An ensemble approach to the representation of subgrid-scale heterogeneity of crop phenology and yield in coarse-resolution large-area crop models

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Abstract

The grid interval of a global climate model (GCM) is generally hundreds of kilometers in latitude and longitude. The spatial heterogeneity of crop condition (*e.g.*, phenology and yields) at that scale could be substantial. Because the atmosphere-cropland exchanges of energy, water, and materials are sensitive to crop condition, this issue poses a question: How can we simulate the condition of a crop of interest on a GCM grid scale while taking into account the spatial heterogeneity of crop condition at a sub-grid scale? We therefore proposed an ensemble approach that uses stochastic parameter values to represent the spatial variation in the phenological and biophysical characteristics of a crop within a given GCM grid box, and tested its feasibility with simulation experiments. The combination of the Soil and Water Assessment Tool (SWAT) applied to maize in the Central Great Plains, United States, and coarse-resolution ($2.5^\circ \times 2.5^\circ$) reanalysis data was taken as the example. The ensemble simulations successfully captured the spatial variation in the phenology and yield. Our conclusion is that the ensemble approach is feasible and expected to benefit large-area crop modeling when extending those models to include more information on the spatial heterogeneity of crop condition than ever.

Key words: Calibration, Large-area crop model, Markov Chain Monte Carlo method, Soil and Water Assessment Tool (SWAT), Spatial heterogeneity.

1. Introduction

How can we simulate phenology and yield of a crop of interest on a global climate model (GCM) grid scale while taking into account the spatial heterogeneity of crop condition at a sub-grid scale? The issue has become increasingly important to improve large-area crop models (*e.g.*, Challinor *et al.*, 2004; Iizumi *et al.*, 2009) because a GCM grid scale is in general hundreds of kilometers in latitude and longitude and the spatial heterogeneity of crop condition in that scale could be substantial (van Bussel *et al.*, 2011).

One possible approach this study sought to propose is an ensemble approach that conducts many crop growth simulations at a sub-grid scale under given

stochastic parameter values that represent the spatial variation in the phenological and biophysical characteristics of a crop of interest within a GCM grid box. A somewhat similar approach has been proposed for GCM physical parameterizations (Murphy *et al.*, 2007), though it is used for analyzing the uncertainty of climate projection rather than in accounting for spatial heterogeneity.

To that end, this study aimed to examine the feasibility of the approach by taking the combination of the Soil and Water Assessment Tool (SWAT; Neitsch *et al.*, 2005) applied to maize in the Central Great Plains, United States (U.S.), and coarse-resolution ($2.5^\circ \times 2.5^\circ$) National Center for Environmental Prediction-Department of Energy (NCEP-DOE) reanalysis data (Kanamitsu *et al.*, 2002) as an example. The good performance of SWAT with capturing the major observed characteristics of maize growth and yields in the U.S. (*e.g.*, Srinivasan *et al.*, 2010) where over 40% of

Received; May 16, 2013.

Accepted; July 11, 2013.

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the world maize production occurred in 2009 is a reason for selecting the model and region for this analysis.

2. Methods and Data

2.1 Crop model

SWAT is a process-based crop model consisting of submodels for growth and development, dry matter production, yield formation, soil water balance, nitrogen dynamics, and management of sowing, irrigation,

nitrogen, and crop residual operations. More detailed descriptions are available from Neitsch *et al.* (2005).

We selected 10 parameters (Table 1), which are important for determining the crop's characteristics related to the developmental rate, radiation-use efficiency, response to elevated $[\text{CO}_2]$ concentration, and tolerance of several abiotic stresses. Among many candidate parameters, the parameters that appeared in the growth processes likely sensitive to climatic condi-

Table 1. List of abbreviations, units, definitions, prior uniform distributions, and references for the selected parameters for the maize version of SWAT.

Abbr.	Unit	Definition	Prior	Reference(s)
$f_{\text{bion } 0}$	fraction	Threshold fraction of the actual nitrogen content to the optimal value	(0, 1)	Neitsch <i>et al.</i> (2005)
$f_{\text{GDD, sen}}$	fraction	Fraction of the growing season at which senescence becomes the dominant growth process	(0.7, 0.9)	Howell <i>et al.</i> (1996); Steduto and Hsiao (1998)
isolr	fraction	Rate coefficient for adjusting the initial nitrogen content in the soil layers	(0.5, 1)	
LAI_{max}	m^2/m^2	Maximum leaf area index (LAI)	(2, 4)	Williams <i>et al.</i> (1968); Christy and Williamson (1985)
RUE_{hi}	$\text{kg ha}^{-1} \cdot (\text{MJ m}^{-2} \text{ day}^{-1})^{-1}$	Radiation-use efficiency (RUE) at a doubled CO_2 level	(0.3, 0.45)	Stockle <i>et al.</i> (1992)
TGDD	$^{\circ}\text{C days}$	Total growing degree days required for maturity (base temperature is 10°C)	(1000, 1800)	Ko <i>et al.</i> (2009); Roth and Yocum (1997)
T_o	$^{\circ}\text{C}$	Optimal temperature	(25, 30)	Stewart <i>et al.</i> (1998)
vpd_0	kPa	Threshold vapor pressure deficit (VPD) above which the crop will exhibit a reduced RUE	(0, 3)	Stockle and Kiniry (1990)
Δplt	days	Difference in days from the standard sowing date in the area	(-30, 30)	Sacks and Kucharick (2011)
$\Delta \text{RUE}_{\text{decl}}$	$(\text{kg ha}^{-1} \cdot (\text{MJ m}^{-2} \text{ day}^{-1})^{-1} \cdot \text{kPa}^{-1})$	Rate of decline in the RUE per unit increase in VPD	(3, 20)	Neitsch <i>et al.</i> (2005)
σ_1^2	$(\text{Mg ha}^{-1})^2$	Variance of error for the fine-resolution SWAT outputs for the yield	(0.0001, 4)	
σ_2^2	$(\text{days})^2$	Variance of error for the fine-resolution SWAT outputs for the silking date	(0.0001, 100)	
σ_3^2	$(\text{days})^2$	Variance of error for the fine-resolution SWAT outputs for the maturity date	(0.0001, 100)

Fig. 1. Geographical map of topography (shaded) with location of state borders (thin lines) and study area (bold line) (a). Topography (b-c) and maize harvested area fraction (d-e) in the study area at two spatial resolutions (b and d, 2.5°; and c and e, 0.3° in latitude and longitude). A square located within the coarse grid box #4 (c and e) is the selected fine grid for simulation experiments #1–2 (see Table 3).

tions (including an altered climate) were selected by referring to modeling details (Neitsch *et al.*, 2005) and other expert judgments.

Two versions of SWAT, *i.e.*, the fine- and coarse-resolution versions (0.3° and 2.5° in latitude and longitude, respectively), were used. The modeled growth processes were identical between the two versions. The fine- and coarse-resolution models were applied to 404 fine grid boxes and 9 coarse grid boxes, respectively (Figs. 1d and e). The parameter values for the coarse-resolution model were calibrated in this study using the

fine-resolution model outputs as the calibration data. For the fine-resolution model, we used the parameter values at a finer scale than the NCEP-DOE reanalysis determined in previous study (Iizumi *et al.*, 2010).

2.2 Data

Table 2 presents a summary of the data used. SWAT requires daily maximum and minimum temperatures, precipitation, solar radiation, relative humidity, and wind speed. NCEP-DOE reanalysis (Kanamitsu *et al.*, 2002) and the North American regional reanalysis (Mesinger *et al.*, 2006) were used as the weather in-

Table 2. List of datasets used for this study.

Element	Data name ¹	Original resolution		Source
		Spatial	Temporal	
Weather	NCEP-DOE reanalysis	$2.5^{\circ} \times 2.5^{\circ}$	Daily (1979–2009)	Kanamitsu <i>et al.</i> (2002)
	North American regional reanalysis	$0.3^{\circ} \times 0.3^{\circ}$	Daily (1979–2009)	Mesinger <i>et al.</i> (2006)
Soil ²	ISLSCP-II global soil characteristics	$1^{\circ} \times 1^{\circ}$	Constant	Hall <i>et al.</i> (2006)
Nitrogen	Reported nitrogen input	Country	Yearly (1979–2009)	FAO (2010)
Cropland	Global harvested area map	$0.083^{\circ} \times 0.083^{\circ}$	2000	Monfreda <i>et al.</i> (2008)
Irrigation ³	Reported irrigation input	Country	Yearly (1979–2009)	FAO (2010)
	Global irrigation map	$0.083^{\circ} \times 0.083^{\circ}$	2000	Siebert <i>et al.</i> (2005)
CO ₂	CDIAC reported CO ₂	Site (Mauna Loa, Hawaii, U.S.)	Yearly (1979–2009)	Keeling <i>et al.</i> (2009)
Yield	Reported maize yield	County	Yearly (1980–2006)	USDA (2010)
Phenology	Reported dates of sowing, silking, and harvesting of maize	State	Yearly (1980–2006)	USDA (2010)

¹ Abbreviations are as follows: NCEP-DOE, National Center for Environmental Prediction-Department of Energy; CDIAC, Carbon Dioxide Information Analysis Center; ISLSCP-II, International Satellite Land-Surface Climatology Project, Initiative II; FAO, United Nations Food and Agriculture Organization; and USDA, U.S. Department of Agriculture.

² The bottom depth of each soil layer corresponds to 20, 100, 300, 600, 1000, and 1500 mm.

³ In the simulations, the irrigation water was intermittently put into the surface soil layer, although the irrigation input per operation was limited to less than 30% of its yearly value, and the irrigation operation was conducted only when there were more than five consecutive dry days and where there was still irrigation water remaining for the year (a dry day was defined as a day with precipitation $<1 \text{ mm d}^{-1}$).

puts for the coarse- and fine-resolution models, respectively. No bias correction was performed because it can be assumed that the biases of the NCEP-DOE reanalysis are comparable to those of the regional reanalysis (note, however, that bias-corrected or observed coarse-resolution weather inputs are needed when observed crop data are used as the calibration data). Soil data were assigned for six soil layers after regridding to each resolution. The same values of [CO₂] concentration were used for all grid boxes, regardless of the

spatial resolution.

We used the yearly country nitrogen data from the Food and Agriculture Organization (FAO, 2010). Identical values were used across grid boxes and spatial resolutions. The locations where maize was grown were specified using Monfreda *et al.* (2008). The yearly country irrigation data from FAO (2010) were used in a similar manner as described for nitrogen, though the locations where irrigation facilities were equipped were specified using Siebert *et al.* (2005). In

addition, the maize yield and phenology data from the U.S. Department of Agriculture (USDA, 2010) were used when assessing the reliability of the fine-resolution model outputs.

2.3 Calibration method

The Markov Chain Monte Carlo (MCMC) method (Metropolis *et al.*, 1953; Hastings, 1970) was used to calibrate the coarse-resolution model. In this method, parameter values distributed within a known possible range (represented by a uniform distribution; Table 1) were updated using the data (*i.e.*, the fine-resolution model outputs) to form a posterior distribution of a parameter value according to Bayes' theorem:

$$p(\theta|D) = \frac{\pi(D|\theta)p(\theta)}{\int \pi(D|\theta)p(\theta)d\theta}, \quad (1)$$

where $p(\theta|D)$ is the posterior probability distribution of parameter θ under a given data D , $\pi(D|\theta)$ is the likelihood function, $p(\theta)$ is the prior probability distribution of parameter θ , and the denominator of the right-hand side is the normalizing constant.

The likelihood function was specified as:

$$\pi(\theta) = \prod_{i=1}^3 \pi_i(\theta), \quad (2)$$

$$\pi_i(\theta) = \left(2\pi\sigma_i^2\right)^{-\frac{N}{2}} \exp\left\{-\frac{\left(\mathbf{Y}_i - \hat{\mathbf{Y}}_i\right)^T \left(\mathbf{Y}_i - \hat{\mathbf{Y}}_i\right)}{2\sigma_i^2}\right\}$$

where N is the sample size, and $\mathbf{Y}_i$ and $\hat{\mathbf{Y}}_i$ are the vectors of the calibration data and coarse-resolution

model outputs, respectively. The variances of error (σ_i^2) were estimated in parallel with other parameters. The suffix i denotes the i -th metric number of the calibration data (Table 1). For simplicity, the error distribution was assumed to be a multivariate normal distribution, with the nondiagonal elements of the variance-covariance matrix equal to zero.

The MCMC method was performed following the procedures described in Iizumi *et al.* (2009). The iterations of 100,000 Monte Carlo steps with three parallel Markov chains were performed. The convergence was diagnosed in accordance with Gelman and Rubin (1992).

2.4 Simulation experiments

To examine the feasibility of the ensemble approach, we used simulation experiments (Fig. 2). Simulation experiments are free from the lack of dense crop observations, because the crop growth heterogeneity in a given GCM grid box can be directly observed from the given fine-resolution model outputs. Simulation experiments are also free from the unfavorable impacts on model calibration from imperfect modeling, measurement errors, and unknown processes, because the two versions of the model are different only for spatial resolution and are identical for the modeled growth processes.

We first confirmed the sensitivity of the calibration capability of the MCMC method to the sample size of calibration data to demonstrate the robustness of calibrated ensemble simulations to new data (*i.e.*, the vali-

Fig. 2. Schematic diagram of the simulation experiments.

dation data). In experiments #1–2 (Table 3), the coarse-resolution model was calibrated using the coarse-resolution inputs and fine-resolution model outputs at a selected fine grid box for the 10-year period (1979–1988) or 30-year period (1979–2008). While the performance of the calibrated model in part depends on the setup of prior distributions of the parameters if likely parameter values distributed in the tail of the distributions (Makowski *et al.*, 2002), this is not the case for this study because we set the prior distributions as widely as possible based on the information from the literature (Table 1). Therefore, we did not present the sensitivity analysis for prior distributions. After the confirmation, we estimated the posterior distributions of the parameter values for a coarse grid box using the coarse-resolution inputs and fine-resolution model outputs for the 31-year period (1979–2009) at all fine grid boxes located within a given coarse grid box (experiment #3; Table 3). Then we evaluated the spatial variation in the phenology and yield within a coarse grid box simulated using the coarse-resolution inputs and the estimated posterior parameter distributions.

2.5 Analyses

The degree of heterogeneity of crop condition (represented by the long-term mean spatial variation in the fine-resolution model outputs within a coarse grid box) varies from one coarse grid to another (Fig. 3). The spatial variation seems larger when the fine grid boxes with various maize harvested area fractions are mixed (Fig. 1e) or when there are comparatively complex terrains in a coarse grid box (Fig. 1c) (*e.g.*, the yield at coarse grid #4). In this study, we took coarse grid #4 as an example for experiment #3, because this

coarse grid box showed slightly larger spatial variation for both phenology and yield compared with other coarse grid boxes. For experiments #1–2, a fine grid box was located within coarse grid #4 (Fig. 1e), where the largest temporal yield variation was observed.

To evaluate the performance of the approach in capturing the given crop growth heterogeneity, we used two types of statistical tests, the two-sample Kolmogorov-Smirnov (K-S) test and Student's *t*-test. The K-S test was used to compare the whole probability distributions of yield or phenology between the two samples (*i.e.*, the calibration data and calibrated ensemble simulations) year by year. The null hypothesis of the K-S test is that the two samples are drawn from the same distribution. The *t*-test was used to compare the means of two samples year by year with the assumption of non-equal variance. The null hypothesis of the *t*-test is that the means of the two samples are equal.

3. Results

3.1 Evaluation of the fine-resolution model outputs

The fine-resolution model outputs at the 404 fine grid boxes for the period 1979–2009 were compared with the reported data (Fig. 4). The Pearson's correlation coefficients for yield ranged from 0.09 to 0.92 (the mean value was 0.64, and the correlation values for 357 fine grid boxes were statistically significant at the 1% level). The corresponding values for the dates of silking and maturity were 0.16 to 0.90 (0.72; 386 grid boxes) and 0.40 to 0.94 (0.72; 402 grid boxes), respectively. The root-mean-square errors (RMSEs) for yield ranged from 9.6 to 77.3% (the mean value was 29.8%). The corresponding values for the dates of silking and maturity were 3 to 15 days (7 days) and 7

Table 3. List of the simulation experiments.

Experiment #	Description
1	The calibration of the coarse-resolution model using the fine-resolution model outputs at a selected fine grid box in the coarse grid box (#4) for the 10-year period (1979–1988)
2	Same as experiment #1 but for the 30-year period (1979–2008)
3	The calibration of the coarse-resolution model using the fine-resolution model outputs at all fine grid boxes located within a coarse grid box

All experiments determined the posterior distributions of the 13 parameters (including 3 variances of error) for a coarse grid box using the coarse-resolution inputs.

Fig. 3. Long-term mean of the fine-resolution model outputs for yield (a-b), silking date (d-e), and maturity date (g-h) (1979–2009) at two different spatial resolutions. The values for the coarse grid box of 2.5° were calculated by spatially aggregating the data at the fine grid box of 0.3°. The spatial variation of the fine-resolution SWAT outputs located within a coarse grid box (represented by the coefficient of variation, CV) are shown for yield (c), silking date (f), and maturity date (i). The presented CV was calculated year by year and then averaged over the period 1979–2009.

to 40 days (18 days), respectively.

3.2 Sensitivity of calibration capability to the sample size of calibration data

Figure 5 shows the time series of the calibrated ensemble simulations for the fine grid box using the 1,500 sets of the parameter values derived from exper-

Fig. 4. Geographical maps of Pearson's correlation coefficients and root-mean-square errors calculated between the fine-resolution model outputs and reported data for (a-b) yield, (c-d) silking date, and (e-f) maturity date for the period 1979–2009. Circles in correlation maps (a, c, and e) indicate that the correlation value for a fine grid is statistically significant at the 1% significance level.

iments #1 and #2. The correspondences between the calibrated ensemble simulation (represented by the median value) and the fine-resolution model outputs

Fig. 5. Time series of the calibrated ensemble simulations (median, red line; 99% interval, red shaded area) at the selected fine grid box located within the coarse grid box #4 (see Fig. 1 c) from the experiments #1-2. Filled circles indicate the fine-resolution model outputs used for the calibration. The data presented in open circles were not used for the calibration. Pearson's correlation coefficients and root-mean-square errors (in percent for yield, relative to the long-term mean fine-resolution model outputs) are shown for the median of the calibrated ensemble simulations.

for the phenology and yield were comparable across the results of experiments #1 and #2 (Fig. 5), suggesting the performance of the coarse-resolution model calibrated using the MCMC method was rather insensitive to the sample size. In addition, as expected, the 99% interval of the ensemble simulations became narrower as the sample size increased.

3.3 Representation of subgrid-scale heterogeneity of crop condition within a GCM grid box

The time series of the fine-resolution model outputs and the calibrated ensemble simulations (experiment #3) are presented in Fig. 6. The 99% interval of the calibrated ensemble simulations captured the major spatial variation in the given fine-resolution model outputs. Coincidentally, the correspondence in median

values between the ensemble simulations and fine-resolution model outputs is good. For the yield, the correlation (RMSE) value is 0.585 ($p < 0.01$, 13.7%, relative to the long-term mean fine-resolution model outputs). The corresponding value for the silking date and maturity date are 0.924 ($p < 0.01$, 2.5 days) and 0.776 ($p < 0.01$, 8.5 days), respectively. For both phenology and yield, no significant test results for both distributions and means were found.

4. Discussion and Remarks

From the assessment results, the fine-resolution model captured the major patterns of yield and phenology in the study area reasonably well. This fact indicates that the outcomes from the simulation experi-

ments are consistent with reality and have implications for the calibration of a large-area crop model using observed crop data.

The results of experiments #1-2 suggest the low sensitivity of the calibration capability of the MCMC method to the sample size of calibration data. The calibrated ensemble simulations demonstrated a good match with new data (Fig. 5). This is a little bit sur-

prising for the yield because all 10 parameters related to yield were determined using the 10-year data. Although such a characteristic of the MCMC method is consistent with the conclusion of Makowski *et al.* (2002) that the MCMC method can strongly improve the accuracy of crop model predictions even when few data samples are available to estimate the parameters, caution is needed because in this study the calibration

Fig. 6. Time series of the calibrated ensemble simulations in the experiment #3 (median, red line; 50% interval, deep red shaded area; and 99% interval, light red shaded area) in the coarse grid box #4. The box plot indicates the spatial variation of the fine-resolution model outputs in the coarse grid box. The horizontal line within each box indicates the median value. The lower and upper hinges of each box indicate the 25th and 75th percentiles, respectively. The vertical line flanking each box indicates the range covering the mean ± 2 standard deviation. Dots indicate outliers. Pearson's correlation coefficients and root-mean-square errors (in percent for yield, relative to the mean of the fine-resolution model outputs) between the median values of the ensemble simulations and the fine-resolution model outputs are shown as numbers in red.

and simulated data were generated from the same (but different resolution) models. The insensitivity of the MCMC method to the sample size may be lower than that presented in this study when imperfect modeling, measurement errors, and unknown processes matter.

The calibrated ensemble simulations in experiment #3 successfully captured the major characteristics of the spatial heterogeneity of the phenology and yield within a given GCM grid box (Fig. 6), indicating that the ensemble approach is feasible. Namely, the sub-grid-scale spatial heterogeneity of crop condition within a GCM grid box can be simulated by conducting ensemble simulations using the posterior distributions of the parameter values if subgrid-scale crop data were used to determine the posterior distributions. Given limitations due to imperfect modeling, measurement errors, and unknown processes, high-resolution crop data (e.g., leaf area index; Ganguly *et al.*, 2008) from satellite remote sensing may be applicable to the calibration of a large-area crop model in this manner when accounting for the spatial heterogeneity of crop condition into simulations of a large-area crop model.

We conclude that use of the ensemble approach is expected to improve the representation of the consequences of subgrid-scale heterogeneity of crop condition on simulations of the atmosphere-cropland exchanges of energy, water, and materials at a GCM grid box scale. However, note that the proposed approach is designed for coarse-resolution crop models: direct simulations of such effects using high-resolution crop models and downscaled climatic data are another approach (which this study does not deal with) if a dense crop observation network is available (e.g., van Bussel *et al.*, 2011). Given the limited accessibility of high-resolution global, historical crop datasets, the proposed approach will benefit large-area crop modeling as well as dynamic global vegetation modeling (e.g., Bondeau *et al.*, 2007) and land surface modeling (e.g., van den Hoof *et al.*, 2011) when extending such coarse-resolution models to include more heterogeneous natures of crop condition than ever.

Acknowledgements

We acknowledge M. Okada and Y. Numata for their support in data handling. The earlier version of this study was partially supported by the Innovative Program of Climate Change Projection for the 21st Century (KAKUSHIN program). T. Iizumi was supported

by a Grant-in-Aid for Scientific Research (23880030). The final version of this study was supported by the Environment Research and Technology Development Fund (S-10-2) of the Ministry of the Environment, Japan. The computations were carried out on the cluster system at the Computer Center for Agriculture, Forestry and Fisheries Research.

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