1	Supplementary Material (Text, Tables and Figures)
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3	Effects of Environmental and Management Factors on Worldwide Maize and Soybean
4	Yields over the 20 th and 21 st Centuries
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20 Supplementary Text Sections

21

22 Text S1. Bias Correction of Future Climate

The bias correction method proposed by Hawkins et al. (2013) is used in this study to correct the six atmospheric variables, including downward shortwave and longwave radiation, surface pressure, wind speed, surface temperature and specific humidity from CESM outputs. This method considers the mean and variability differences between CRU-NCEP reanalysis and CESM output between year 2006 and 2016:

$$T_{cor} = \overline{T_{obs}} + \frac{\sigma_{obs}}{\sigma_{ref}} \times (T_{raw} - \overline{T_{ref}})$$
(SE1)

where T_{cor} is bias-corrected CESM variables, $\overline{T_{obs}}$ represents mean CRU-NCEP outputs from the historical reference period, T_{raw} is raw datasets from historical or future CESM variables, $\overline{T_{ref}}$ is a mean CESM output from the same historical reference period, σ_{obs} and σ_{ref} represents the standard deviation in the reference period of CRU-NCEP and CESM variables, respectively. The data are corrected every six hour averaged from eleven years. This method not only considers the mean values but also involves the temporal variance of the model outputs in accordance with the observations (Ho et al., 2012).

36 The correction of future precipitation is calculated using the following equation:

37

$$P_{cor} = P_{raw} \times \frac{\overline{P_{obs,m}}}{\overline{P_{raw,m}}}$$
(SE2)

where P_{cor} is bias-corrected model precipitation, P_{raw} stands for uncorrected corresponding precipitation, $\frac{P_{obs,m}}{P_{raw,m}}$ is the ratio of monthly mean precipitation from CRU-NCEP to that from CESM for the same reference period (Déqué et al., 2007). This method reduces mean biases between models and observations; however, it does not take coefficient of variance of the modeled precipitation into account.

44 Text S2. Estimation of Crop Specific Harvested Area for Irrigated and Non-Irrigated

45 Conditions

LUH2 provides the 5-category cropland distributions (C3 annual crops, C3 perennial crops, C4 46 47 annual crops, C4 perennial crops, and C3 nitrogen-fixing crops) during the historic period 1850-2015 and 2016-2100 for SSP scenarios (Hurtt et al., in preparation), while both MIRCA2000 48 (Portmann et al., 2010) and M3 (Monfreda et al., 2008) data set include crop-specific cropland 49 areas and harvested areas, but for the year 2000. The process for generating crop-specific harvested 50 areas consisted of four steps (Eq. S18): (i) since the LUH2 cropland area amount is not the same 51 as for M3 data in year 2000, we divide the M3 data by LUH2 to calculate the bias factor $\left(\frac{M3_a}{LUH2_a}\right)$, 52 (ii) calculate the ratio of crop-specific harvested areas to cropland areas from M3 data set $(\frac{M3_o}{M3_o})$, 53 (iii) calculate the ratio of crop-specific rainfed and irrigated harvested areas to the crop-specific 54 harvested areas from MIRCA2000 (apply for the period 850-2015) or LUH2 (apply for scenarios 55

for the period 2016-2100) $\left(\frac{FR_{i,0}}{FR_{o}}\right)$, (iv) multiplying each factor from step (i), (ii), (iii) by timevarying LUH2 cropland areas to calculate fraction of crop-specific; irrigated or rainfed harvested areas over 0.5 degree grid cell areas from year 850 to 2100.

59
$$\operatorname{Crop}_{i,o} = \frac{M_{3a}}{LUH_{2a}} \times \frac{M_{3o}}{M_{3a}} \times \frac{FR_{i,o}}{FR_o} \times \frac{LUH_{2a}}{Grid}$$
(SE3)

60 where subscripts *a*: total cropland areas; *i*: irrigated or rainfed conditions; *o*: crop-specific types; 61 $FR_{i,o}$: crop-specific irrigated or rainfed harvested areas from MIRCA2000 data; FR_o :crop-specific 62 total (rainfed plus irrigated) harvested areas from MIRCA2000 data; $M3_o$: crop-specific total 63 (rainfed plus irrigated) harvested areas from M3 data; $M3_a$:cropland areas from M3 data; LUH2_{*a*}: 64 cropland areas from LUH2 data; Grid : 0.5 degree grid cell areas.

To compare the annual maize and soybean yields with published datasets, the simulated yields are weighted to combine yields under fully irrigated assuming no water stress and rainfed (no irrigation) conditions to grid-cell levels, regional as well as global scales using the following equation.

where Yield_F represents crop-specific yields (t/ha) by aggregating yields with irrigated areas and rainfed areas; Yield_{ir} is yield (t/ha) produced from simulations with applying irrigation; Yield_{rf} is

yield (t/ha) produced from simulations without irrigation (rainfed conditions); harea_{ir} is irrigated

harvested areas (ha), and harea $_{rf}$ is rainfed harvested areas (ha).

74

75 Text S3. Estimation of Crop Specific N Inputs at Spatial Scale

We use crop-specific spatially resolved M3 data (Mueller et al., 2012) for N input (sum of N 76 fertilizer, deposition, and manure), which is available for the year 2000, and spatial and temporal 77 78 varying N fertilizer input data of LUH2 (Hurtt et al., in preparation) for C3 and C4 crops. The 79 LUH2 data is available for the historical time period and for the two future scenarios. We first 80 separate the of M3 N input data into fertilizer, deposition, and manure by using N input data of Liu et al. (2010), which provides the percentage contribution of fertilizer, deposition, and manure 81 to the total N input at a continental scale. We apply these percentages to M3 N input data to obtain 82 the N fertilizer, deposition, and manure for each crop of M3 at a spatial scale. Then we use 83 84 following procedure to obtain the spatial distribution of N fertilizer amount: (1) divide the cropspecific N fertilizer rate to total N fertilizer rate from M3 cropland to calculate the fraction of 85 fertilizer amount (FFA) for individual crop, (2) divide the total M3 fertilizer amount to that of the 86 LUH2 amount to calculate the bias factor (BF), and (3) multiply LUH2-based time varying values 87 88 of fertilizer amount with FFA and BF to calculate the fertilizer application amount.

The historical and future deposition data is taken from Lamarque et al. (2011). For crop specific N manure application data, we use M3 data for year 2000 and assume that it changes over the 91 historcal and under two future scenarios at the same rates as the N fertilizer amount. Then we add

- 92 spatial and time varying N fertilizer N manure, and N deposition amounts to estimate N input.
- 93

94 Text S4. Estimation of Irrigation Water Amount

The irrigation amount (W_{irrig}) is estimated as the soil moisture deficit between irrigation target (W_t) and soil water content (W_{liq}) within the root-zone as follows:

97

$$W_{irrg} = W_t - W_{liq}$$
(SE5)

98 where W_t is defined as soil moisture content without water stress (i.e., WS is 1.0) for crop 99 photosynthesis during the growing period.

The irrigation scheme adds W_{irrig} directly to the topsoil layer, analogously to drip irrigation. 100 The estimated W_{irrig} is withdrawn first from surface runoff and drainage. If surface runoff plus 101 drainage is less than W_{irrig}, the remaining requirement of irrigation is extracted from river water 102 storage (i.e., accumulated total runoff). To estimate these water we have incorporated a river 103 transport module (RTM) into ISAM (Sharma et al, 2018). RTM is used to distribute total runoff 104 from the land surface model to the downstream systems such as rivers and oceans. In RTM the 105 water is routed from each grid cell to the neighboring grid cell by using a linear transport scheme 106 107 (Oleson et al., 2013). However, the water demand for crops may still not be met with these sources in some dry seasons or areas, because the water resources and management, such as dynamic 108 reservoir operations, are not accounted for in the model. This deficit of irrigation demand causes 109 negative values of river water storages which should be met by water diversion from outside the 110 111 rivers (Leng et al., 2015)(Leng et al., 2015). In this study we assume that the deficit of irrigation demand is met by the groundwater. 112

Irrigation is applied at each time step when the leaf area index (LAI) of the crop is greater than 113 zero and root-zone soil water stress (WS) is less than 1.0 (i.e., water is limiting photosynthesis). 114 115 The WS is expressed as an index ranging from 0 to 1in ISAM (Song et al., 2016). The closer WS is to 1, the lower the effect of water stress on crop photosynthesis. The model estimated annual 116 applied irrigation water is evaluated with 11 global gridded crop models, which participated in 117 AgMIP project (Müller et al. 2019). The simulation input data, including the weather data and N 118 fertilizer inputs, were obtained from Müller et al. (2019). More details of the experimental setup 119 120 and weather datasets can be found in Müller et al. (2019). We calculated the global irrigation water for ISAM by aggregating all grid cell values according to the fraction of irrigation areas, as 121 described by MIRCA2000 (Portmann et al., 2010). Our model estimated irrigation demand due to 122 growing maize and soybean on irrigated croplands are approximately 47.6 km³/yr and 8.0 km³/yr, 123 124 which fall within AgMIP estimated range values (Figure S5).

125

126 Text S5. Estimation of Crop Specific Planting Time

127 The planting time (DOY_{planting}) (Defined as the Julian day of the year) for maize and soybean at 128 each grid cell is estimated to be the later of that estimated from climate (temperature and 129 precipitation) conditions (DOY_{climate}), and that estimated from phenological heat unit values 130 (DOY_{phu}):

$$DOY_{planting} = max (DOY_{climate}, DOY_{phu})$$
 (SE6)

For the calculation of DOY_{climate} we assume that the planting time is dependent on inter-annual 132 precipitation and temperature variability. For example, planting time in tropical regions, where 133 134 distinct wet and dry periods exist, usually happens when the first rainy season of the year starts. In contrast, sowing processes in temperate regions start right after the winter season, as long as the 135 136 temperature is sufficiently warm to avoid frostiness (Sacks et al., 2010). Since the planting time could vary with the season, we define different seasonality types for planting time, which are 137 determined by calculating annual average variation coefficients (CV) for temperature and 138 precipitation using monthly CRU-NCEP climate data for the period 1901-1950 (Waha et al., 2012). 139 The CV is calculated for temperature (K) and precipitation (mm) respectively as follows: 140

141
$$CV = \frac{\sum_{y=1}^{N} CV_y}{N}$$
(SE7a)

142
$$CV_y = \frac{\sigma_y}{\mu_y}$$
(SE7b)

143 where *y* is the year, CV_y is the variation coefficient of temperature or precipitation in year *y*, *N* is 144 the number of years, σ_y is the standard deviation of temperature or precipitation in year *y*, and μ_y 145 the annual mean temperature or precipitation in year *y*. The following equations are used to 146 calculate σ_y and μ_y :

147
$$\sigma_y = \sqrt{\frac{1}{12-1} \times \sum_{m=1}^{12} \overline{Z_{m,y}} - \mu_y}$$
(SE8)

148
$$\mu_y = \frac{1}{12} \times \sum_{m=1}^{12} \overline{Z_{m,y}}$$
(SE9)

149
$$\overline{Z_{m,y}} = \alpha \times Z_{m,y} + (1 - \alpha) \times \overline{Z_{m,y-1}}$$
(SE8)

where $Z_{m,y}$ is the mean temperature or precipitation of the month *m* in year *y*, $\overline{Z_{m,y}}$ is the exponential weighted moving average temperature or precipitation of a month *m* in year *y*, and α is the coefficient representing the degree of weighting (with a value of 0.05). For the first year of $Z_{m,y}$ (y=1), α is 1.0.

The seasonality types are determined based on the multi-year average of variation coefficients for temperature (CV_t) and precipitation (CV_p) and then classify into following four seasonality types:

- 157(1) Temperature seasonality: $CV_t > 0.01$ and $CV_p <= 0.4$ 158(2) Precipitation seasonality: $CV_t <= 0.01$ and $CV_p > 0.4$ 159(3) No temperature and precipitation seasonality: $CV_t <= 0.01$ and $CV_p <= 0.4$
- 160 (4) Both temperature and precipitation seasonality: $CV_t > 0.01$ and $CV_p > 0.4$

For planting time decisions, we distribute each seasonality types into three planting conditions, temperature-limited (1), precipitation-limited (2), and non-climate-limited (3). In situations where both temperature and precipitation seasonality co-exist (4), we distinguish them by the difference in multi-year mean of daily minimum temperature (T_{min}). If T_{min} is equal to or below 283.16 K, the temperature is a determining factor for planting time. If T_{min} is higher than 283.16 K, precipitation is the determining factor, which uses the same algorithm of planting as precipitationlimited planting.

168 Maize and soybean must meet the following requirements for planting day.

169	$DOY_{climate} \ge DOY_{min}$	(SE9)
170	$DOY_{climate} \le DOY_{max}$	(SE10)
171	$T_{air7d} > T_{base}$	(SE11)
172	$T_{soil8d} > T_{soil_min}$	(SE12)
173	$P_{d8} > P_{min}$	(SE13)

174
$$P_{m_avg} > P_{m_avg_min}$$
(SE14)

where T_{air7d} is the 7-day running mean of daily air temperature, T_{soil8d} 8-day running mean of daily root-zone average soil temperature, P_{d8} accumulated precipitation of the past eight consecutive days, and P_{m_avg} 50-year average of monthly precipitation. Other crop-specific variables are defined in Table S1.

179 The second method to calculate the planting day (DOY_{phu}) assumes the day when the 180 accumulated phenological heat unit (PHU₀) reaches a certain minimum threshold (β *PHU_{min}). 181 PHU₀ is calculated by subtracting the threshold temperature of 273.16 K from the average daily 182 air temperature (T_{air}) as follows.

183

184

$$PHU_0 = PHU_0 + T_{air} - 273.16 \quad \text{if } T_{air} > 273.16 \text{ K} \quad (SE15)$$
$$DOY_{phu} = DOY \quad \text{if } PHU_0 \ge PHU_{min} \times \beta \quad (SE16)$$

where PHU_{min} is the mean of annual PHU₀ for the period 1901-1950. β is the fractional parameter for maize (0.1) and soybean (0.12).

We evaluate simulated planting time with the data compiled by AgMIP (Elliott et al., 2015). 187 This data is compiled using planting time data from two global crop calendars SAGE (Sacks et al., 188 2010) and MIRCA2000 (Portmann et al., 2010), as well as using a land surface model (LPJmL) 189 driven data (Waha et al., 2012). The data availability and details can be found in Elliott et al. (2015). 190 Overall, the simulated spatial patterns of planting days for both crops match fairly well with 191 the AgMIP data (Figure S6). For the regions NA, EU, and Northeastern CHN, which fall in the 192 temperature-limited planting regions, the calculations for maize planting day appear to be similar 193 to AgMIP data, whereas regions SA, SSEA, and AF, which fall in precipitation-limited and non-194

climate-limited regions, the estimated results are somewhat inconsistent with AgMIP data. For 195 example, the main disagreements are shown for maize in countries like Thailand, Indonesia, 196 Malaysia, Vietnam, and southeast CHN where simulated planting day is prior to AgMIP data. Our 197 study findings are similar to the findings of previous studies (Deryng et al., 2011; Stehfest et al., 198 199 2007). This suggests that the algorithm for non-climate-limited planting is not well calibrated to reproduce planting time, which may not be determined based on the climatic conditions, but 200 determined somewhat arbitrary. In regions of precipitation-limited planting, our estimation does 201 not consider any effects of irrigation and soil moisture on planting time for maize, which may also 202 make the difference in choice of planting time. Similar discrepancies are found for soybean. 203 204 Simulated results are different in SSEA, SA, and Australia, which are in the precipitation-limited 205 or non-climate-limited planting regions.

206

207 Text S6. Seeding and Plant Residue Removal Rates

The carbon stored in the seeds ($C_{storage}$) during the emergence period is determined based on the following equation (Song et al., 2013):

210
$$C_{\text{storage}} = C_{\text{storage}_ref} \times \frac{R_{\text{seed}}}{R_{\text{seed}_ref}}$$
 (SE17)

where R_{seed} : seeding rate; R_{seed_ref} : reference seeding rate; and $C_{storage_ref}$: referenced carbon storage in seed.

In the previous version of ISAM, R_{seed}, R_{seed_ref}, and R_{seed_ref} kept constant at each grid cell according to the collected data in the United States (US) for maize and soybean (Table S2) (Song et al., 2013; 2016). We now assume varying values for R_{seed} and C_{storage_ref} in ISAM based on the literature as changing seeding rate is found to influence the soybean yield (De Bruin & Pedersen,

217 2008),.

In the temperate regions with higer seasonal temperature variations, such as EU, NA, and CHN, (Text S5), we use the values for sybean based on Song et al. (2013) (Table S2). For other regions, such as areas in AF and SSEA, we use the seeding rate and initial carbon storage in seed as referenced seeding rate from a farmers' guide based on Dugje et al., (2009) (Table S2). For maize, the seeding rates are assumed to be the same for all regions based on Song et al. (2013).

Similar to the difference in planting processes, the removal of residue (in %) at the harvest 223 time is chosen from the previous studies in Africa and the US. In Sub-Saharan Africa 85% of 224 above-ground crop residues are assumed to be removed at the harvest time (Doraiswamy et al., 225 226 2007; Folberth et al., 2012). In contrast, about 30% of the crop residues are recycled in North America (Liu et al., 2010; Drewniak et al., 2015). For eaxmple, 30% of residue is removed in the 227 US (Drewniak et al., 2015). Therefore, we assume residue removal of 30% for grids showing the 228 229 temperature seasonality (Text S5) and 85% for other grid cells. The rest of the residue is assumed 230 to return to the soil surface (e.g., Kucharik & Brye, 2003; Verma et al., 2005)

231

232 Text S7. ISAM Model Simulations Yields for Maize and Soybean for FACE Sites

Two FACE sites data, which we used in this study to evaluate the model performance, conducted experiments in fully open-air, field conditions with increase in atmospheric CO₂ concentration ([CO₂]) from baseline (around 380 ppm) to 550 ppm. Table S3 summarizes two FACE site locations and elevated atmospheric CO₂ concentration.

237 Soybean FACE site (SoyFACE) in Illinois, the US is the first FACE study of soybean (Morgan et al., 2005). SoyFACE performs ambient and elevated CO₂ treatments for 2002–2011. The [CO₂] 238 for the ambient case varies between 370 and 392 ppm for this period (hereafter referred to as 239 ambient) and for the elevated case [CO₂] was set to 550 ppm for 2002-2008 and 585 ppm for 2009-240 2011 (hereafter referred to as elevated) according to the filed treatment (Gray et al., 2016). Maize 241 was grown over two years (2007-2008) at FACE site in Germany. The circular main plot was 242 spitted into a well-watered (WET) and a dry (DRY) semicircular subplot (Manderscheid et al., 243 2014). The WET conditions keep sufficient water supply under ambient $[CO_2]$ (378 ppm) and 244 elevated [CO₂] (550 ppm) concentrations. The model is run with site-specific planting and harvest 245 246 times, seeding density, actual period of $[CO_2]$ enrichment and irrigation, and amounts of N fertilizer and irrigation. We only compare the modeled irrigated yield with WET FACE condition, 247 because the sufficient information was not provided in the literature for the DRY FACE condition 248 (Deryng et al., 2016). 249

For the simulation for these sites, the model was first spun-up using climate forcing and input for soil variables. Next, the model was run for two cases. The first was the ambient [CO₂] case, and the second was elevated [CO₂] case.

For the SoyFACE site simulations we use half-hourly time step climate forcing data compiled 253 from the Bondville, IL site, which is the nearest Surface Radiation Network (SURFRAD) station 254 255 (40.05°N, 88.37°W) and Willard airport (40.04°N, 88.27°W) site. We used precipitation data from the Willard airport and other meteorological data from SURFRAD site (Vanloocke et al., 2010). 256 The missing data for SURFRAD site was filled with the data collected at Willard Airport. For 257 German FACE site runs we use hourly time step climate forcing data of CRU-NCEP for the period 258 259 2007-2008. For each face site we prescribe layer-specific soil dataset, for example, the sand/clay fraction, organic matter, bulk density, and other hydraulic parameters. These parameter values for 260 SoyFACE site are taken from the soil survey geographic database (SSURGO) database (USDA, 261 2019) and for German FACE site from the Global Soil Dataset for use in Earth System Models 262 263 (GSDE, Shangguan et al., 2014).

The evaluation of ISAM results with FACE sites show that the original version of ISAM (ISAM_O) estimated effects of $[CO_2]$ enrichment on crop yields for maize was consistent with FACE site data, but overestimated for soybean for elevated $[CO_2]$ case (Figure S7a), because, the electron transport rate (*J*) calculation used the linear function of the light response curve (Chen et al., 2011):

269

$$J = \varepsilon \alpha \emptyset \tag{SE18}$$

where ε is 0.04 mol mol⁻¹ for maize (Arora, 2003); and 0.08 for Soybean (Sellers et al., 1996) is quantum yield of electron transport, α (=4.6 µmol J⁻¹) is conversion from photosynthetically

- active radiation to photosynthetic photon flux, and \emptyset (W m⁻²) is absorbed photosynthetically active radiation, which is calculated from solar fluxes using the two-stream approximation and varies between sunlit and shaded leaves for photosynthesis (Song et al., 2013).
- To address this issue, we added curvature to the light response curve in J for the revised version of the ISAM (ISAM_R) (Bonan et al., 2011):

277
$$J = \min(\varepsilon \alpha \emptyset, J_{\max}/4)$$
(SE19)

where J_{max} is maximum potential electron transport rate (Bonan et al., 2011; Song et al., 2013).

After implementation of curvature to the light response curve, ISAM_R estimated results were consistent with the measured values (Figure S7a). For example, ISAM_R estimated yields for the average ambient and elevated measured yields were 353 ± 40 g/m² and 416 ± 40 g/m² compared to the measured values of 382 ± 38 g/m² and 425 ± 44 g/m² over the 5-year (2002, 2004-2007) growing season (Twine et al., 2013).

The simulated canopy temperature and stomatal conductance are also evaluated with measured 284 data in years 2004-2011 (Figures S7b and S7c). Our results indicated that after revised 285 photosynthetic pathway calculated by ISAM_R is also able to reduce the biases in the simulated 286 magnitudes of stomatal conductance under ambient and elevated [CO₂]. The modeled stomatal 287 288 conductance was decreased by 21%, and observation show a 30% average decrease due to CO₂ fertilization effect. In addition, canopy temperature increased because of decrease in stomatal 289 290 conductance under elevated [CO₂]. ISAM_R estimated average canopy temperature increased by 291 0.28K (1.1%), which was similar to observed values of around 0.21K (0.9%) (Figure S7b).

292

293 Text S8. Implementation of the N Stress Effect on Carbon Allocation

We evaluate ISAM estimated maize yield response to different application rates of N fertilizer with published results from six different site-level field experiments (Table S5). Our modeling analysis suggests that the biases in the original version of ISAM (ISAM_O) estimated maize yield is large for the lower N input cases (Figure S8a) because the model underestimates the effect of N stresses (i.e., ratio of N supply and N demand) on grain formation and carbon allocation.

299 The field experiment studies suggest that the maize growth slows down at the lower N supply rates, causing decline in maize yield (Alemayehu et al., 2015; Gehl et al., 2005; Getachew & Belete, 300 2013; Hammad et al., 2011) and harvest index (ratio of harvested grain to above ground biomass) 301 (Akinnifesi et al., 2007; Attia et al., 2015; Kucharik & Brye, 2003; Nangia et al., 2008; Puntel et 302 al., 2016). However, the model is overestimating the maize yields and harvest index at the lower 303 N application rates, because the model overestimates the amount of carbon allocated to the grain 304 305 formation under the N stress (i.e., ratio of N supply and N demand). However, model results for soybean are consistent with the measured data (Figure S8b). To overcome this deficiency, we 306 implement in the model with N stress effect on carbon allocated to grain during initial and post-307 308 reproductive (grain-filling) periods (hereafter this version of the model is called ISAM_R). 309 Therefore, at a lower N fertilizer rate, ISAM_R shows a stronger N stress, lower carbon allocation to grain formation and harvest index compared to ISAM_O case (Figure S8a). 310

We validate the modeled maize yield with site-specific observed values. Overall, ISAM_R estimated maize yields for different N fertilizer rates are compared well with the observation data (Figure S8a).

314

315 Text S9. Heat Stress effect on Crop Productivity

The model calculates the impact of heat stress on reduction in the carbon allocation amount to grain during the reproductive stage of the phenology as follows:

(SE20)

$$A_{g} = A_{g \max} * HS$$

where
$$A_g$$
 is the updated and maximum carbon allocated fraction of net assimilated carbon to the

where A_g is the updated and maximum carbon allocated fraction of net assimilated carbon to the grain pool during the reproductive stage of the phenology, A_{g_max} is an initial calibrated parameter without heat stress impact (Song et al., 2013), and HS is heat stress factor calculated based on Challinor et al. (2005) and has also been used in other studies (e.g., Deryng et al., 2014; Moriondo et al., 2011; Teixeira et al., 2013):

324

325
$$HS = \frac{1}{24} \sum_{i=1}^{24} \begin{cases} 1.0 & T_{mean_i} \leq T_{crit} \\ \frac{T_{limit} - T_{mean_i}}{T_{limit} - T_{crit}} & T_{crit} < T_{mean_i} < T_{limit} \\ 0.0 & T_{mean_i} \geq T_{limit} \end{cases}$$
(SE21)

326

where T_{limit} is limiting temperature at which full heat stress reaches, T_{mean_i} is hourly canopy temperature during the initial and reproductive or flowering stages of the phenology, and T_{crit} the critical temperature at which heat stress starts. For the temperature input in HS, we use crop canopy temperature calculated based on ISAM as the average between the temperatures of the sunlit and shaded leaf weighted by the fraction of sunlit and shaded leaf areas.

T_{crit} and T_{limit} vary among crop types taken in consideration current literature (Deryng et al., 2014; Teixeira et al., 2013). Here, T_{crit} for mize and soybean are 32°C and 35°C, whereas T_{limit} are 45°C and 40°C.

335

339

Text S10. The Calculation of the Percent Bias (PBIAS)

The PBIAS is calculated to compare modeled yield with measured yield at regional and globalscales:

 $PBIAS = \frac{\sum_{i=1}^{M} \sum_{j=1}^{N} (Y_{i,j}^{o} - Y_{i,j}^{m})}{\sum_{i=1}^{M} \sum_{j=1}^{N} Y_{i,j}^{o}} \times 100\%$ (SE22)

340 where $Y_{i,j}^{o}$ and $Y_{i,j}^{m}$ are the observed and modeled yearly yields for the available data *i* in the year *j*.

341 M is the number of available data points. N is the number of years for each available data.

The positive PBIAS means the model yield is consistently underestimated compared to the observed yield. The closer the value of PBIAS to zero means the higher the accuracy of the model results (Song et al., 2015).

346 Text S11. Calculation of Detrended Yield

Following the method of Müller et al. (2017), we first aggregate ISAM estimated yields to regional
values using equation (SE4). For the consistent purpose, ISAM follow the region definition of

FAOstat (2017). We then calculate 5-year moving average (t-2 to t+2) yields based on ISAM and

FAOstat over the period 1981-2007 and 3-year moving (t-1 to t+1) average yields at the boundary

351 of this time period to get the yield trends at a regional and global scales. We eliminate the trend

from ISAM model results and FAOstat data by subtracting the trended yield from actual yield.

Note that no de-trended yields appear at boundary years, 1981 and 2007. So, de-trended yield shown in Figure S9 cover the period 1982-2006.

355

356 Text S12. CLM and AgMIP Model Results for the FACE Sites

357 To assess the performance models against FACE site data in Table S4, AgMIP project selected

358 corresponding yield from the 6 AgMIP model simulations for climate change (CC) w/ CO_2 and

359 CC w/o CO₂ at the grid cells matching the coordinates of FACE observations (Deryng et al., 2016).

360 But temperatures are held constant for the AgMIP models experiment results reported in Table S6.

Ambient $[CO_2]$ in the FACE experiments varied between 360 and 380 ppm and elevated $[CO_2]$

362 corresponds to 550 ppm. So, AgMIP used 10-year average estimates around the year 2050, which
 363 corresponds to the same increment of [CO₂] level rise relative to the baseline (550 ppm in 2050 to

364 380 ppm in 2000, respectively). We use the same method to extract yields from the CLM outputs

of Ren et al. (2018). Given these limitation, the comparison of AgMIP and CLM model results

366 with FACE sites should not be considered as a direct comparison. However, the comparisons can

367 still demonstrate the difference between observed yield changes and simulated values from global

368 crop models

369 Supplementary Tables

- 370
- **Climate-limited regions Definition (Symbol)** Maize Soybean Minimum planting day Precipitation-limited 120 (270) 160 (314) (DOY_{min})* Temperature-limited 80 (296) 100 (314) Non-climate limited 115 (115) 115 (314) Maximum planting day 166 (346) 181 (361) (DOY_{max})* Base temperature for crop 283.16 281.16 planting and growth (T_{base}, K) Critical soil temperature for Precipitation-limited 285.2 285.2 planting (T_{soil min}, K) Temperature-limited 285.16 283.16 Non-climate limited 0 0 Minimum accumulated 8-Precipitation-limited 1 1 day precipitation for 0 0 Temperature-limited planting (P_{min}, mm) Non-climate limited 0 0 Annual average monthly Precipitation-limited 60 60 precipitation requirement Temperature-limited $(P_{m_avg_min}, mm)$ 0 0 Non-climate limited 0 0
- Table S1. Parameters of planting day for maize and soybean.

372 373 *The maximum and minimum planting days are in the Northern Hemisphere, the corresponding days in the Southern Hemisphere are shown in brackets.

- Table S2. The initial carbon storage in seed as referenced ($C_{storage_ref}$), reference seeding rates
- (R_{seed_ref}) , and seeding rates (R_{seed}) for maize and soybean by climate-limited regions*.

Crop type	Climate-limited planting regions	Reference Carbon Storage in Seed (gC/m ²)	Referenced seeding rate (seeds/acre)	Seeding rate (seeds/acre)	Reference
Maize	Precipitation-limited Temperature-limited Non-climate limited	20	62236	35000	Song et al.
	Temperature-limited	30	370644	370000	(2013, 2010)
Soybean	Precipitation-limited Non-climate limited	5	370644	179860	Dugje et al. (2009)

377 *See Supplementary Text S6

380 Table S3. Summary of two FAC	CE sites.
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Crop	Site location	Latitude	Longitude	Ambient	Elevated	Reference
		(deg.)	(deg.)	CO_2	CO_2	
				(ppm)	(ppm)	
Maize	Braunschweig,	52.30	10.43	378	550	Manderscheid et al.
	Germany					(2014)
Soybean	Illinois, USA	40.05	-88.20	370-392	550, 585	Bernacchi et al.
						(2006); Gray et al.
						(2016); Morgan et al.
						(2005)

Table S4. ISAM estimated change (%) in maize and soybean yields due to elevated $[CO_2]$ concentration are compared with FACE site data and CLM and AgMIP model results under wet/irrigated conditions¹.

Crop	FACE		Model	
		ISAM ⁴	CLM ⁷	AgMIP ⁷
Maize	-1.0^{2}	0.2	0.9	0.2 - 7.7
Soybean	14.4 ± 12.5^3	17.5 ± 2.7^5	22	5.2 - 44.4
		$(32.1\pm4.3)^6$		

- 1 The positive values are net sink of C by the terrestrial ecosystem
- 388 ²German- FACE site
- 389 ³SoyFACE site
- ⁴See supplementary Text S7 for ISAM simulations
- ⁵Calculated by the revised version of ISAM
- ⁶Calculated by the original version of ISAM
- ⁷Deryng et al. (2016) (See Text S11 for CLM and AgMIP models simulations)
- 394
- 395

- Table S5. Information for various sites, which are used to evaluate the model response to different
- 398 level of N fertilizer applicate rates.

Site	Location	Lat. (deg)	Long. (deg)	N fertilizer (kgN/ha/yr)	Year	Soil	Reference
			Maize				
Wisconsin's Agricultural Research Station (WARS)	Arlington, WI, USA	43.28° N	89.37° W	0, 180	1995- 2000	silt loam	Kucharik & Brye (2003)
Agricultural Engineering & Agronomy Research Farm (AEARF)	Ames, IA, USA	42.01° N	93.79° W	0, 67, 134, 201, 268	1999- 2014	loam	Puntel et al. (2016)
University of Tennessee Milan Research and Education Center (UTMREU)	Milan, TN, USA	35.93° N	88.72° W	0, 61.6, 123.2, 184.8, 246.4	2007- 2011	silt loam	Boyer et al. (2013)
Florence	Florence, SC, USA	34.24° N	79.81° W	68, 101, 135, 169	1999- 2001	loam sand	Stone et al., (2010)
Oakes	Oakes, ND, USA	46.07° N	98.10° W	0, 45, 90, 135, 180, 225	1990- 1995	loam sand	Derby et al. (2005)
Brunswick	Brunswick, NE, USA	42.33° N	79.92° W	0, 56, 112, 168, 224, 280	2006- 2008	loam sand	Attia et al. (2015)
			Soybean				
University of Nebraska Field Laboratory at Mead	Mead, NE	41.169 °N	96.466° W	0, 56, 112	1974, 1976	Silty clay loam	Al-Ithawi et al. (1980)

400

- 401 Table S6. Maize and soybean yields (t/ha) at global and regional scales averaged over the period
- 402 1996-2005 for the reference case (E_{Ref}) and for the [CO₂] (E_{CO2}), climate (E_{Cli}), irrigation (E_{Irr}),
- 403 nitrogen input (E_{Nit}) and harvest areas (E_{Har}) factor cases; and the % contribution of individual
- factor to the Reference case yield over the average period 1996-2005*. The lowest two panels
- show the the contribution of individual factor change (%) to the yield change from 1996-2005 to
 2090s under RCP4.5 and RCP 8.5 scenarios**.

	Reference [CO ₂] Climate		nate	N input		Irrigation		Harvest Area				
Global/Region	Maize	Soy	Maize	Soy	Maize	Soy	Maize	Soy	Maize	Soy	Maize	Soy
	1		Averag	e crop vi	eld over t	he period	1996-200)5. t/ha	l		I.	1
Global	4.52	2.12	4.32	1.77	4.41	2.03	2.92	1.97	4.20	2.07		
North America	7.86	2.68	7.48	2.37	7.48	2.56	5.27	2.59	7.31	2.62		
(NA)								,				
South America	3 25	1 75	3.16	1 38	3.28	1.69	2.23	1.62	3 20	1 75		
(SA)	5.25	1.75	5.10	1.50	5.20	1.07	2.23	1.02	5.20	1.75		
(SA)	5 70	256	5 16	2.25	5.60	2.44	2.74	2.50	5 25	2.26		
Europe (EU)	3.78	2.30	3.40	2.23	3.02	2.44	5.74	2.30	1.92	2.20		-
Alfica (AF)	1.93	0.97	1.82	0.69	1.95	1.00	1.01	0.90	1.82	0.90		
China (CHN)	5.40	2.40	5.21	1.96	5.47	2.32	2.71	2.07	4.69	2.27		
South and South East Asia (SSEA)	1.91	0.89	1.85	0.56	1.88	0.86	1.15	0.60	1.86	0.88		
	Contrib	ution of	individua	l factor	(%) to the	e referenc	e case ov	er the pe	eriod 199	6-2005*		
Global			4.38	16.40	2.27	3.92	35.37	7.08	7.05	2.09		
North America			4.86	11.31	4.79	4.19	33.01	3.14	7.02	2.15		
(NA)												
South America			2.88	21.60	-0.91	3.55	31.49	7.53	1.65	0.15		-
(SA)												
Europe (EU)			5.56	12.26	2.77	4.61	35.33	2.40	7.39	11.95		-
Africa (AE)			5 71	28.22	0.78	0.74	16.06	7.14	5.80	6.65		
China (CUN)			2.56	19 22	-0.78	-9.74	10.90	12.05	12.14	5.71		
South and			2.30	26.00	-1.52	2.32	49.80	22.21	2 27	0.67		
South East			2.70	30.99	1.32	2.80	39.85	52.21	2.57	0.07		
Asia (SSEA)												
Cont	ribution o	f individ	ual factor	• to the v	ield chan	ge from 1	996-2005	and 209	0s under 1	RCP4.5	(%)**	.I
Global	1.00	15.44	7.04	27.90	-6.59	-4.31	53.46	15.19	3.46	1.82	-19.75	-7.16
North America	7.79	12.94	7.94	20.29	-2.89	-3.95	53.03	2.91	5.63	1.93	-3.60	-1.48
(NA)												
South America	51.84	35.41	8.69	34.64	-14.37	-2.04	87.26	22.90	1.53	0.36	0.80	-5.59
(SA)												
Europe (EU)	11.73	-4.25	13.98	19.25	-12.03	-17.41	56.82	2.69	3.49	9.76	-6.28	-9.22
Africa (AF)	35.51	27.30	8.38	42.98	-6.15	-24.39	64.60	28.31	2.06	4.63	-22.64	-6.42
China (CHN)	-6.81	10.13	5.63	27.72	-4.22	-10.73	51.92	20.37	8.07	4.96	-6.91	-1.33
South and	41.94	56.48	6.70	67.24	-9.44	-18.83	83.35	40.49	6.17	12.46	8.86	17.54
South East												
Asia (SSEA)												
Contribution of individual factor to the yield change (%) from 1996-2005 and 2090s under RCP8 5 (%)**												
Global	-22.05	13.95	9.64	46.50	-11.03	-30.15	31.51	9.34	2.83	2.19	-13.28	-4.24
North America	-10.53	13.50	9.53	33.20	-14.63	-26.12	41.59	2.05	2.70	1.06	-0.82	0.44
(NA)												
South America	-8.82	28.02	8.09	58.23	-6.30	-33.41	33.79	11.71	1.75	1.36	8.89	1.75
(SA)												
Europe (EU)	4.36	4.18	27.08	43.10	-14.68	-38.62	44.98	2.38	5.61	23.73	-2.13	2.37
Africa (AF)	5.53	49.17	9.23	77.42	-9.70	-44.13	31.31	18.90	1.30	6.35	0.01	2.57

China (CHN)	-19.60	8.97	12.66	47.67	-25.20	-37.18	37.38	17.73	7.42	4.72	-2.82	-0.21
South and	-11.63	65.73	5.63	105.0	-4.73	-56.07	36.76	39.88	3.03	12.76	1.74	9.72
South East				9								
Asia (SSEA)												

407 *(E_{Ref} in 1996-2005 - E_{XXX} in 1996-2005)/E_{Ref} in 1996-2005. E_{XXX} represents E_{CO2}, E_{Cli}, E_{Irr}, E_{Nit} or E_{Har}

408 **(E_{Ref} in 2090s - E_{XXX} in 2090s)/E_{Ref} in 1996-2005. E_{XXX} represents E_{CO2}, E_{Cli}, E_{Irr}, E_{Nit} or E_{Har}

Supplementary Figure Captions 410

Figure S1. Regional distributions map. The acronym for each region is in parentheses. 411

413

Figure S2. Global total (a) harvested areas (Million ha) and (b) nitrogen input amount (deposition, 414 manure, and fertilizer) (trillion gram N) for maize and soybean from 1950 to 2100. The harvested 415 areas and N input amount for the historical time period are calculated using the method described 416

- 417 in Supplementary Text S2 and Text S3. The result for the period 2016-2100 are based on RCP 4.5
- 418 and RCP 8.5 scenarios.
- 419

Figure S3. Harvested area fraction plotted at 0.5° x 0.5° grid resolution for maize (left panel) and 420

- 421 soybean (right panel) for 1996-2005 (top row) and 2090s (2090-2099) under RCP4.5 (middle row) and RCP8.5 (bottom row).
- 422
 - 423 Figure S4. Nitrogen input rate (kgN/ha for 0.5° x 0.5° grid) for maize (left panel) and soybean
 - (right panel) for 1996-2005 (top row), and 2090s (2090-2099) under RCP4.5 (middle row) and 424
 - 425 RCP8.5 (bottom row).
- 426

427 Figure S5. Comparison of ISAM estimated global total irrigated water for (a) maize and (b)

- 428 soybean with AgMIP models (Müller et al., 2019) for the period 1905-2012. The green solid line 429 shows the AgMIP ensemble median values and the shaded area shows the interquartile range.
- 430

431 Figure S6. Comparison of ISAM estimated spatial distributions of maize and soybean planting 432 days (Julian day of the year) averaged for year 1996-2005 with AgMIP data (Elliott et al., 2015).

433

Figure S7. Comparison of measured (red bars) and modeled (orginal version represented by 434

- ISAM_O (dark gray bars), and revise version by ISAM_R (bright gray bars) at the SoyFACE for 435
- 436 (a) ratio of yield in elevated to ambient [CO₂] for the year 2002, and 2004-2008, (b) change in
- canopy temperature in elevated relative to ambient CO₂ during daylightwhen photosynthetically 437
- active radiation is $> 50 \ \mu mol/m^2/s$ for 2004-2011, and (c) midday stomatal conductance under 438
- ambient and elevated CO₂ for 2004-2011. The error bar in (a) shows one standard deviation of 439
- observed yield with 7 different cultivars and in (b) and (c) are means \pm standard errors of 440 441 temporal variability.
- 442

443 Figure S8a. Measured and simulated yields of maize with different N fertilizer levels at (a) WARS, (b) AEARF, (c) UTMREU, (d) Florence, (e) Oakes, and (f) Brunswick sites (Table S3). The red 444 445 solid dots show measured values, green solid triangles show simulated results with original version 446 of ISAM (ISAM_O), and blue solid diamonds for revised version of ISAM (ISAM_R). Bars show 447 \pm standard deviation indicating the temporal variability in measured yields of maize.

448

Figure S8b. Same as Figure S8a, but for soybean with different N fertilizer levels at University of 449 Nebraska Field Laboratory, Mead site. 450

451	
452 453	Figure S9. Comparision of ISAM estimated detrending maize (left panel), and soybean (right panel) yields (t/ha) for regional and global scale for the the period 1982-2006 with FAOstat data
454 455	set. The " <i>r</i> " value in each figure is the correlation coefficient.
456 457 458	Figure S10. Maize (left panel) and soybean (right panel) changes in yields (%) for the 2090s relative to the 1996-2005 under RCP4.5 (top row) and RCP 8.5 scenarios (bottom row). Results are plotted at 0.5° x 0.5° degree spatial resolution
459	are protect at 0.5° x 0.5° degree spatial resolution.
460 461 462 463	Figure S11a. Maize and soybean yield changes (%) averaged for 1996-2005 due to effects of CO ₂ , climate, irrigation and nitrogen inputfactors. Simulated areas are masked by crop-specific harvested areas averaged for 1996-2005.
464 465 466	Figure S11b. Same as Figure S12a, but the changes (%) from 1996-2005 and to 2090s under RCP4.5.
467 468 469	Figure S11c. Same as Figure S11a, but the changes (%) from 1996-2005 and to 2090s under RCP8.5.
470 471 472	Figure S12. Peak leaf area index (LAI) for maize and soybean averged for 1996-2005 and 2090 under RCP 4.5 and RCP8.5 scenarios.
473 474 475	Figure S13 Simulated leaf net photosynthetic rates for C4 crops, maize and C3 crops, soybean response to leaf temperature. Solid line is maize and dashed line is soybean.
476 477 478 479	Figure S14. Maps of effect of heat stress on maize and soybean yield (%) for RCP4.5 and RCP8.5 in the 2090s. Values show (yield w/ heat stress minus yield w/o heat stress) / (yield w/o heat stress) *100%.
480 481 482 483	Figure S15. Changes in harvested areas (solid bars) and production (hatched bars) for (a) maize and (b) soybean under RCP4.5 and RCP8.5 scenarios (red bars) by the 2090s relative to the period of mean 1996-2005.



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Figure S2. Global total (a) harvested areas (Million ha) and (b) nitrogen input amount (deposition,
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- 511



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(a) ratio of yield in elevated to ambient $[CO_2]$ for the year 2002, and 2004-2008, (b) change in canopy temperature in elevated relative to ambient CO_2 during daylightwhen photosynthetically

canopy temperature in elevated relative to ambient CO₂ during daylightwhen photosynthetically active radiation is > 50 μ mol/m²/s for 2004-2011, and (c) midday stomatal conductance under

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- 538
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548



- relative to the 1996-2005 under RCP4.5 (top row) and RCP 8.5 scenarios (bottom row). Results
- are plotted at $0.5^{\circ} \ge 0.5^{\circ}$ degree spatial resolution.



Figure S11a. Maize and soybean yield changes (%) averaged for 1996-2005 due to effects of
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560 Figure S11b. Same as Figure S12a, but the changes (%) from 1996-2005 and to 2090s under

561 RCP4.5.



Figure S11c. Same as Figure S11a, but the changes (%) from 1996-2005 and to 2090s under
RCP8.5.



Figure S12. Peak leaf area index (LAI) for maize and soybean averged for 1996-2005 and 2090under RCP 4.5 and RCP8.5 scenarios.



571 Figure S13 Simulated leaf net photosynthetic rates for C4 crops, maize and C3 crops, soybean

572 response to leaf temperature. Solid line is maize and dashed line is soybean.



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Figure S15. Changes in harvested areas (solid bars) and production (hatched bars) for (a) maize
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