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Jing Huang
Southwest University of Science and Technology

Laura Scherer
Leiden University

Kelly Thorp
United States Department of Agriculture

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Advancing the application of a model-independent open-source geospatial tool for national-scale spatiotemporal simulations

Jing Huang [a, b]*, Laura A. Scherer [b], Kang Lan [a], Fu Chen [c], Kelly R. Thorp [d]

[a] College of Life Science and Engineering, Southwest University of Science and Technology (SWUST), Mianyang 621010, China

[b] Institute of Environmental Sciences (CML), Leiden University, Leiden 2333 CC, Netherlands

[c] College of Agronomy, China Agricultural University, Beijing 100193, China

[d] USDA-ARS, U.S. Arid Land Agricultural Research Center, Maricopa AZ 85138, USA

*Corresponding author.

E-mail address: huang.jing@swust.edu.cn (J. Huang).

Abstract

The growing demand for geospatial application of environmental models has led to the development of tools for conducting simulations spatially. A model-independent and open-source tool named Geospatial Simulation (GeoSim) has been developed previously. Based on previous applications at field scale, this study advances GeoSim application for national-scale and multi-year simulations. The widely-applied FAO AquaCrop model was implemented by GeoSim to simulate wheat yield and irrigation requirements on a daily timestep across China from 2000 to 2009. The spatial inputs required by AquaCrop were minimized to four attributes in GeoSim's base shapefile. 6,915 unique response units were identified among the primary 116,801 polygons. Approximately 20 hours were required to perform 69,150 simulations (10 years). Post-processing of simulation outputs permitting mapping at the original resolution of 5 arc-minutes. The novel methods developed in this study demonstrate new opportunities for efficiently managing environmental simulations for large scales and multiple years with high resolution.

Key words: Geospatial simulation; AquaCrop; High spatiotemporal resolution; Water consumption; Yield

1. Introduction

Over the past decades, applications of agroecosystem system models have rapidly expanded, and the models have been applied in numerous areas such as resource use and efficiency, food security, and environmental performance (Holzworth et al., 2015). There are more than 100 crop models available, and they have been applied for the simulation of about 150 crops or land uses (Rivington and Koo, 2010). With the expanding application domain, models are increasingly applied at diverse spatiotemporal scales (Bryan, 2013; Folberth et al., 2012; Liu, 2009; Zhao et al., 2013). This has required spatial simulation capability to be added to the models or the construction of model wrappers that provide this capability. In recent years, progress has been made on the development of geographic information systems (GIS) to handle geo-processing tasks, store geo-spatial data, manage input and output data from the simulation model and visualize the results spatially (Bryan, 2013; Holzworth et al., 2015; Thorp et al., 2008; Thorp and Bronson, 2013). A few agroecosystem models have been improved as GIS-based modelling systems allowing simulations at multiple locations to be run simultaneously with dynamic interactions, e.g. Apollo-DSSAT for DSSAT (Thorp et al., 2008), GEPIC for EPIC (Liu, 2009), and Grid-Parallel-APSIM for APSIM (Zhao et al., 2013).

However, many GIS-based modelling systems have been developed for a specific application or model. That said, these systems are model-dependent and are useful only for limited purposes. In addition, some systems, which may be proprietary, computer platform dependent, now obsolete, or cost prohibitive, are not available for all users (Thorp and Bronson, 2013). To avoid these problems, Thorp and Bronson (2013) developed a tool called Geospatial Simulation (GeoSim), which is a model-independent open-source system for managing point-based model simulations at multiple locations. The tool has been demonstrated on the widely-applied AquaCrop and DSSAT models (Memic et al., 2018; Thorp et al., 2015; Thorp and Bronson, 2013). Although GeoSim does not restrict model applications to any specific spatial scale, the past applications of GeoSim were all conducted at the field scale. To date, no study has demonstrated GeoSim for broader spatial scales, although it can potentially be applied as such.

To demonstrate its applicability for national-scale multi-year simulations, this study used GeoSim to implement the widely-applied FAO AquaCrop model for simulating wheat yield and net irrigation water requirements across China from 2000 to 2009. Alternative tools such as AquaCrop-GIS (Lorite et al., 2013) and AquaCrop-OS (Foster et al., 2017) have also been designed to implement AquaCrop for multiple simulations. However, these tools work with old AquaCrop versions and have limitations, such as low simulation efficiency or need for programing skills, which can constrain the model applicability. The objective of this study was to 1) demonstrate that GeoSim can efficiently work with AquaCrop for modelling at large spatiotemporal scales with high resolution and 2) to highlight how decisions on setting up the simulations can improve efficiency. While beyond the scope of this study, GeoSim also has the potential to work with other models following a similar approach. As such, it facilitates addressing global challenges such as food security and environmental security by efficiently extending models for spatial simulations.

2. Methods

2.1. GeoSim and AquaCrop

GeoSim was designed to facilitate spatial simulations for any point-based model which uses ASCII files for input and output (Thorp and Bronson, 2013). It was developed as a plug-in for Quantum GIS (QGIS, https://www.qgis.org), and both of these software programs are open-source and freely available. GeoSim provides an interface to run point-based models using geospatial data contained in a QGIS database. Six tools are currently available in GeoSim. These tools enable the system to prepare and process the required shapefile, to manage input and output data for the polygons in that shapefile, and to optimize model parameters to minimize errors.

FAO's AquaCrop is a water-driven dynamic model which can simulate the potential yields of herbaceous crops under various management and environmental conditions (Vanuytrecht et al., 2014). It derives biomass gain as a function of water consumption under rain-fed or different irrigation conditions on a daily step (Raes et al., 2009; Steduto et al., 2009). The model performance has been widely tested for numerous crops under diverse environments and agricultural production systems around the world (Vanuytrecht et al., 2014). This study applied the most recent release of AquaCrop (version 6.1) (http://www.fao.org/aquacrop).

2.2. Pre-processing of spatial inputs

GeoSim automates simulations by passing geospatial data from polygons in a base shapefile to the model input files, and it then similarly passes targeted model outputs back to the base shapefile (Thorp and Bronson, 2013). A "control" file within GeoSim uses "template" files to interface with the model input files and uses "instruction" files to search model output files for the geospatial data to be returned to the base shapefile. The flexibility of GeoSim permits a user to pass any spatial input data to the model files, such as climate data and soil parameters. However, to minimize the input spatial variables, this case study applied GeoSim by passing spatial data only to AquaCrop's project file (*.PRM) which controls AquaCrop simulations (Fig.1). All the unique input files required by AquaCrop were prepared separately, prior to conducting simulations with GeoSim (see next paragraph).

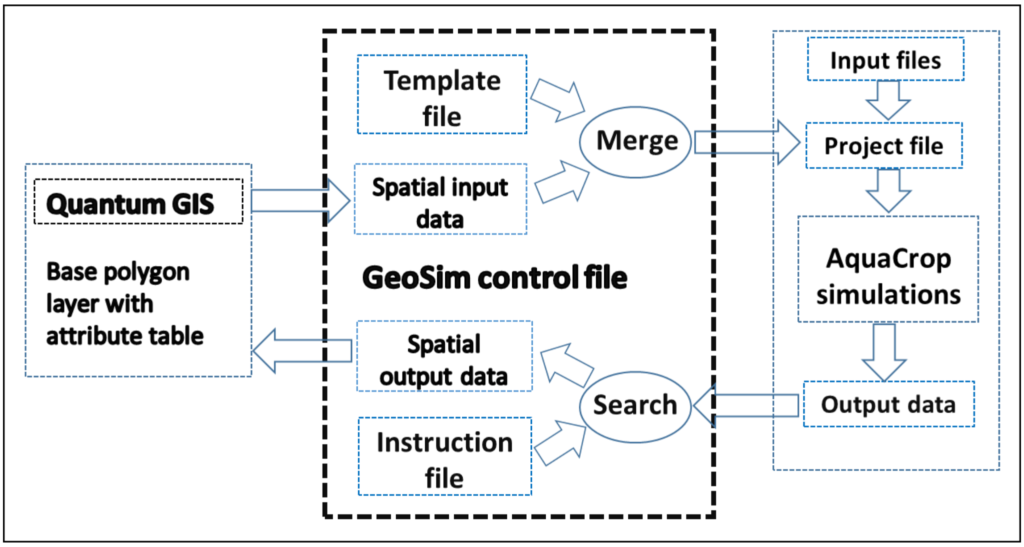


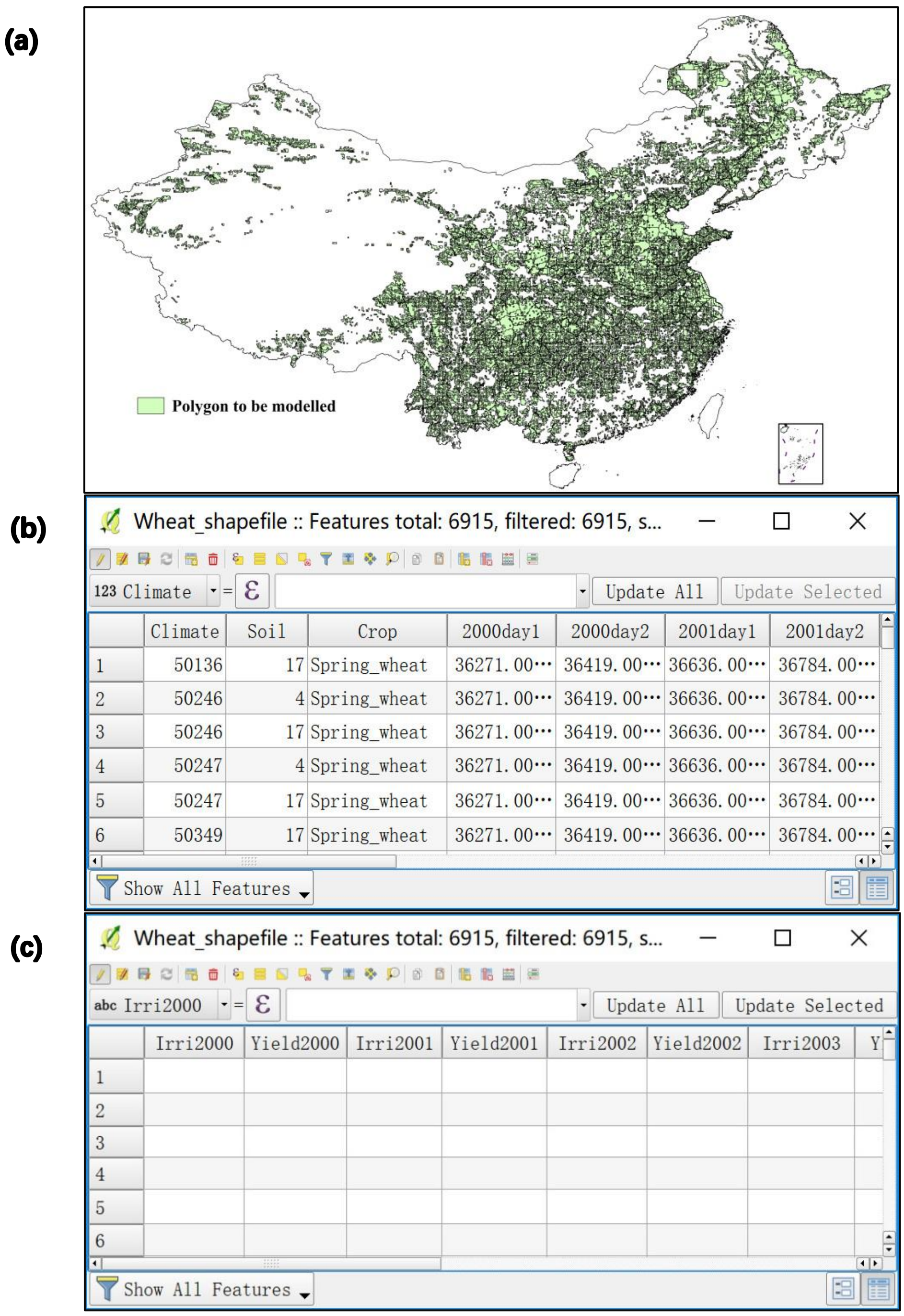
Fig.1. Framework of GeoSim application for AquaCrop, adapted from (Thorp and Bronson, 2013).

Six types of input data were used for the simulations of wheat yield and irrigation requirement across China from 2000 to 2009: 1) crop distribution; 2) climate data; 3) crop parameters; 4) soil parameters; 5) initial soil water conditions; and 6) management data. A shapefile (vector data) of national wheat distribution was converted from a raster dataset with a resolution of 5 arc-minutes in the year 2000 (section 1.1 in Appendix A). Climate files were prepared according to the AquaCrop formats based on daily data from 825 meteorological stations (http://data.cma.cn). The coordinates of all meteorological stations were used to generate a shapefile containing the station codes (section 1.2 in Appendix A). The default file for atmospheric CO_2 concentration in the AquaCrop database was used. Crop files for both spring and winter wheat containing numerous parameters were prepared according to the AquaCrop formats (section 1.3 in Appendix A). Day numbers, which indicate the first and last days of cropping and simulation periods, were calculated for China's 41 agro-ecological zones (AEZ) and included in the attribute table of the AEZ shapefile (Fig.A.3 in Appendix A). The crop type, which indicates whether the crop was spring or winter wheat, was also included in the AEZ shapefile. A soil shapefile containing 39 soil codes was prepared with national coverage (section 1.4 in Appendix A). Furthermore, 39 soil files containing soil hydraulic parameters for each soil code in the shapefile were prepared according to the AquaCrop formats. Initial soil water contents were assumed to be at field capacity. To model the net irrigation water requirement of wheat, the "determination of net irrigation requirements" option was selected in AquaCrop to create an irrigation file. Other management effects such as fertilizer application and ground surface cover were disregarded. Groundwater was not considered due to lacking detail in the national dataset.

All the prepared climate, crop, soil, irrigation, and initial condition files were stored in a directory (can be several directories) which was specified in AquaCrop's project file (*.PRM). Then GeoSim was used to pass only the names of these files as spatial variables to the project file, rather than passing the specific numerous parameters for each input file. To further reduce the spatial variables, the climate files for each simulation were named as the same code of the meteorological station where the climate data were from. GeoSim passed a station code to different locations where the climate file names were required in the project file.

2.3. Identification of unique response units

The shapefiles for wheat distribution, meteorological station, AEZ, and soil were used to create a base polygon shapefile required by GeoSim. By intersecting these layers, a new shapefile with 116,801 polygons was generated. However, efficiency of spatial simulations could be improved by combining some of these polygons. For example, because the wheat distribution information was only used to indicate the location of wheat cropping, this spatial attribute information did not need to be passed to AquaCrop. The only required attributes for geospatial AquaCrop simulations, as managed by GeoSim, were meteorological station code, wheat type, soil code, and day numbers. As some polygons shared these attributes in common, there was opportunity to eliminate redundant AquaCrop simulations. To identify the unique response units, which were defined as polygons with unique combination of meteorological station code, wheat type, soil code, and day numbers, the "Dissolve" tool in QGIS was applied to merge polygons with the same information. Finally, only 6,915 polygons remained in the base shapefile to be modelled (Fig.2a). This demonstrates an advantage of using GeoSim within QGIS. By using QGIS tools to identify identical spatial zones, the efficiency of simulations managed by GeoSim could be improved. The input information for each polygon were appended in the different columns of the attribute table (Fig.2b), while 20 blank columns (two outputs with 10 years) were set up to receive output data (Fig.2c).



	Climate	Soil	Crop	2000day1	2000day2	2001day1	2001day2
1	50136	17	Spring_wheat	36271.00…	36419.00…	36636.00…	36784.00…
2	50246	4	Spring_wheat	36271.00…	36419.00…	36636.00…	36784.00…
3	50246	17	Spring_wheat	36271.00…	36419.00…	36636.00…	36784.00…
4	50247	4	Spring_wheat	36271.00…	36419.00…	36636.00…	36784.00…
5	50247	17	Spring_wheat	36271.00…	36419.00…	36636.00…	36784.00…
6	50349	17	Spring_wheat	36271.00…	36419.00…	36636.00…	36784.00…

	Irri2000	Yield2000	Irri2001	Yield2001	Irri2002	Yield2002	Irri2003	Y
1								
2								
3								
4								
5								
6								

Fig.2. The base polygon shapefile (a) and excerpts from the attribute table (b and c). The first three columns “Climate”, “Soil” and “Crop” in (b) indicate meteorological station codes, soil codes, and wheat type respectively, while remaining 20 columns indicate the day numbers, i.e. the first and last day numbers for the 10 years. (c) shows the blank spaces to be overwritten by the results from the output files. There were 20 columns for receiving all the target results, yield and irrigation estimates, for each of 10 years.

2.4. Template, instruction, and control files

In this study, GeoSim was applied to manage only the project file (*.PRM) of AquaCrop, which contains all the required information for simulations in successive years. The template file (*.gst) is a replicate of the AquaCrop's project file (*.PRM). Within the template file, "unique codes" were included at the locations of day numbers and the names of climate, crop, and soil files. Each unique code can be used more than once if the same information in the base shapefile needs to be passed to several locations in the template file. As this case study conducted simulations in 10 years, there were 10 sections indicating the simulation for each year in the template file. Prior to running a model for a polygon, GeoSim searched the template file for each unique code and overwrote it with the data value for that polygon.

An instruction file (*.gsi) was created to retrieve information from the AquaCrop output files that contained spatial results to be passed back to the base shapefile. The instruction file told GeoSim how to read the output files and extract the data values. There were 20 lines of commands to acquire the irrigation and yield results for each of the 10 years.

The control file (*.gsc) instructed GeoSim how to use the template and instruction files to control AquaCrop simulations for each polygon. In this file, the names of the attributes in the base shapefile and their corresponding unique codes in the template file were provided.

Excerpts from the template, instruction and control files are presented in Appendix A. Further information for developing these GeoSim files can be found in Thorp and Bronson (2013) and the GeoSim manual. After setting up the GeoSim files, GeoSim conducted the simulations for all the polygons in the base shapefile.

2.5. Post-processing of spatial outputs

As the model completed the simulations, results for wheat yield and irrigation requirement in each of the 10 years for each polygon were transferred from the model output files to the attribute table of the base shapefile. Then the "Vector Geoprocessor" tool within GeoSim was applied to calculate the mean values of irrigation and yield from 2000 to 2009, and the results were appended to the base shapefile.

To disaggregate the unique response units back to the original resolution, we intersected the base shapefile with the primary wheat distribution layer. This new shapefile contained 116,801 polygons as opposed to 6,915 polygons used during the modelling. The large number of spatial units equaled those resulting from the intersection of wheat distribution, meteorological station, AEZ, and soil layers (section 2.3), and also contained all the result attributes. The yield and irrigation attributes in the new shapefile were then converted to raster datasets with a resolution of 5 arc-minutes. By pairing native QGIS tools with GeoSim to improve the efficiency of spatial simulations, a novel method to develop national-scale maps of wheat yield and irrigation requirements was demonstrated.

3. Results and discussion

3.1. Case study

The total running time to complete 69,150 simulations (6,915 polygons with 10 years) was about 20 hours with single-core processing. Average results of wheat yield and net irrigation requirements from 2000 to 2009 for the modelled 6,915 polygons are presented in Appendix A. The grid-based results with a resolution of 5 arc-minutes are presented in Fig.3. By spatially applying AquaCrop using GeoSim, the detailed spatial and temporal variability of crop yield and irrigation requirements was easily demonstrated across China.

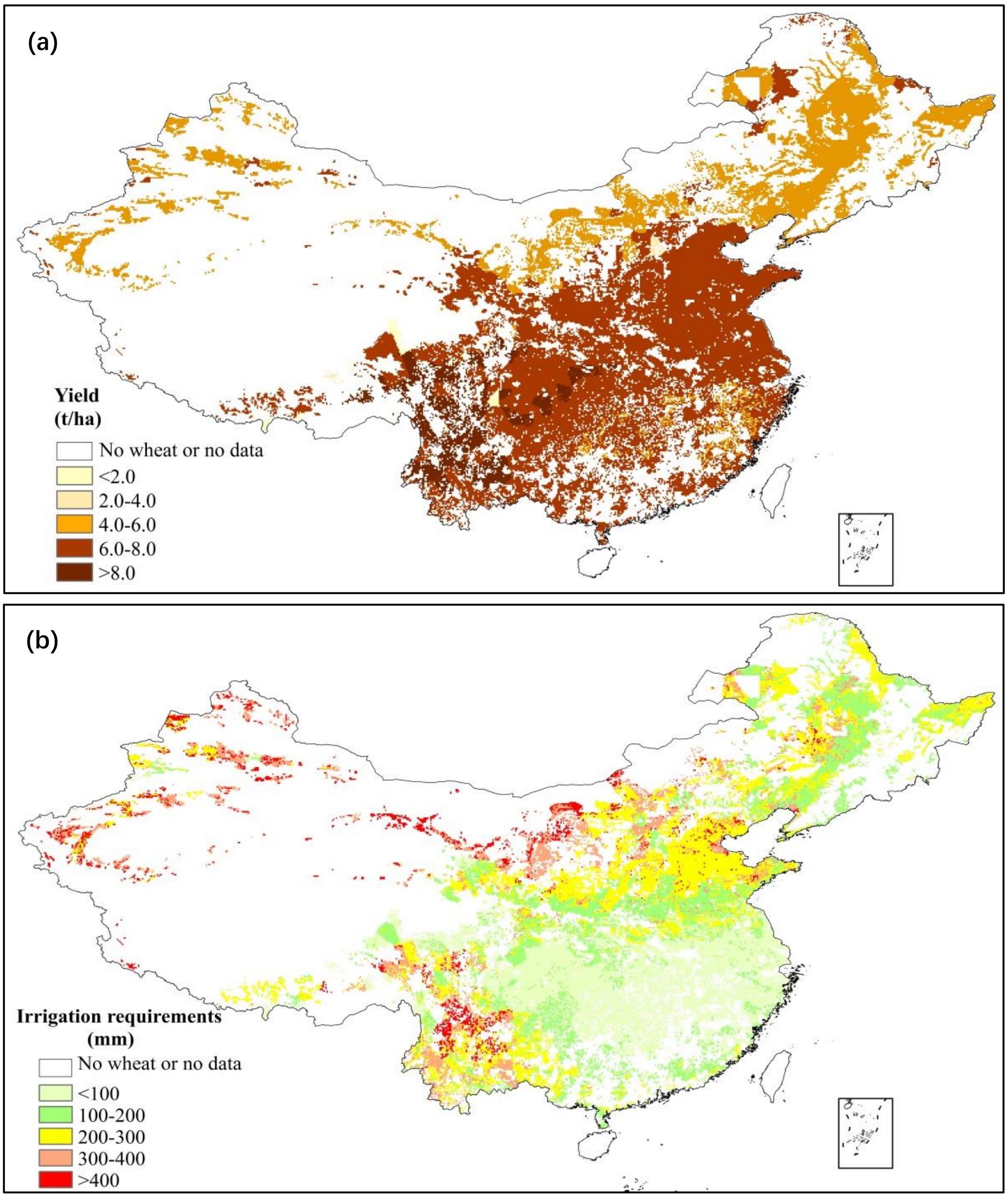


Fig.3. Average wheat yield (a) and net irrigation water requirements (b) during 2000-2009.

3.2. Advancement of GeoSim application

Previous application of GeoSim at the field scale used the tool to pass spatial input data to AquaCrop's soil file, initial soil water file, and irrigation files (Thorp and Bronson, 2013). However, for large spatiotemporal simulations at the national scale, a simpler approach was to pass spatial input data only to AquaCrop's project file. By setting up all of AquaCrop's input files in a specific directory, GeoSim was used to pass only four spatial variables (meteorological station code, crop type, soil code, and day numbers) to the project file. Although GeoSim can be used to pass any spatial input data required by AquaCrop, passing data to the climate and soil files would have resulted in a massive and cumbersome base shapefile and required several template files to receive these data. By directly incorporating spatial input data into unique climate and soil files and using GeoSim to adjust file names assigned to each spatial zone, this study demonstrated an efficient way to use a base shapefile with few columns and used only one template file. Thus, the effort for pre-processing the GeoSim files was greatly reduced. It also demonstrated the flexibility of GeoSim to be used in numerous different ways depending on the goals of simulation analysis.

To reduce the modelling time, 6,915 unique response units were identified in the base shapefile among the 116,801 primary polygons. Because QGIS allowed the post-processing of outputs, the original resolution of the analysis could be regained. By conducting simulations only for the unique spatial zones and subsequently expanding the simulation results to the primary zones, simulation efficiency was improved by over 16 times, while the primary spatial resolution was not changed. These pre-processing and post-processing activities demonstrated the advantage and flexibility of using GeoSim in combination with native QGIS functionality to achieve efficient simulation analyses at the national scale.

3.3. Comparison with alternative AquaCrop wrappers

Compared with AquaCrop-GIS (Lorite et al., 2013), which is currently recommended by FAO for a high number of simulations (http://www.fao.org/aquacrop), GeoSim significantly reduced the simulation time. AquaCrop-GIS uses an Excel spreadsheet to control AquaCrop, and it creates all the possible combinations of inputs for each polygon. Thereby, AquaCrop-GIS wastes time by doing irrelevant simulations. For example, it will do 5,393,700 simulations (6,915 polygons × 39 soils ×2 wheat types ×10 years) when applied for our case study. In contrast, GeoSim only passes polygon information to AquaCrop that is of interest for the study. Therefore, GeoSim required only 69,150 AquaCrop simulations, almost 80 times less. Moreover, it may be impossible for a modern desktop computer to complete all the 5,393,700 simulations with AquaCrop-GIS in a reasonable time. It would also be time consuming to split the work into several parts. Also, selecting targeted results from numerous output files would be cumbersome and time consuming with AquaCrop-GIS, but GeoSim automates this.

Foster et al. (2017) developed the AquaCrop-OS model, which also facilitates large numbers of AquaCrop simulations. However, this model is not GIS-based and requires the user to have programming experience. In addition, it has its own format requirements for input files and the user must define separate sets of input files for each simulation run. Unlike AquaCrop-OS, GeoSim does not change the formats of any input files required by AquaCrop. All GeoSim does is help users manage the geospatial model inputs and outputs within QGIS. A user who knows how to conduct the stand-alone AquaCrop simulations can easily learn to apply GeoSim for geospatial simulations.

4. Conclusions

By using native QGIS geo-processing functions with GeoSim, the efficiency of AquaCrop for conducting national-scale simulations was improved. The flexibility of GeoSim permits its implementation in numerous different ways depending on the goals of the analysis. Other tools exist for spatial extension of AquaCrop, but none could perform with the ease and efficiency of GeoSim. This study demonstrated a novel approach to apply GeoSim for national-scale spatiotemporal simulations with high resolution. GeoSim is a model-independent tool and it can always work with the latest version of the model. Also, as GeoSim was developed as open-source software, users can improve or expand the source code for customized purposes.

Acknowledgements

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Appendix A. Supplementary data

Supplementary data related to this article can be found at

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1. Data source

1.1. Wheat distribution

The national wheat distribution dataset with a resolution of 5 arc-minutes in the year 2000 was obtained from China's National Basic Research Program (Grant numbers: 2010CB9515) (personal communication). The development of the dataset was based on the statistics of wheat area at China's county level using a Spatial Production Allocation Model (Liu et al., 2013). The raster dataset was then converted to a vector dataset (Fig.A.1).

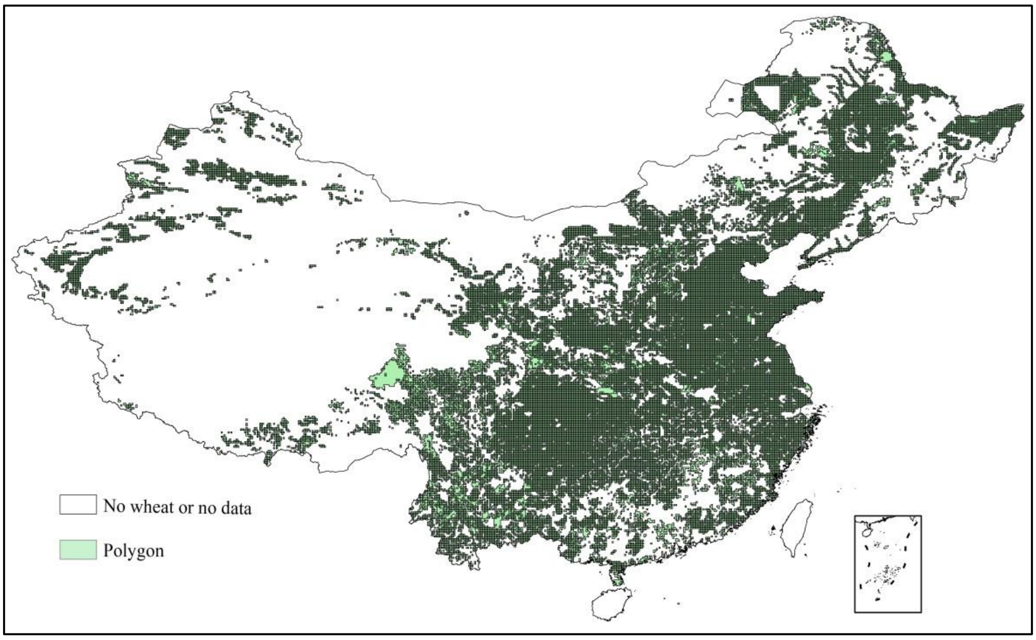

Fig.A.1. Polygon layer for wheat distribution. The total number of the polygons was 46,197. The wheat area in each polygon was higher than 0.

1.2. Climate data

Daily climate data from 825 meteorological stations across China from 2000 to 2009 were obtained from the National Meteorological Information Center (NMIC, http://data.cma.cn). Then input files for daily maximum and minimum temperature (*.TMP), precipitation (*.PLU), reference evapotranspiration (ET0) (*.ETo) which was calculated following the FAO-56 guidelines (Allen et al., 1998), as well as the covering climate files (*.CLI) were prepared and stored in a specific directory. The climate files for each simulation were named using the same code as the meteorological station where the data were from. The coordinates of the 825 meteorological stations were used to generate a raster dataset with a resolution of 5 arc-minutes by applying the Euclidean Allocation Tool (ArcGIS 10.2). The raster dataset was then converted as polygon layer containing the station codes (Fig.A.2). For atmospheric CO_2 concentrations, the default file which contains the mean annual atmospheric CO_2 concentration since 1958 in the AquaCrop database was used.

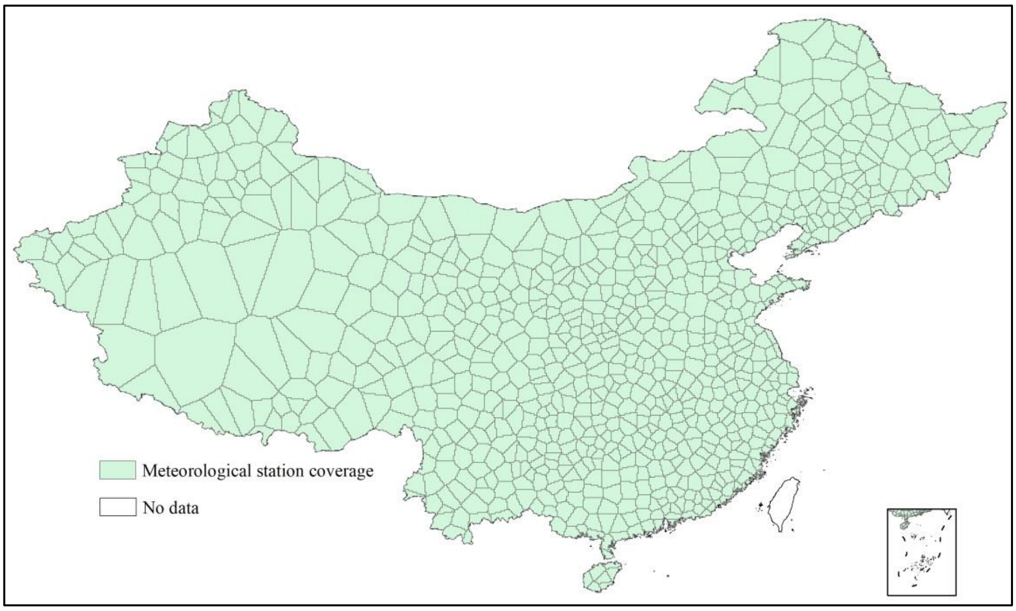

Fig.A.2. The polygon layer of the coverage of the 825 meteorological stations. Station codes were appended in a column titled “Climate” in the attribute table.

1.3. Crop parameters

Crop parameters including sowing dates, sowing density, growing stages and harvest dates were also obtained from the NMIC. But these data were not available for all the meteorological stations in wheat production areas. The other crop data such as crop transpiration, yield formation, and soil water stresses were based on the conservative wheat parameters provided by the AquaCrop reference manual and several studies which have calibrated and validated AquaCrop for both spring and winter wheat production modelling in

China (Chai, 2016; Fu, 2012; Iqbal et al., 2014; Jin et al., 2014; Liu, 2017; Ma et al., 2013; Xing, 2018; Yin, 2013; Zhao, 2017). Crop files (*. CRO) for both spring and winter wheat were prepared and stored in a specific directory. Day numbers which indicate the first and last days of cropping and simulation periods for each year were calculated based on the sowing and harvest dates. However, AquaCrop adjusted the "last day number" according to the temperature regimes of the distinctive years. If the calculated value of "last day number" was lower than the adjusted value by AquaCrop, the model simulation terminated before wheat maturity was reached. To avoid this problem, an extra 50 days was added to the harvest day to ensure that the last day of the crop cycle was always later than the crop maturity day. This study specified the simulation period as the same as the cropping period. Then the first and last day numbers were re-calculated as the average for each of China's agro-ecological zones (AEZs), which were defined based on climatic, soil and landform characteristics (Liu and Chen, 2010). Average first day numbers and last day numbers for each AEZ in each year were appended in the attribute table of the AEZ shapefile (Fig.A.3). The crop type which indicates whether the wheat was spring or winter wheat was also included in the attribute table of the AEZ shapefile.

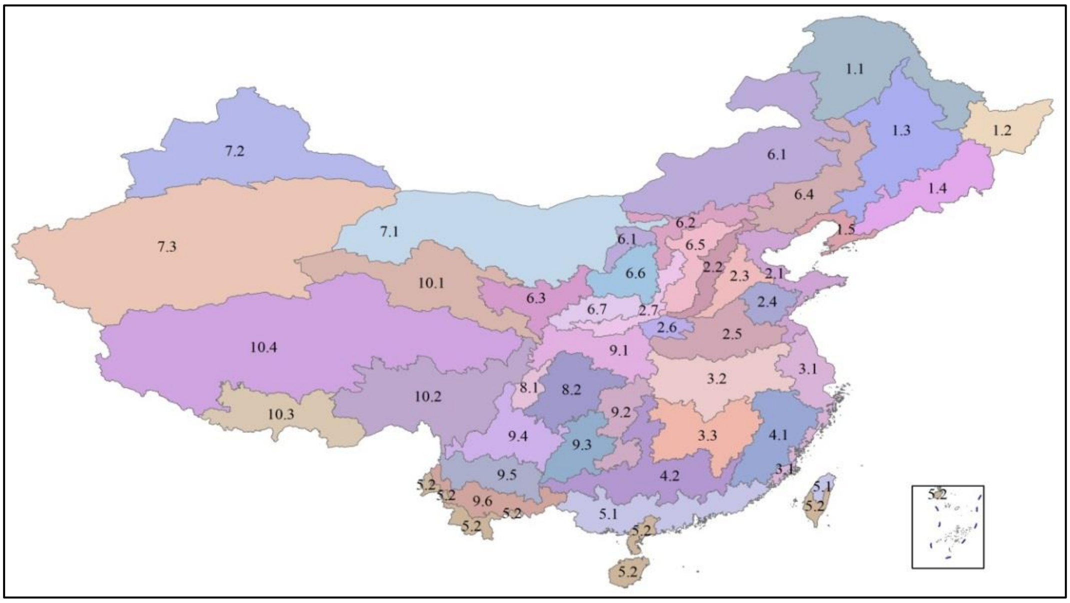

Fig.A.3. Polygon layer of China’s 41 agro-ecological zones (AEZ). The float number in the map indicates the code of each zone. Details for each zone can be found in Liu and Chen (2010). Annual average day numbers from 2000 to 2009 for each AEZ were appended in the attribute table.

1.4. Soil parameters

Primary soil data on the fraction of clay, sand and silt were obtained from the Harmonized World Soil Database (HWSD) (Wieder et al., 2014). Both topsoil (0-30 cm) and subsoil (30-100 cm) were presented in the raster dataset at 0.05-degree spatial resolution. Soil texture was identified by the USDA-developed Soil Texture Calculator (https://www.nrcs.usda.gov). A raster dataset containing 39 soil codes (combinations of the topsoil and subsoil texture) was obtained with a national coverage and resampled with a resolution of 5 arc-minutes. The raster data was then converted to a polygon layer (Fig.A.4). The indicative values of several soil hydraulic parameters for each soil type were obtained from the AquaCrop reference manual. Then 39 soil files (*.SOL) according to the 39 soil codes in the shapefile were prepared and stored in a specific directory.

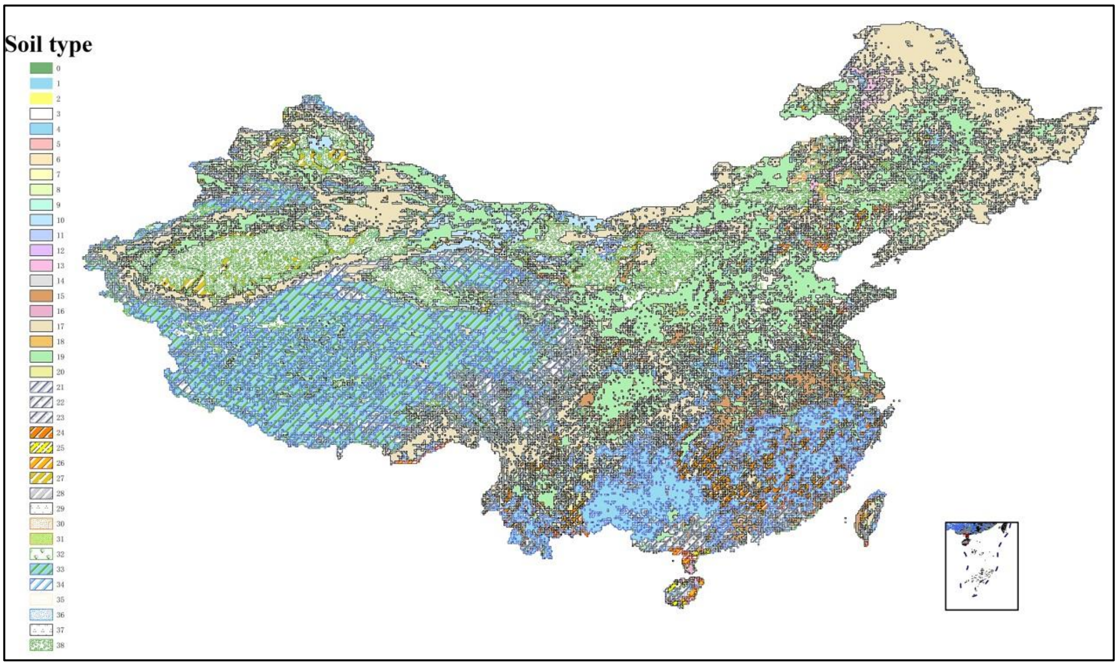

Fig.A.4. The polygon layer of China’s 39 soil types. Soil codes are appended in the attribute table.

1.5. Other parameters

To avoid modeling failures caused by low soil water content affecting the canopy senescence, the initial soil water contents were assumed to be at field capacity, which was the default value of AquaCrop. To model the net irrigation water requirement of wheat, the "determination of net irrigation requirements" option in AquaCrop was selected to create the irrigation file. The threshold for the allowable root zone depletion was set as 50% of readily available soil water, which can result in obtaining high wheat yield and avoiding irrigation water waste (Zhang et al., 2015).

2. Template, instruction and control files

The excerpts of template, instruction and control files are presented in Fig.A.5, Fig.A.6, and Fig.A.7, respectively.

(a)

```
Wheat.PRM.gst - Notepad
File  Edit  Format  View  Help
Geospatial Simulation Template (GST) File
Wheat 2000
      6.1        : AquaCrop Version (May 2018)
  #DAY11          : First day of simulation per
  #DAY12          : Last day of simulation per
  #DAY11          : First day of cropping peri
  #DAY12          : Last day of cropping perio
      4          : Evaporation decline factor f
      1.10       : Ke(x) Soil evaporation coeff
      5          : Threshold for green CC below
     70          : Starting depth of root zone
      5.00       : Maximum allowable root zone
     -6          : Shape factor for effect wate
     20          : Required soil water content
      1.0        : Adjustment factor for FAO-ad
      3          : Number of days after which d
      1.00       : Exponent of senescence facto
     12          : Decrease of p(sen) once ear
     10          : Thickness top soil (cm) in w
     30          : Depth [cm] of soil profile a
      0.30       : Considered depth (m) of soi
      1          : CN is adjusted to Antecedent
     20          : salt diffusion factor (capac
    100          : salt solubility [g/liter]
     16          : shape factor for effect of s
     12.0        : Default minimum temperature
     28.0        : Default maximum temperature
      3          : Default method for the calcu
-- 1. Climate (CLI) file
   #CLIM.CLI
   C:\AquaCrop\Climate\
   1.1 Temperature (TMP) file
   #CLIM.TMP
    C:\AquaCrop\Climate\
   1.2 Reference ET (ETo) file
   #CLIM.ETo
    C:\AquaCrop\Climate\
   1.3 Rain (PLU) file
   #CLIM.PLU
     C:\AquaCrop\Climate\
   1.4 Atmospheric CO2 (CO2) file
   MaunaLoa.CO2
     C:\AquaCrop\
-- 2. Crop (CRO) file
   #CROFILE.CRO
    C:\AquaCrop\
-- 3. Irrigation (IRR) file
   Irrigation.IRR
     C:\AquaCrop\
-- 4. Management (MAN) file
   (None)
   (None)
-- 5. Soil profile (SOL) file
    #SOLFILE.SOL
    C:\AquaCrop\Soil\
-- 6. Groundwater (GWT) file
   (None)
   (None)
-- 7. Initial conditions (SW0) file
   Wheat.SW0
     C:\AquaCrop\
-- 8. Off-season conditions (OFF) file
   (None)
   (None)
```

(b)

```
  #DAY21          : First day of simulation per
  #DAY22          : Last day of simulation per
  #DAY21          : First day of cropping perio
  #DAY22          : Last day of cropping perio
-- 1. Climate (CLI) file
   #CLIM.CLI
   C:\AquaCrop\Climate\
   1.1 Temperature (TMP) file
   #CLIM.TMP
    C:\AquaCrop\Climate\
   1.2 Reference ET (ETo) file
   #CLIM.ETo
    C:\AquaCrop\Climate\
   1.3 Rain (PLU) file
   #CLIM.PLU
     C:\AquaCrop\Climate\
   1.4 Atmospheric CO2 (CO2) file
   MaunaLoa.CO2
     C:\AquaCrop\
-- 2. Crop (CRO) file
   #CROFILE.CRO
    C:\AquaCrop\
-- 3. Irrigation (IRR) file
   Irrigation.IRR
     C:\AquaCrop\
-- 4. Management (MAN) file
   (None)
   (None)
-- 5. Soil profile (SOL) file
    #SOLFILE.SOL
    C:\AquaCrop\Soil\
-- 6. Groundwater (GWT) file
   (None)
   (None)
-- 7. Initial conditions (SW0) file
   Wheat.SW0
     C:\AquaCrop\
-- 8. Off-season conditions (OFF) file
   (None)
   (None)
```

Fig.A.5. Excerpts from the template file (*.gst). (a) shows the first section for the first year simulation and (b) shows the second section for the second year simulation. In total, there are 10 sections for 10-year simulations. The locations of the unique codes which start with "#" are where day numbers, climate code, crop code and soil code will be overwritten, respectively.

```
WheatPRMseason.OUT.gsi - Notepad
File  Edit  Format  View  Help
Geospatial Simulation Instruction (GSI) File
Irri2000,Plus4,Get73:82
Yield2000,Plus4,Get294:303
Irri2001,Plus5,Get73:82
Yield2001,Plus5,Get294:303
Irri2002,Plus6,Get73:82
Yield2002,Plus6,Get294:303
Irri2003,Plus7,Get73:82
Yield2003,Plus7,Get294:303
Irri2004,Plus8,Get73:82
Yield2004,Plus8,Get294:303
Irri2005,Plus9,Get73:82
Yield2005,Plus9,Get294:303
Irri2006,Plus10,Get73:82
Yield2006,Plus10,Get294:303
Irri2007,Plus11,Get73:82
Yield2007,Plus11,Get294:303
Irri2008,Plus12,Get73:82
Yield2008,Plus12,Get294:303
Irri2009,Plus13,Get73:82
Yield2009,Plus13,Get294:303
```

Fig.A.6. Excerpt from the instruction file (*.gsi). The commands of “plus” and “get” were applied to acquire the target data values. Further information can be found in GeoSim user’s manual.

```
Wheat.gsc - Notepad
File  Edit  Format  View  Help
Geospatial Simulation Control (GSC) File

*GSC1: ModelDirectory
C:\AquaCrop\

*GSC2: BaseLayer
wheat_shapefile

*GSC3: TemplateFile,InputFile
LIST\\wheat.PRM.gst,LIST\\wheat.PRM

*GSC4: InputAttribute,Code
Climate,#CLIM
Soil,#SOLFILE
Crop,#CROFILE
2000day1,#DAY11
2000day2,#DAY12
2001day1,#DAY21
2001day2,#DAY22
2002day1,#DAY31
2002day2,#DAY32
2003day1,#DAY41
2003day2,#DAY42
2004day1,#DAY51
2004day2,#DAY52
2005day1,#DAY61
2005day2,#DAY62
2006day1,#DAY71
2006day2,#DAY72
2007day1,#DAY81
2007day2,#DAY82
2008day1,#DAY91
2008day2,#DAY92
2009day1,#DAY01
2009day2,#DAY02

*GSC5: InstructionFile,OutputFile
OUTP\\wheatPRMseason.OUT.gsi,OUTP\\wheatPRMseason.OUT

*GSC6: OutputAttribute,Type

Irri2000,real(4.1)
Yield2000,real(4.3)
Irri2001,real(4.1)
Yield2001,real(4.3)
Irri2002,real(4.1)
Yield2002,real(4.3)
Irri2003,real(4.1)
Yield2003,real(4.3)
Irri2004,real(4.1)
Yield2004,real(4.3)
Irri2005,real(4.1)
Yield2005,real(4.3)
Irri2006,real(4.1)
Yield2006,real(4.3)
Irri2007,real(4.1)
Yield2007,real(4.3)
Irri2008,real(4.1)
Yield2008,real(4.3)
Irri2009,real(4.1)
Yield2009,real(4.3)

*GSC7: CommandLine
ACsav60.exe
```

Fig.A7. Excerpt from the control file (*.gsc).

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Appendix A. Supplementary information

1. Data source

1.1. Wheat distribution

The national wheat distribution dataset with a resolution of 5 arc-minutes in the year 2000 was obtained from China's National Basic Research Program (Grant numbers: 2010CB9515) (personal communication). The development of the dataset was based on the statistics of wheat area at China's county level using a Spatial Production Allocation Model (Liu et al., 2013). The raster dataset was then converted to a vector dataset (Fig.A.1).

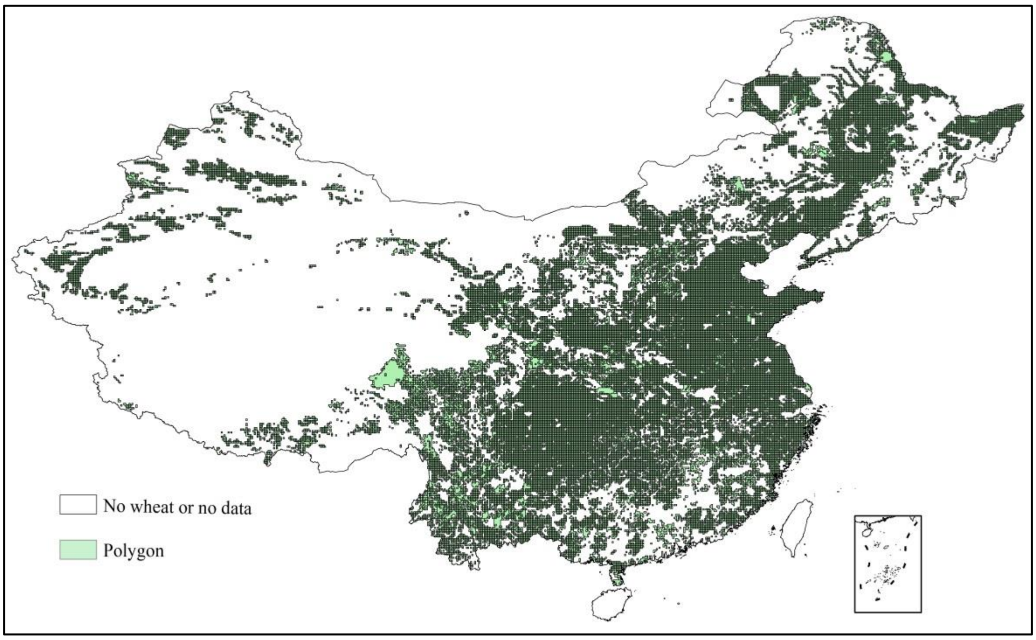

Fig.A.1. Polygon layer for wheat distribution. The total number of the polygons was 46,197. The wheat area in each polygon was higher than 0.

1.2. Climate data

Daily climate data from 825 meteorological stations across China from 2000 to 2009 were obtained from the National Meteorological Information Center (NMIC, http://data.cma.cn). Then input files for daily maximum and minimum temperature (*.TMP), precipitation (*.PLU), reference evapotranspiration (ET0) (*.ETo) which was calculated following the FAO-56 guidelines (Allen et al., 1998), as well as the covering climate files (*.CLI) were prepared and stored in a specific directory. The climate files for each simulation were named using the same code as the meteorological station where the data were from. The coordinates of the 825 meteorological stations were used to generate a raster dataset with a resolution of 5 arc-minutes by applying the Euclidean Allocation Tool (ArcGIS 10.2). The raster dataset was then converted as polygon layer containing the station codes (Fig.A.2). For atmospheric CO_2 concentrations, the default file which contains the mean annual atmospheric CO_2 concentration since 1958 in the AquaCrop database was used.

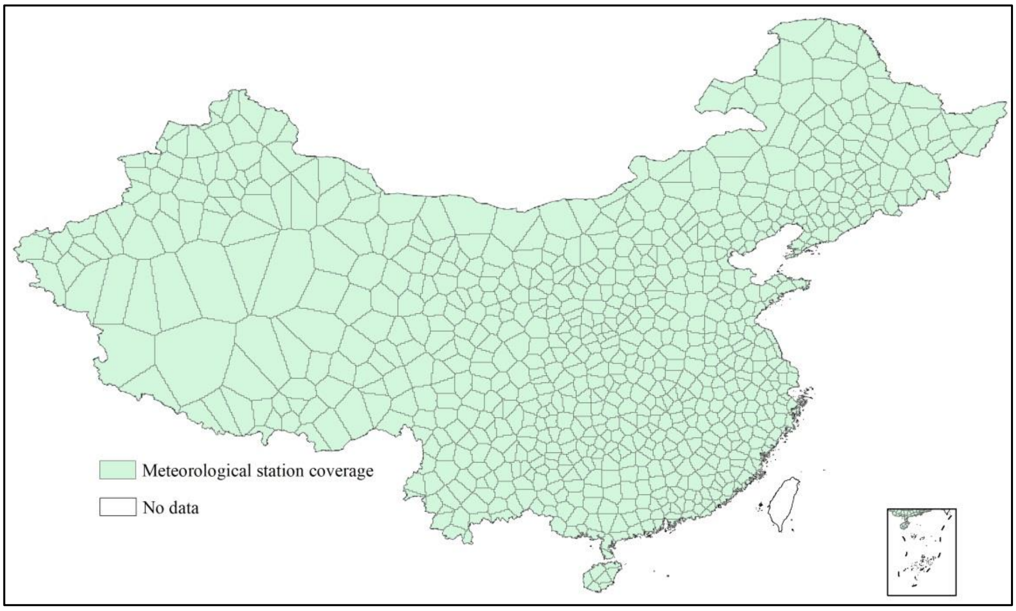

Fig.A.2. The polygon layer of the coverage of the 825 meteorological stations. Station codes were appended in a column titled “Climate” in the attribute table.

1.3. Crop parameters

Crop parameters including sowing dates, sowing density, growing stages and harvest dates were also obtained from the NMIC. But these data were not available for all the meteorological stations in wheat production areas. The other crop data such as crop transpiration, yield formation, and soil water stresses were based on the conservative wheat parameters provided by the AquaCrop reference manual and several studies which have calibrated and validated AquaCrop for both spring and winter wheat production modelling in China (Chai, 2016; Fu, 2012; Iqbal et al., 2014; Jin et al., 2014; Liu, 2017; Ma et al., 2013; Xing, 2018; Yin, 2013; Zhao, 2017). Crop files (*. CRO) for both spring and winter wheat were prepared and stored in a specific directory. Day numbers which indicate the first and last days of cropping and simulation periods for each year were calculated based on the sowing and harvest dates. However, AquaCrop adjusted the “last day number” according to the temperature regimes of the distinctive years. If the calculated value of “last day number” was lower than the adjusted value by AquaCrop, the model simulation terminated before wheat maturity was reached. To avoid this problem, an extra 50 days was added to the harvest day to ensure that the last day of the crop cycle was always later than the crop maturity day. This study specified the simulation period as the same as the cropping period. Then the first and last day numbers were re-calculated as the average for each of China’s agro-ecological zones (AEZs), which were defined based on climatic, soil and landform characteristics (Liu and Chen, 2010). Average first day numbers and last day numbers for each AEZ in each year were appended in the attribute table of the AEZ shapefile (Fig.A.3). The crop type which indicates whether the wheat was spring or winter wheat was also included in the attribute table of the AEZ shapefile.

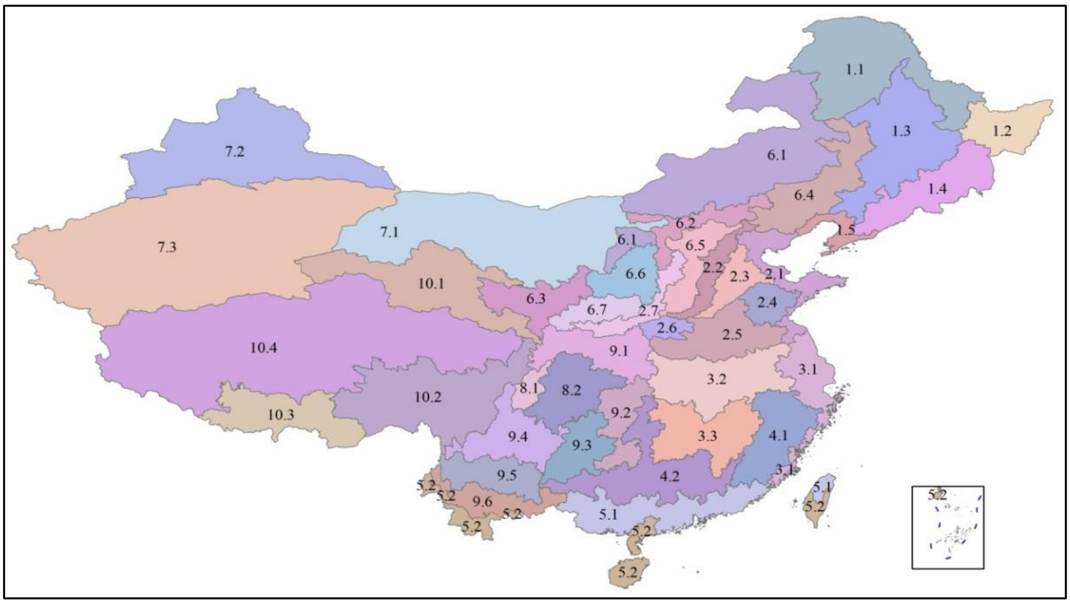

Fig.A.3. Polygon layer of China's 41 agro-ecological zones (AEZ). The float number in the map indicates the code of each zone. Details for each zone can be found in Liu and Chen (2010). Annual average day numbers from 2000 to 2009 for each AEZ were appended in the attribute table.

1.4. Soil parameters

Primary soil data on the fraction of clay, sand and silt were obtained from the Harmonized World Soil Database (HWSD) (Wieder et al., 2014). Both topsoil (0-30 cm) and subsoil (30-100 cm) were presented in the raster dataset at 0.05-degree spatial resolution. Soil texture was identified by the USDA-developed Soil Texture Calculator (https://www.nrcs.usda.gov). A raster dataset containing 39 soil codes (combinations of the topsoil and subsoil texture) was obtained with a national coverage and resampled with a resolution of 5 arc-minutes. The raster data was then converted to a polygon layer (Fig.A.4). The indicative values of several soil hydraulic parameters for each soil type were obtained from the AquaCrop reference manual. Then 39 soil files (*.SOL) according to the 39 soil codes in the shapefile were prepared and stored in a specific directory.

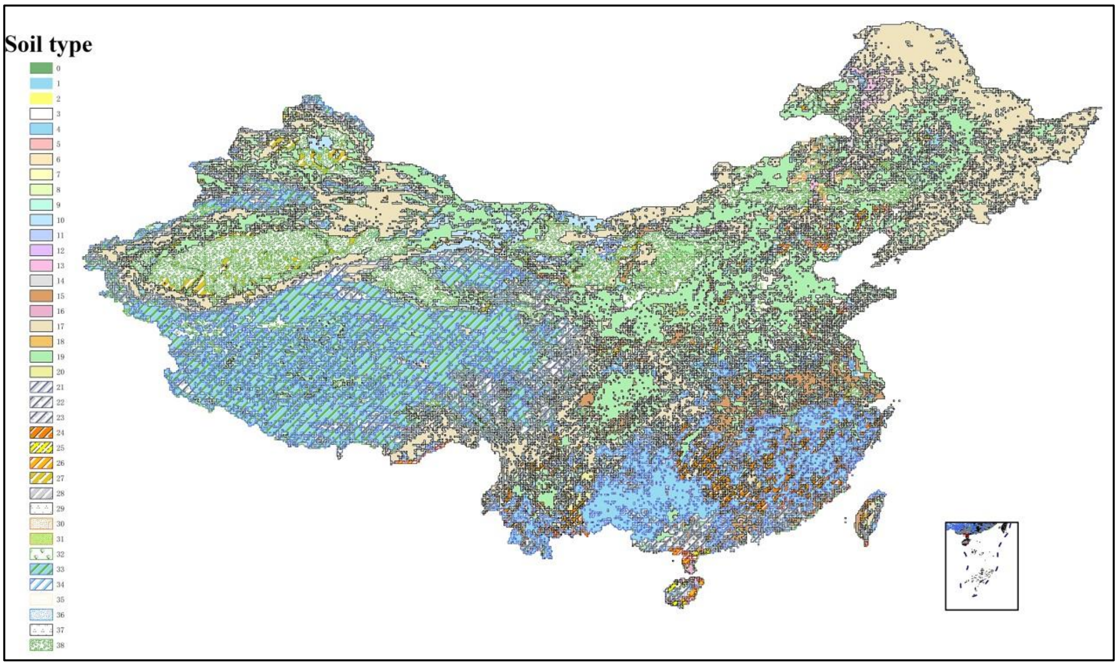

Fig.A.4. The polygon layer of China's 39 soil types. Soil codes are appended in the attribute table.

1.5. Other parameters

To avoid modeling failures caused by low soil water content affecting the canopy senescence, the initial soil water contents were assumed to be at field capacity, which was the default value of AquaCrop. To model the net irrigation water requirement of wheat, the "determination of net irrigation requirements" option in AquaCrop was selected to create the irrigation file. The threshold for the allowable root zone depletion was set as 50% of readily available soil water, which can result in obtaining high wheat yield and avoiding irrigation water waste (Zhang et al., 2015).

2. Template, instruction and control files

The excerpts of template, instruction and control files are presented in Fig.A.5, Fig.A.6, and Fig.A.7, respectively.

(a)

```
Wheat.PRM.gst - Notepad
File  Edit  Format  View  Help
Geospatial Simulation Template (GST) File
Wheat 2000
      6.1       : AquaCrop Version (May 2018)
  #DAY11         : First day of simulation per
  #DAY12         : Last day of simulation per
  #DAY11         : First day of cropping peri
  #DAY12         : Last day of cropping perio
       4        : Evaporation decline factor f
       1.10     : Ke(x) Soil evaporation coef
       5        : Threshold for green CC belo
      70        : Starting depth of root zone
       5.00     : Maximum allowable root zone
      -6        : Shape factor for effect wat
      20        : Required soil water content
       1.0      : Adjustment factor for FAO-a
       3        : Number of days after which
       1.00     : Exponent of senescence fact
      12        : Decrease of p(sen) once ear
      10        : Thickness top soil (cm) in
      30        : Depth [cm] of soil profile
       0.30     : Considered depth (m) of soi
       1        : CN is adjusted to Antecedent
      20        : salt diffusion factor (capa
     100        : salt solubility [g/liter]
      16        : shape factor for effect of
      12.0      : Default minimum temperature
      28.0      : Default maximum temperature
       3        : Default method for the calc
-- 1. Climate (CLI) file
   #CLIM.CLI
   C:\AquaCrop\Climate\
   1.1 Temperature (TMP) file
   #CLIM.TMP
    C:\AquaCrop\Climate\
   1.2 Reference ET (ETo) file
   #CLIM.ETo
    C:\AquaCrop\Climate\
   1.3 Rain (PLU) file
   #CLIM.PLU
     C:\AquaCrop\Climate\
   1.4 Atmospheric CO2 (CO2) file
   MaunaLoa.CO2
     C:\AquaCrop\
-- 2. Crop (CRO) file
   #CROFILE.CRO
    C:\AquaCrop\
-- 3. Irrigation (IRR) file
   Irrigation.IRR
     C:\AquaCrop\
-- 4. Management (MAN) file
   (None)
   (None)
-- 5. Soil profile (SOL) file
    #SOLFILE.SOL
    C:\AquaCrop\Soil\
-- 6. Groundwater (GWT) file
   (None)
   (None)
-- 7. Initial conditions (SW0) file
   Wheat.SW0
     C:\AquaCrop\
-- 8. Off-season conditions (OFF) file
   (None)
   (None)
```

(b)

```
  #DAY21         : First day of simulation per
  #DAY22         : Last day of simulation per
  #DAY21         : First day of cropping peri
  #DAY22         : Last day of cropping perio
-- 1. Climate (CLI) file
   #CLIM.CLI
   C:\AquaCrop\Climate\
   1.1 Temperature (TMP) file
   #CLIM.TMP
    C:\AquaCrop\Climate\
   1.2 Reference ET (ETo) file
   #CLIM.ETo
    C:\AquaCrop\Climate\
   1.3 Rain (PLU) file
   #CLIM.PLU
     C:\AquaCrop\Climate\
   1.4 Atmospheric CO2 (CO2) file
   MaunaLoa.CO2
     C:\AquaCrop\
-- 2. Crop (CRO) file
   #CROFILE.CRO
    C:\AquaCrop\
-- 3. Irrigation (IRR) file
   Irrigation.IRR
     C:\AquaCrop\
-- 4. Management (MAN) file
   (None)
   (None)
-- 5. Soil profile (SOL) file
    #SOLFILE.SOL
    C:\AquaCrop\Soil\
-- 6. Groundwater (GWT) file
   (None)
   (None)
-- 7. Initial conditions (SW0) file
   Wheat.SW0
     C:\AquaCrop\
-- 8. Off-season conditions (OFF) file
   (None)
   (None)
```

Fig.A.5. Excerpts from the template file (*.gst). (a) shows the first section for the first year simulation and (b) shows the second section for the second year simulation. In total, there are 10 sections for 10-year simulations. The locations of the unique codes which start with "#" are where day numbers, climate code, crop code and soil code will be overwritten, respectively.

```
WheatPRMseason.OUT.gsi - Notepad
File  Edit  Format  View  Help
Geospatial Simulation Instruction (GSI) File
Irri2000,Plus4,Get73:82
Yield2000,Plus4,Get294:303
Irri2001,Plus5,Get73:82
Yield2001,Plus5,Get294:303
Irri2002,Plus6,Get73:82
Yield2002,Plus6,Get294:303
Irri2003,Plus7,Get73:82
Yield2003,Plus7,Get294:303
Irri2004,Plus8,Get73:82
Yield2004,Plus8,Get294:303
Irri2005,Plus9,Get73:82
Yield2005,Plus9,Get294:303
Irri2006,Plus10,Get73:82
Yield2006,Plus10,Get294:303
Irri2007,Plus11,Get73:82
Yield2007,Plus11,Get294:303
Irri2008,Plus12,Get73:82
Yield2008,Plus12,Get294:303
Irri2009,Plus13,Get73:82
Yield2009,Plus13,Get294:303
```

Fig.A.6. Excerpt from the instruction file (*.gsi). The commands of “plus” and “get” were applied to acquire the target data values. Further information can be found in GeoSim user’s manual.

```
Wheat.gsc - Notepad
File  Edit  Format  View  Help
Geospatial Simulation Control (GSC) File

*GSC1: ModelDirectory
C:\AquaCrop\

*GSC2: BaseLayer
Wheat_shapefile

*GSC3: TemplateFile,InputFile
LIST\\Wheat.PRM.gst,LIST\\Wheat.PRM

*GSC4: InputAttribute,Code
Climate,#CLIM
Soil,#SOLFILE
Crop,#CROFILE
2000day1,#DAY11
2000day2,#DAY12
2001day1,#DAY21
2001day2,#DAY22
2002day1,#DAY31
2002day2,#DAY32
2003day1,#DAY41
2003day2,#DAY42
2004day1,#DAY51
2004day2,#DAY52
2005day1,#DAY61
2005day2,#DAY62
2006day1,#DAY71
2006day2,#DAY72
2007day1,#DAY81
2007day2,#DAY82
2008day1,#DAY91
2008day2,#DAY92
2009day1,#DAY01
2009day2,#DAY02

*GSC5: InstructionFile,OutputFile
OUTP\\WheatPRMseason.OUT.gsi,OUTP\\WheatPRMseason.OUT

*GSC6: OutputAttribute,Type

Irri2000,real(4.1)
Yield2000,real(4.3)
Irri2001,real(4.1)
Yield2001,real(4.3)
Irri2002,real(4.1)
Yield2002,real(4.3)
Irri2003,real(4.1)
Yield2003,real(4.3)
Irri2004,real(4.1)
Yield2004,real(4.3)
Irri2005,real(4.1)
Yield2005,real(4.3)
Irri2006,real(4.1)
Yield2006,real(4.3)
Irri2007,real(4.1)
Yield2007,real(4.3)
Irri2008,real(4.1)
Yield2008,real(4.3)
Irri2009,real(4.1)
Yield2009,real(4.3)

*GSC7: CommandLine
ACsaV60.exe
```

Fig.A7. Excerpt from the control file (*.gsc).

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