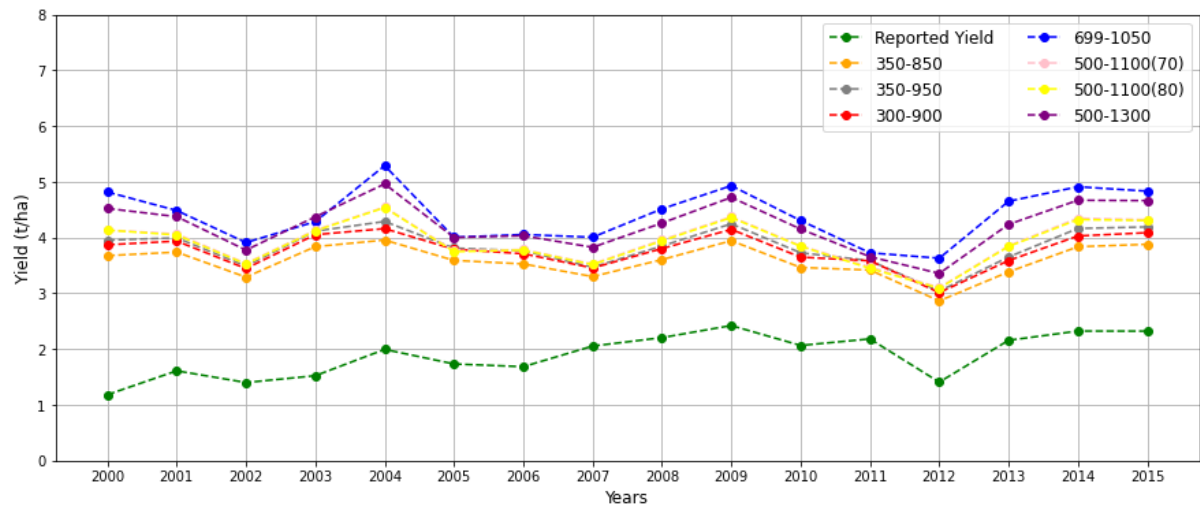
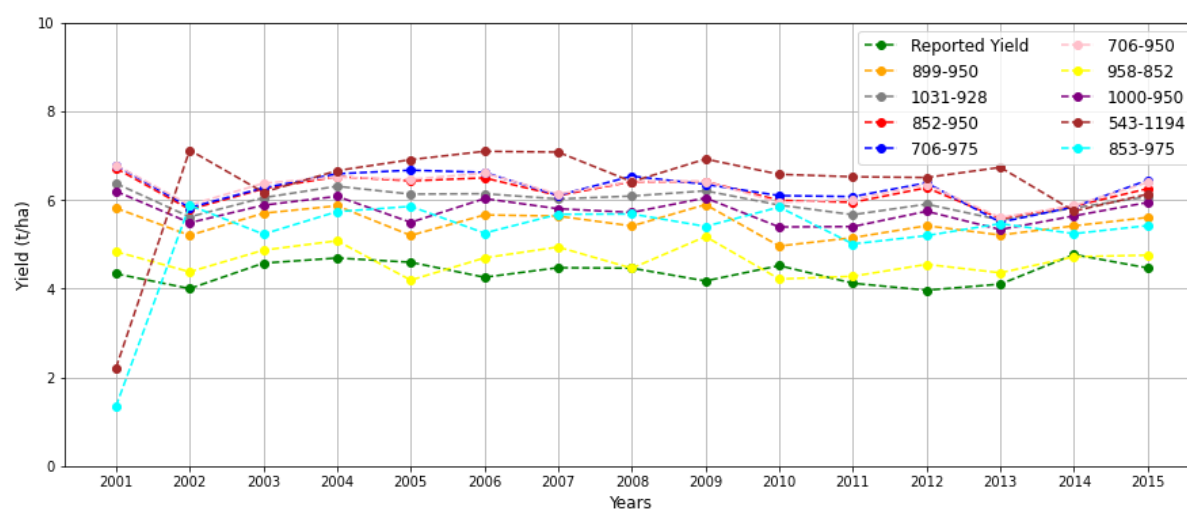


Figure S2: Reported yield and simulated yield of cultivars for irrigated and rainfed soybean.

Wheat Irrigated



Wheat Rainfed

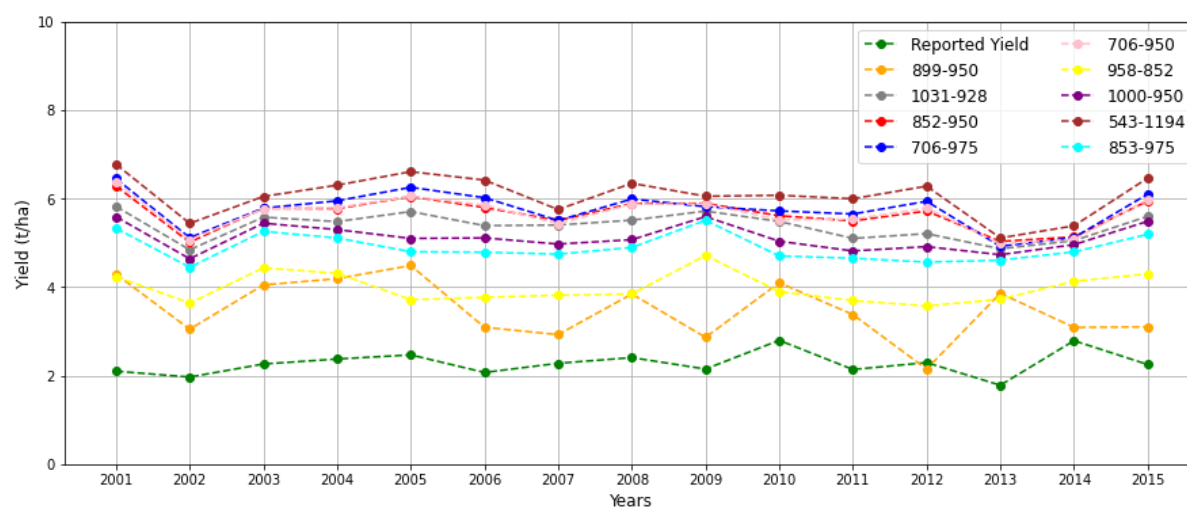


Figure S3: Reported yield and simulated yield of cultivars for irrigated and rainfed wheat.

S3. Soil hydrology and crop yield

Simulations with WOFOST Stand-Alone (SA) and the coupled varieties in which information is exchanged between PCR-GLOBWB 2 with WOFOST (one-way coupled, OW), and back (two-way coupled, TW; Fig. 3) give different yields as a result of the influence of soil moisture availability on transpiration. In case soil moisture availability is too low, water stress will occur and assimilation and biomass accumulation in the different plant compartments, including the storage organs (crop yield) will be affected. This explains the different crop yields of Fig. 4 and Fig. 5 in the main text.

Here, we investigate the effect of soil hydrology and crop yield in our models in detail by evaluating the development of soil moisture, evapotranspiration and biomass over time for rainfed and irrigated maize at two contrasting locations in the USA, being a cell in Georgia (32.79° N, 83.79° W) and one in the High Plains (33.29° N, 98.88° W). These locations receive different rainfall amounts, Georgia experiencing less water stress than the High Plains as a result. Furthermore, to increase the contrast, two years were selected being 2009 and 2012, a normal and a drier year, respectively.

Table S2: Seasonal rainfall during the crop growing period at the two locations for the years 2009 and 2012.

Locations	Rainfall (mm) over a growing season	
	2009 (normal year)	2012 (dry year)
Georgia – 32.79° N, 83.79° W	612.0	244.1
High Plains – 33.29° N, 98.88° W	278.2	234.2

S3.1. Biomass accumulation and yield

The effect of water stress on the final biomass accumulation in the plant compartments is shown in Fig. S4-S5. In case of irrigation, water stress is largely avoided by applying water, and the accumulated biomass, including the crop yield (storage organs), is almost the same per location and year for all three model variants (SA, OW, TW). Only for the two-way coupled model version, the values are sometimes lower as irrigation scheduling in PCR-GLOBWB 2 can be sub-optimal, whereas in WOFOST, water stress does not occur by keeping the soil moisture at optimal levels. The total biomass differs for the two locations for the two years, the total biomass being greater for the drier year 2012 than for the normal year 2009. The reason for this higher biomass is the fact that in the drier year, more shortwave radiation is available to sustain photosynthesis, and no water stress is incurred as any soil moisture deficit is replenished by irrigation. The subdivision of the accumulated biomass into the different biomass compartments varies between locations and years. This is mostly the result of the higher temperatures in the drier year that shift the moments the different growth stages are reached in WOFOST due to the accumulated growth temperature (e.g., anthesis). In particular, for Georgia, the increase in yield is higher in the drier year than in the normal year. In contrast, the

increase in total biomass is not so large, and the totals are similar for both years 2009 and 2012 and both locations ($15 - 17 \cdot 10^3$ kg /hectare per year).

For the rainfed conditions, the differences in biomass components are larger. First, the total biomass and yield are the same for Georgia in the normal year 2009, in which no water stress occurs. When water stress occurs, the values are different. At the High Plains location water stress occurred already in 2009, and the yields differed between the model variants, the stand-alone (SA) version giving the lowest yield, followed by the two-way coupled version (TW), then the one-way coupled version (OW). This pattern is similar for the drier year 2012 at both Georgia and the High Plains. For this year, the yields fall strongly, and this reduction appears to be stronger than for the other plant compartments, which suggests that water stress occurs later in the growing season, when the other plant compartments (roots, stems and leaves) are already largely set. For rainfed crops, the higher yields for the one-way coupled model version are also found here. A remarkable point here is that the crop yield at the location in Georgia for 2012 exceeds all other yields, including the ones under irrigation. The explanation for this is that the two cultivation types (irrigation, rainfed) consider different crop types or cultivars for maize (see section S2) and that, as a result rainfed maize has a slightly larger growing season and, as a result can accumulate storage organs longer and to a higher amount than irrigated maize.

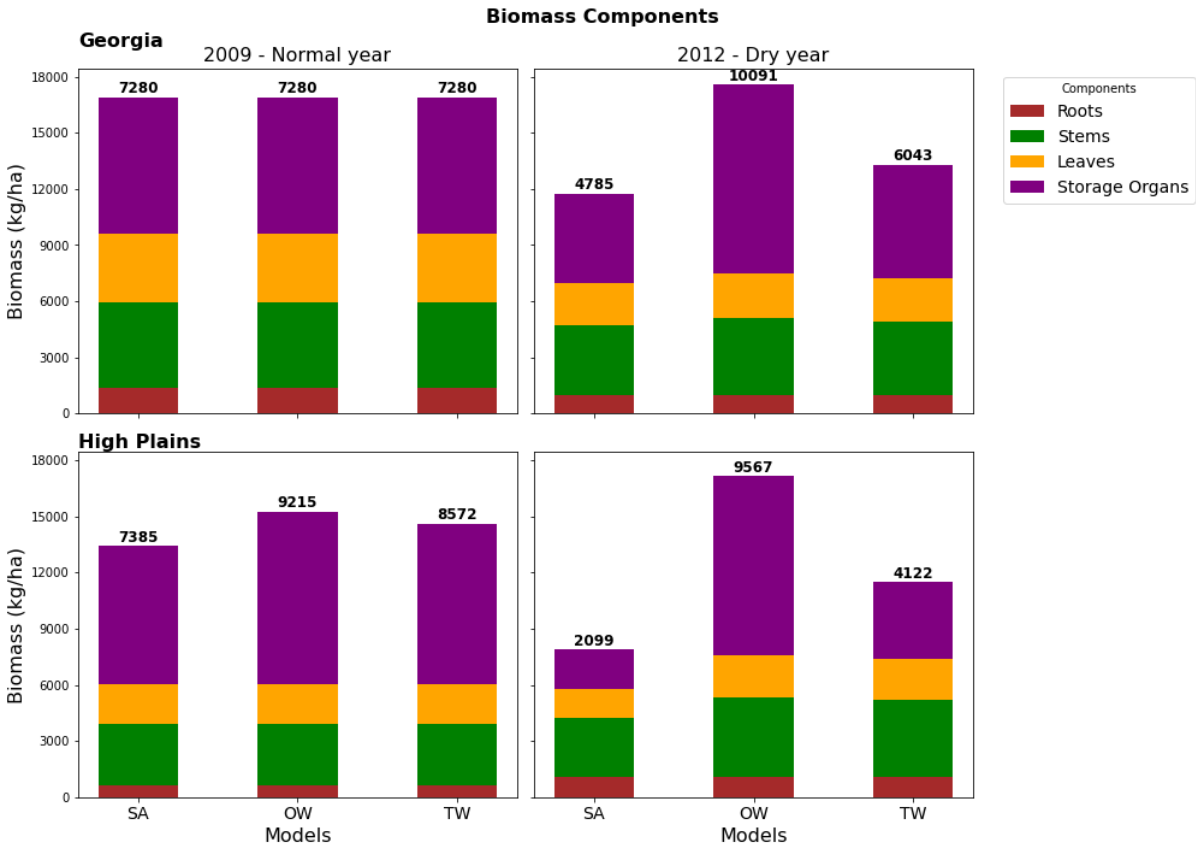


Figure S4: Biomass components (Roots, Stems, Leaves, Storage Organs/Yield) for three model approaches, Stand-alone, One-way and Two-way coupling during normal year (2009) and dry year (2012) for rainfed maize in the Georgia (32.79° N, 83.79° W) and High Plains (33.29° N, 96.61° W).

98.88° W). The value given at the top of each bar is the accumulated mass of storage organs at the end of the growing season (crop yield)

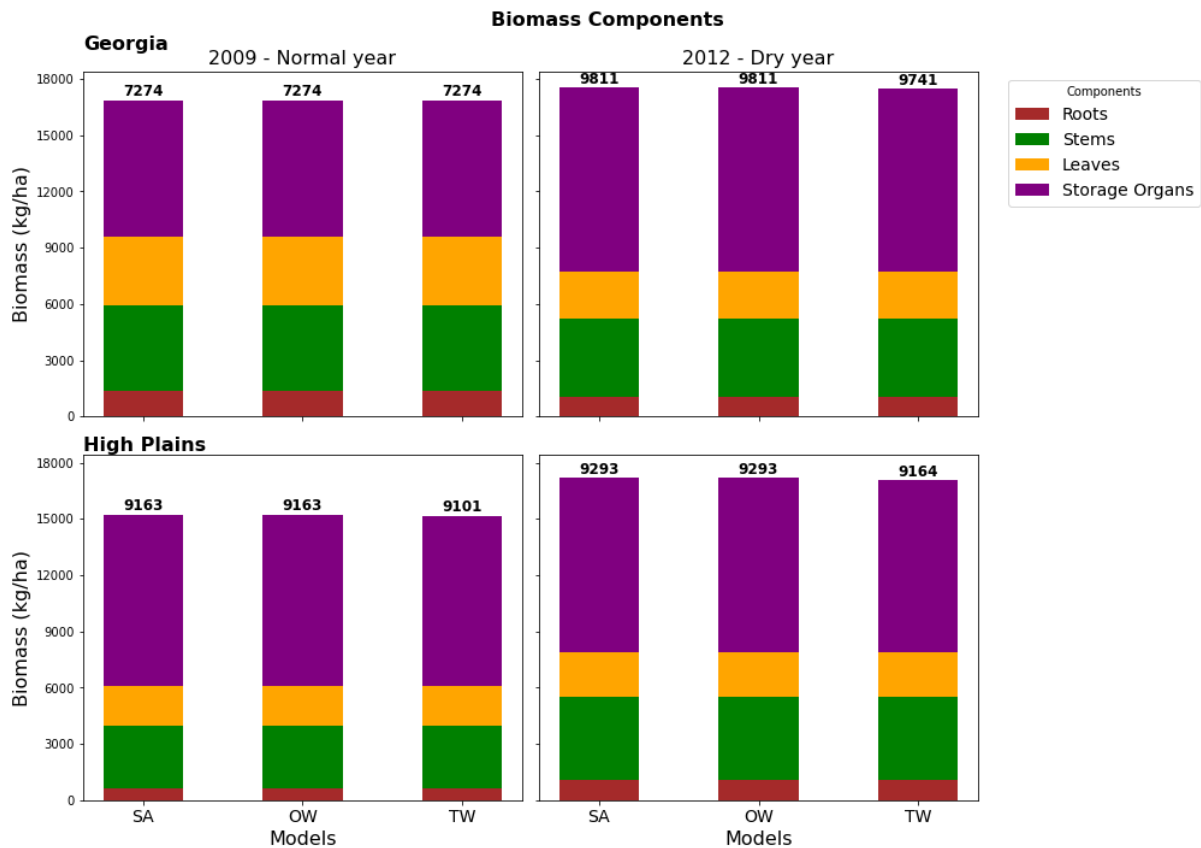


Figure S5: Biomass components (Roots, Stems, Leaves, Storage Organs/Yield) for three model approaches, Stand-alone, One-way and Two-way coupling during normal year (2009) and dry year (2012) for irrigated maize in the Georgia (32.79° N, 83.79° W) and High Plains (33.29° N, 98.88° W). The value given at the top of each bar is the accumulated mass of storage organs at the end of the growing season (crop yield).

S3.2. Soil hydrology, water stress and crop growth

We evaluated the influence of the soil hydrology on the crop growth over the growing season for the three model variants (SA, OW, TW) for the two locations (Georgia, High Plains) and the normal year 2009 and drier year 2012. In all cases, the assimilation in WOFOST is dependent on the transpiration that is derived from a single root zone that can span the two soil layers in PCR-GLOBWB 2. The transpiration in WOFOST occurs over the part of the surface covered by the crop canopy and is limited by the potential rate, with the remainder of the potential evapotranspiration passed to the bare-soil evaporation. In WOFOST, transpiration and bare soil evaporation are reduced depending on soil moisture availability. For transpiration, this is based on the soil moisture directly; and for the bare soil evaporation, the rate decreases asymptotically to zero as a function of the number of days since the last rain. Water stress in WOFOST reduces assimilation and thus crop growth. It is defined as the ratio of the actual transpiration over the potential transpiration and occurs only if the soil moisture in the root zone is below a threshold of the depletion factor. Thus, lower than potential transpiration rates

are not limiting for rainfed crops at the start of the growing season when soil moisture is still high; only later on, when the soil moisture falls below the depletion factor, does water stress occur. In the case of irrigated crops, water stress is generally avoided, as the soil moisture is kept at levels that sustain transpiration at the optimum rate. In WOFOST stand-alone (SA), this is achieved by setting the soil moisture at field capacity throughout the simulation. In PCR-GLOBWB 2, the FAO guidelines (Allen et al., 1998) are used that replenish the soil moisture whenever it falls below a given threshold, based on the aforementioned depletion factor. Overall, the effect is the same, except that the soil moisture in PCR-GLOBWB 2 under irrigation still varies over time and irrigation occurs at variable moments of time, mimicking irrigation scheduling in real life. Under rainfed cultivation, the soil moisture can vary freely, and it depends on the values that are simulated in WOFOST Stand-Alone (SA) or in PCR-GLOBWB 2 (one-way, OW, and two-way, TW, coupling) and how this is passed to WOFOST to simulate crop growth.

Figures S6-S9 show in detail how soil hydrology and crop growth (biomass) develop over time. All figures follow the same format, with the normal year 2009 being plotted to the left and the drier year 2012 to the right. The first row shows the biomass accumulation for the three model variants (SA, OW, TW) and root depth relative to the thickness of the soil layers of PCR-GLOBWB 2 (horizontal line showing the limit of the top layer of 30 cm thick). Note that the root depth develops over time at a fixed rate until the maximum depth is reached. This shows, however, that for most of the time, the crop has access to the soil moisture in the second soil layer of PCR-GLOBWB 2 (after ~10 days) and that this at its maximum after ~40 days of the growing season for the rainfed crops. So, for most of the time, the crop has access to the moisture of the first and second soil layers of PCR-GLOBWB 2. For irrigated cultivation, a different cultivar is used with a greater maximum root depth, meaning the roots reach the maximum depth slightly later and more of the second layer is penetrated. With the different cultivars and depending on the soil moisture conditions, sowing dates and growing season lengths can vary slightly but do not vary appreciably between locations, treatments and years. Hence, all plots use the same horizontal axis for time, spanning the growing season in terms of Julian days. Also, different model variants are shown with consistent colours, being blue for WOFOST stand-alone (SA), green for one-way coupled version (OW) and red for two-way coupled version (TW).

To show the evaporative fluxes by means of a stacked bar chart, the growing season has been broken down into a total of five 20-day periods to show totals for all the model variants, and a comparison between the WOFOST fluxes and the PCR-GLOBWB 2 ones have been made when possible. Hence, two stacked columns are shown for OW and TW with matching colours. The WOFOST values amount to the potential evaporation per 20-day period and have been broken down into the bare soil evaporation, the transpiration -the effective evaporative flux contributing to crop growth- and the remainder, which is the amount of the atmospheric demand that cannot be met. As mentioned above, this is not directly affecting crop growth, provided the soil moisture does not fall below a preset level in the root zone of WOFOST. This is shown in the first panel, second row of Fig. S6, where there is no water stress (first panel, third row), but the atmospheric demand is consistently not met. Note that in all bar plot graphs

(Fig. S6-S9), the total column height of the WOFOST bars match as they depend on the imposed meteorological forcing, but the subdivision into the actual components can vary.

The third row shows the water stress (1 in the case water is abundant and there is no stress, 0 in the case there is no water and stress completely limits growth). The water stress develops in line with the soil moisture content, which is plotted on the bottom row. Solid lines represent the volumetric moisture content (VMC) of the root zone (first panel) for the three variants that allow direct comparison. However, the soil moisture content as water slice is given for the two PCR-GLOBWB 2 models (top layer 1 extending 30 cm below the surface, the bottom layer 2 120 cm below this). Since this is total soil moisture storage, the absolute values are different, as the one layer is four times thicker than the other. Considering a typical porosity of 0.4, full saturation would be 0.12 [m] for the top layer and 0.48 for the bottom layer, which is fairly consistent with the unsaturated conditions depicted for all simulations. Note that the plotted volumetric moisture contents are based on the harmonized soil hydrological properties that are passed from PCR-GLOBWB 2 to WOFOST, which does not consider the residual moisture content of the soil. For irrigation (Fig. S8-9), when the water stress is repressed automatically in WOFOST SA, its soil moisture content is not given, as it is fixed at field capacity and no water stress occurs.

A first observation from Fig. S6-S9 is that the accumulated biomass is the same and the subdivision into the different evapotranspiration fluxes is the same if no water stress occurs. However, the volumetric moisture contents can vary between the model variants. Evidently, water stress is virtually absent in the case of irrigated agriculture (Fig. S8-S9), and the yields are higher for the drier year 2012 because of the improved growing conditions (radiation, growth temperature) if water stress is removed (see also Fig. S5).

At the same time, it is evident that when water stress occurs, the growth becomes impaired and that the subdivision into the different evapotranspiration changes. Generally, water stress occurs longer and more intense at the High Plains than at the Georgia location under rainfed cultivation and particularly in the dry year (2012). Among the model versions, the SA model is more sensitive to water stress than the coupled versions, and the volumetric moisture content over the root zone is lower than that of the PCR-GLOBWB 2 based versions, which is computed from the layer-specific moisture contents. For rainfed crops, the water stress in WOFOST stand-alone (SA) is correspondingly larger than in the coupled versions. For the coupled versions, the two-way coupling (TW) still shows water stress, whereas the one-way coupling (OW) shows hardly any water stress (except for 2012 for the High Plains, Fig. S8).

The water stress for rainfed crops (Fig. S6-S7) develops later in the growing season when the available soil moisture falls. Water stress only depends on the ratio of the actual transpiration and the potential transpiration and the available soil moisture content. When water stress occurs, less biomass is accumulated as can be observed in the graphs for the increase in biomass for stand-alone (SA) to two-way coupling (TW) to one-way coupling (OW) versions when stress occurs. The accumulation of biomass also feeds back into the evapotranspiration fluxes of the model variants, as more (less) biomass leads to more (less) leaves and greater canopy closure. With more canopy closure, more of the potential evapotranspiration becomes potential transpiration, and if this potential transpiration can be met by the available soil moisture, this

leads to more growth. Consequently, the subdivision into the evapotranspiration fluxes changes when water stress occurs (e.g., Fig. S6 for 2012, Fig. S7 for 2009 and 2012). In principle, higher actual transpiration does not directly lead to more biomass accumulation in WOFOST, as this is dependent on the assimilation, which is light dependent. However, more leaf area leads to more photosynthesis and, therefore, larger growth. As the OW coupled version experiences hardly any water stress, this effect is more prominent in this case than in the case of the TW coupled version of PCR-GLOBWB 2-WOFOST.

In summary, the simulated hydrology and crop growth for the model variants are dependent on the following aspects:

- Subdivision into evapotranspiration fluxes on canopy closure;
- The scaling of potential transpiration to actual transpiration based on water stress.

Both are dependent on the way how soil moisture is passed from PCR-GLOBWB 2 to WOFOST for OW and TW coupling and how actual soil evaporation and actual transpiration are passed from WOFOST to PCR-GLOBWB 2 in the two-way coupling (TW). The first also depends on the consistency of the coupling with the phenology.

S3.3. Difference between one-way (OW) and two-way (TW) coupling

In the case of the one-way coupling (OW), only the soil moisture is passed from PCR-GLOBWB 2 to WOFOST (Fig. 3). The volumetric moisture content is the weighted average over the root zone of WOFOST from the two soil layers from PCR-GLOBWB 2. The evapotranspiration fluxes are not passed from WOFOST to PCR-GLOBWB 2 and as a consequence, soil moisture depends on the evapotranspiration fluxes that are computed in PCR-GLOBWB 2. A key issue that arises is that this ignores the actual crop growth, and the fluxes depend on the prescribed -fixed- phenology of PCR-GLOBWB 2 only. The amount of potential bare soil evaporation is proportional to the minimum crop factor ($k_{cmin} = 0.20$) and this leads to a deviation between the evapotranspiration considered in WOFOST and those in PCR-GLOBWB 2 (see the different height of the stacked bar of OW on the second row for S6 for 2012 and S7 for 2009 and 2012). Moreover, the potential transpiration in PCR-GLOBWB 2 is partitioned over the two soil layers based on the layer thickness and the root content that is constant in time. This has two major consequences that lead to higher soil moisture contents in the later part of the growing seasons that are beneficial to the simulated crop growth: (i) initially, due to a faster development of crop biomass in the beginning of the growing season in WOFOST compared to the standard phenology in PCR-GLOBWB 2, the amount of evapotranspiration in WOFOST is higher than in PCR-GLOBWB 2 OW, which leads to a lower decrease in soil moisture in PCR-GLOBWB 2 OW that remains available for later in the season; (ii) the transpiration is taken from a relatively large reservoir in the second soil layer (which also contains moisture below the active root zone), while the soil evaporation only affects the upper layer. Once averaged over the root zone and passed to WOFOST, this leads to a higher average soil moisture over the WOFOST root zone and, therefore, less water stress. These two differences favour more growth in the later part of the growing season compared to SA and TW as these model versions experience water stress.

In the two-way coupling (TW), more consistency is reached in the coupling of the soil hydrology and the crop growth. While the soil moisture content is computed again as a weighted average over the extent of the root zone in WOFOST in the two soil layers of PCR-GLOBWB 2, now the actual bare soil evaporation and actual transpiration from WOFOST are passed back to PCR-GLOBWB 2 (Fig. 3). These fluxes are in line with the canopy closure, thus reflecting the phenology, and match the reduction of the potential to the actual evapotranspiration in WOFOST (see the matching height of the stacked bar of TW on the second row for S6 and S7 for all years). With the two-way coupling (TW), further steps have to be incorporated to exchange the actual bare soil evaporation and actual transpiration from WOFOST to PCR-GLOBWB 2. The actual bare soil evaporation from WOFOST is passed directly to the topsoil of PCR-GLOBWB 2, which is directly consistent with the PCR-GLOBWB 2 conceptualization (Fig. 3). To incorporate the actual transpiration, some additional steps have to be taken: first, the depth of the root zone is passed from WOFOST to PCR-GLOBWB 2, and with it the potential transpiration in PCR-GLOBWB 2 is partitioned over the two soil layers; second, the potential transpiration is then reduced on the basis of the soil moisture availability to get the actual transpiration for each of the two layers. This transpiration per layer is then used to subdivide the actual transpiration from WOFOST over the two layers. Next, in PCR-GLOBWB 2, the soil moisture of each PCR-GLOBWB 2 layer is reduced by the actual transpiration derived from WOFOST. The fact that the transpiration is partitioned on the basis of the increasing root depth, leads to a better approximation of the dynamics as initially all transpiration is taken out of the first layer and only later from the second layer (see e.g., Fig. S6, row 2, panel 1). As a consequence, the weighted volumetric moisture content over the root zone of TW is more similar to the SA values for the rainfed crops (Fig. S6-S7), and also, the change in the total soil moisture for the two layers is different in TW compared to OW. In TW, the lower soil moisture leads to water stress, albeit it is lower than in the SA version, where the water balance is evaluated over the entire root zone. When comparing the response in the two soil layers for OW and TW, respectively, it can be observed that the TW version experiences a greater reduction in the soil moisture in the deeper, second layer than the OW version, whereas the soil moisture in the top layer remains more similar. This is the result of the upward flux from the second layer to the top layer when the latter dries out. Later on, as the deeper layer gets drier, this leads to a reduced response with depth, with more of the precipitation of irrigation water (see below) ending up in the top soil, which explains the more similar response of the top layer for both the OW and TW versions of the model for the normal year 2009. It should be mentioned that in PCR-GLOBWB 2, the soil moisture can also be maintained by capillary rise from the underlying groundwater reservoirs, although that in the presented cases would probably only have a marginal influence.

For rainfed crops, these different approaches lead to different soil moistures, evapotranspiration fluxes, and biomass accumulation. For irrigated crops (Fig. S8- S9), the water stress in WOFOST SA disappears completely and is virtually absent for the coupled versions. As a result, the WOFOST evapotranspiration fluxes are the same for all versions. Due to the two-way coupling, the TW version has the same actual evapotranspiration fluxes for PCR-GLOBWB 2. However, the fluxes of the OW version are very different because the evapotranspiration fluxes of WOFOST are not passed to PCR-GLOBWB 2. Consequently, the

two coupled model versions have different soil moisture contents (see also above), especially during the drier year 2012, but experience hardly any water stress. Only in the TW version, sub-optimum irrigation scheduling can lead to small periods of water stress (Fig. S8-S9). This has a negligible impact on the growth as reflected by the lower reported yields for TW compared to SA and OW in Fig. S5.

S3.4. Difference between two-way (TW) coupling and stand-alone WOFOST (SA)

All-in-all, the coupled versions lead to a different response than WOFOST stand-alone. In the case of TW, the withdrawal of the actual transpiration for the second layer from the entire soil moisture storage is slightly inconsistent but at the same time, the total soil water balance is evaluated consistently. In addition, the penetration of the root zone into the soil is simulated consistently and gradually adds part of the second layer once the root zone extends below the top soil. The weighted soil moisture content in TW approaches that of the single-layer value of SA, although it remains a bit higher leading to less stress.

In comparison with TW, the stand-alone WOFOST SA uses a simplified single-layer soil moisture approach, where soil moisture availability is updated directly based on root extension, evapotranspiration losses, and soil moisture redistribution. As the root depth increases, soil moisture from the lower zone gradually becomes available to the expanding root system. However, in the WOFOST stand-alone version: a) evaporation comes out of the entire root zone layer which compromises average soil moisture later in the season compared to TW as in PCR-GLOBWB 2 the lower soil compartment is not affected; b) roots cannot tap into the soil moisture stored in PCR-GLOBWB 2 layer 2 below the root zone, while this is possible in PCR-GLOBWB 2; c) lacks a representation of capillary rise that could supply moisture from the second to the upper soil layer and from groundwater to the lower soil layer. These differences (a-c) between the SA and TW makes that soil moisture of the TW is generally a slightly higher under stressed conditions leading to larger yields.

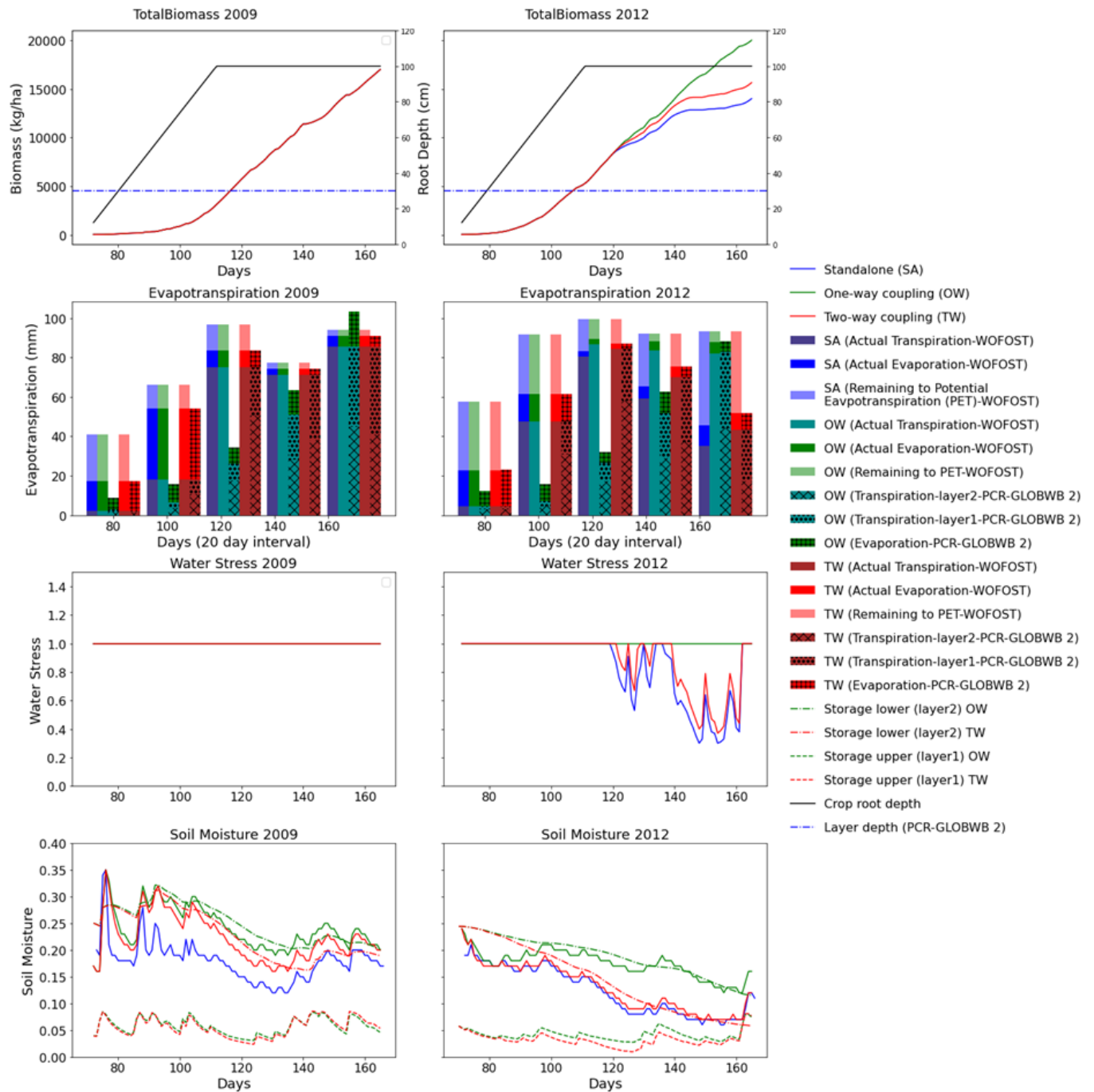


Figure S6: Responses in hydrological variables (evapotranspiration, water stress, soil moisture) for rainfed maize in Georgia during a normal (2009) and dry (2012) year.

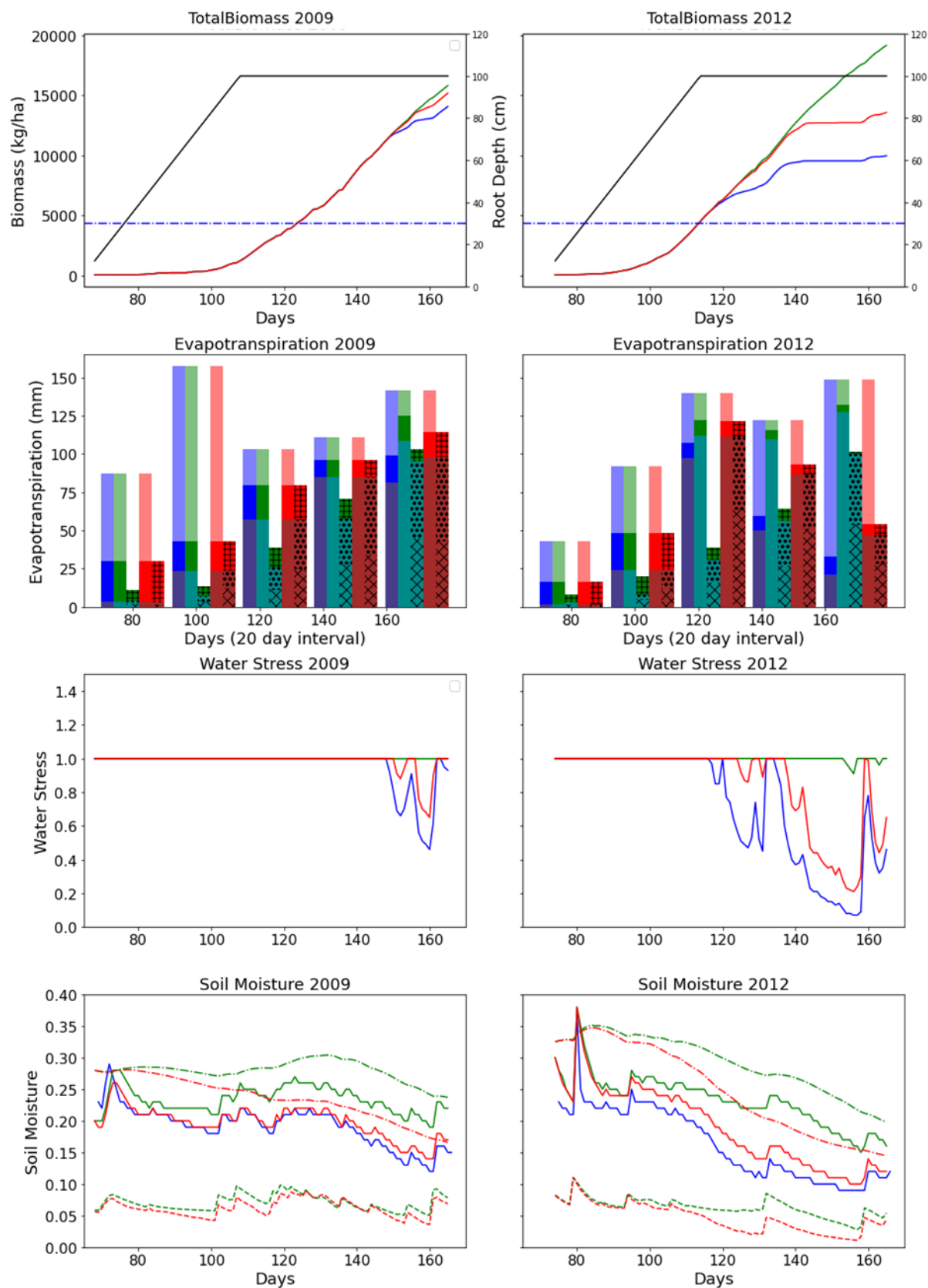


Figure S7: Responses in hydrological variables (evapotranspiration, water stress, soil moisture) for rainfed maize in Greater high plains during a normal (2009) and dry (2012) year. For legend, we refer to Fig. S6.

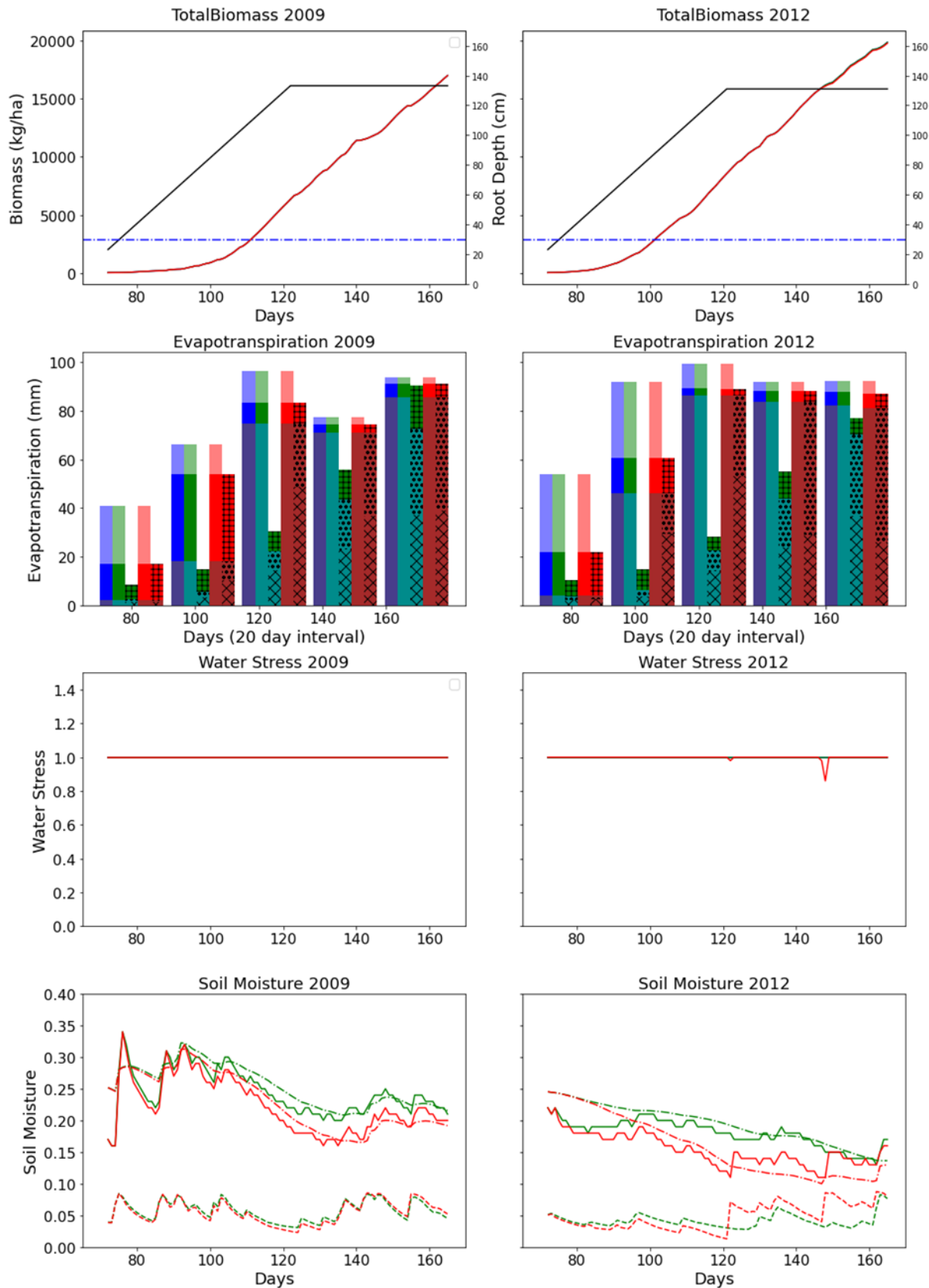


Figure S8: Responses in hydrological variables (evapotranspiration, water stress, soil moisture) for irrigated maize in Georgia during a normal (2009) and dry (2012) year. For legend, we refer to Fig. S6.

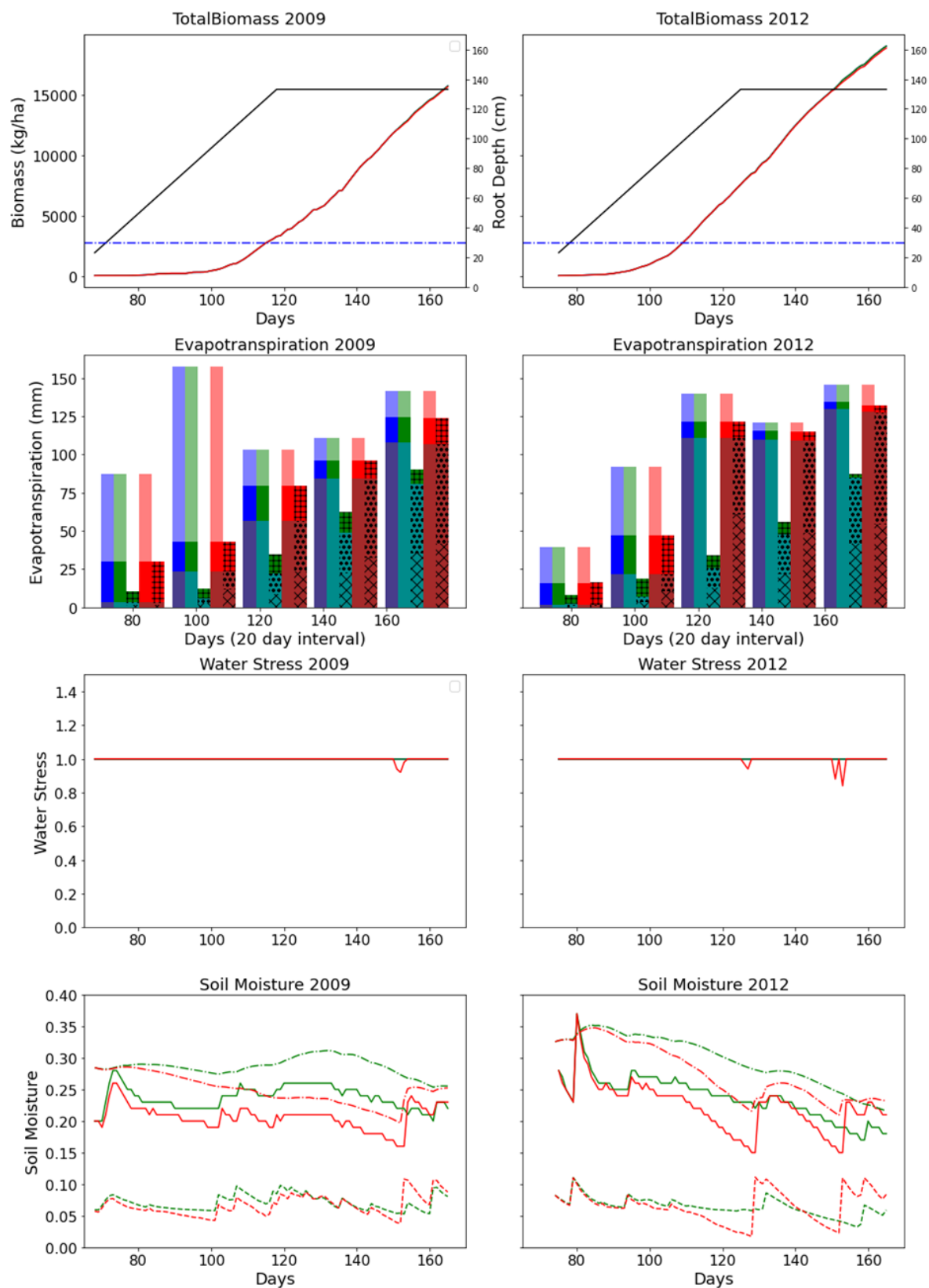


Figure S9: Responses in hydrological variables (evapotranspiration, water stress, soil moisture) for irrigated maize in Greater high plains during a normal (2009) and dry (2012) year. For legend, we refer to Fig. S6.

S4. Model performance metrics

The below Table S3 presents model performance metrics from the spatial analysis.

Table S3: Model performance metrics (i.e. correlation, normalized RMSE and normalized bias) for simulated irrigated and rainfed maize, soybean, and wheat.

S.NO	Metrics	Maize			Soybean			Wheat		
Irrigated crops		Stand alone	One-way	Two-way	Stand alone	One-way	Two-way	Stand alone	One-way	Two-way
1	Correlation	0.24	0.27	0.28	0.28	0.35	0.35	0.73	0.74	0.65
2	Normalized RMSE	0.14	0.14	0.14	0.20	0.18	0.18	0.25	0.25	0.23
3	Normalized Bias	-0.01	-0.01	-0.01	0.12	0.09	0.09	0.10	0.10	0.00
Rainfed crops										
1	Correlation	0.68	0.80	0.80	0.81	0.59	0.62	0.41	0.47	0.49
2	Normalized RMSE	0.34	0.50	0.35	0.74	1.00	0.91	0.66	1.17	0.59
3	Normalized Bias	0.06	0.44	0.27	0.73	0.97	0.86	0.36	1.00	0.37

S5. Relative difference maps

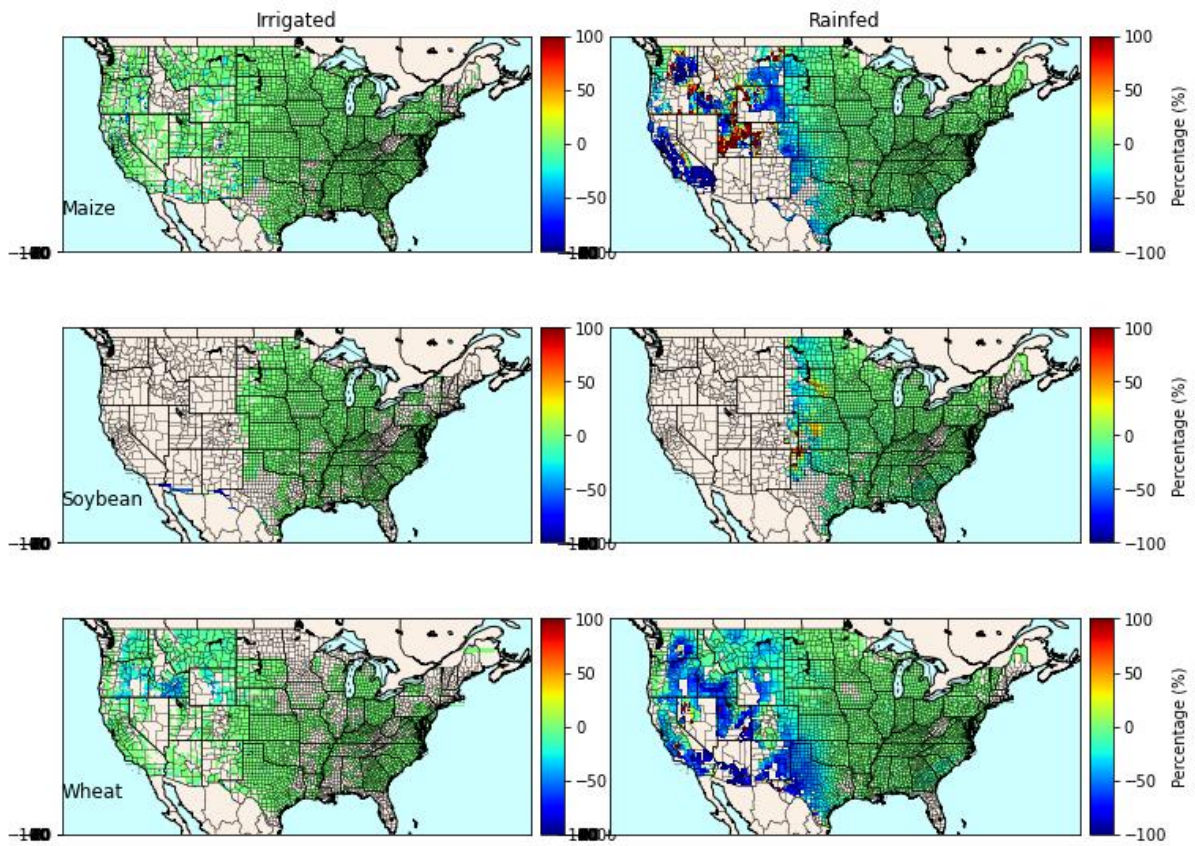


Figure S10: Relative difference in 1979-2019 mean between two-way and one-way coupling for irrigated and rainfed maize, soybean, and wheat crops.

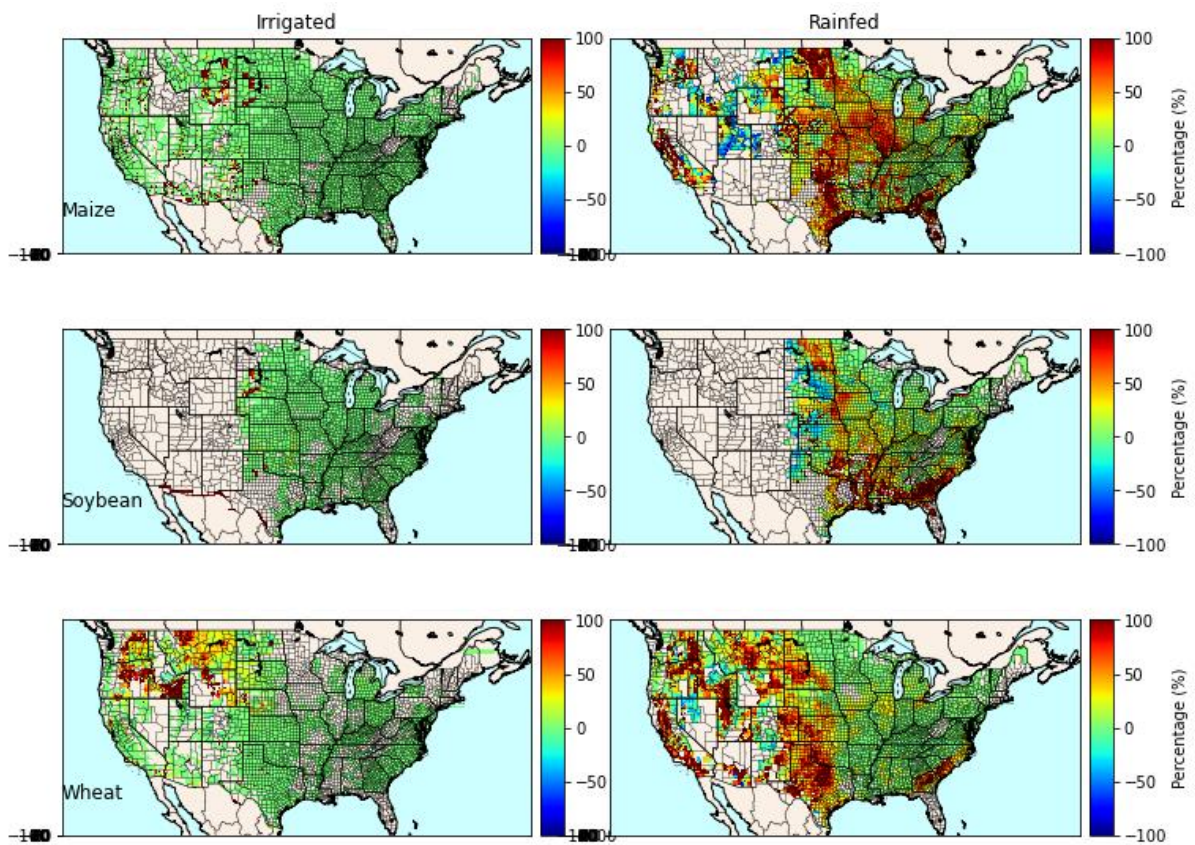


Figure S11: Relative difference in 1979-2019 Coefficient of variance (CV) between two-way and one-way coupling for irrigated and rainfed maize, soybean, and wheat crops.

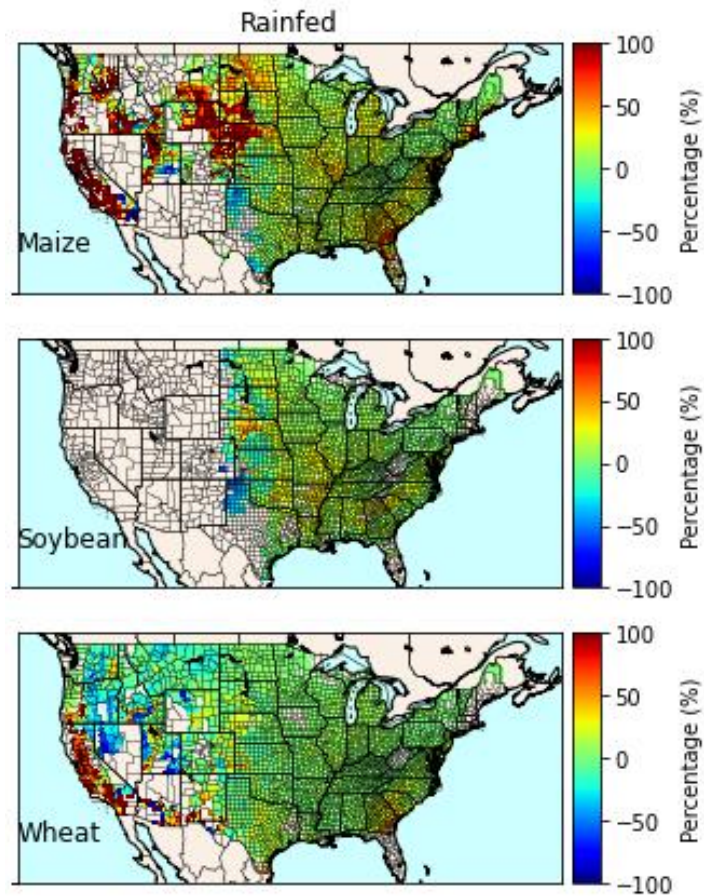


Figure S12: Relative difference in 1979-2019 mean between two-way coupling and stand-alone for rainfed maize, soybean, and wheat crops.

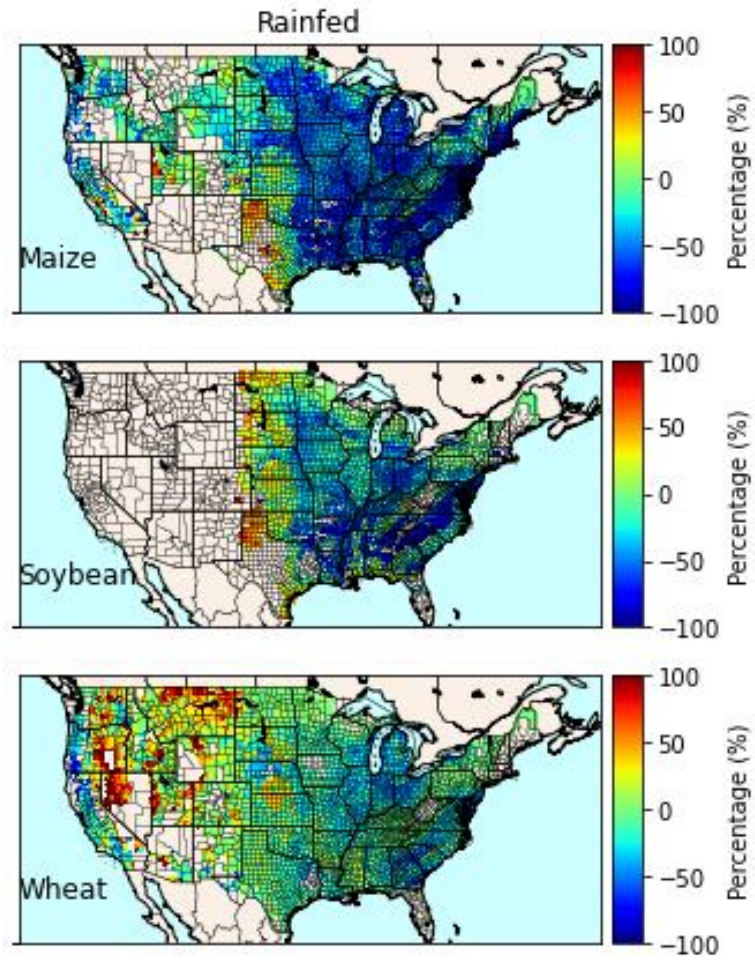


Figure S13: Relative difference in 1979-2019 Coefficient of variation (CV) between two-way coupling and stand-alone for rainfed maize, soybean, and wheat crops.

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