SIMPLE-G: A Multiscale Framework for Integration of Economic and Biophysical Determinants of Sustainability

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Abstract: We introduce SIMPLE-G, a Simplified International Model of agricultural Prices, Land use, and the Environment- Gridded version, which is a novel tool for evaluating sustainability policies in a global context, while factoring in local heterogeneity in land and water resources and natural ecosystem services. This multi-scale model can provide boundary conditions for local decision makers, as well as capturing feedbacks from local policies to national and global scales. To illustrate its value in environmental analysis, we provide two applications of the model. First, we quantify the local stresses on land and water resources due to global changes in population, income, and productivity. Second, we quantify the global impacts of local policy responses and adaptations to water scarcity.

Highlights:

- Novel global-to-local-to-global modelling framework introduced
- Model condensation permits rapid solution with millions of grid cells
- GeoHub implementation allows users to run the model and explore results via the web
- Subtotals allow for attribution of local stresses to individual global change drivers

Keywords: Sustainability, agriculture, environmental stresses, multiscale modelling, global change, water scarcity

Software and data availability: SIMPLE-G web application, SIMPLE-G-US web application

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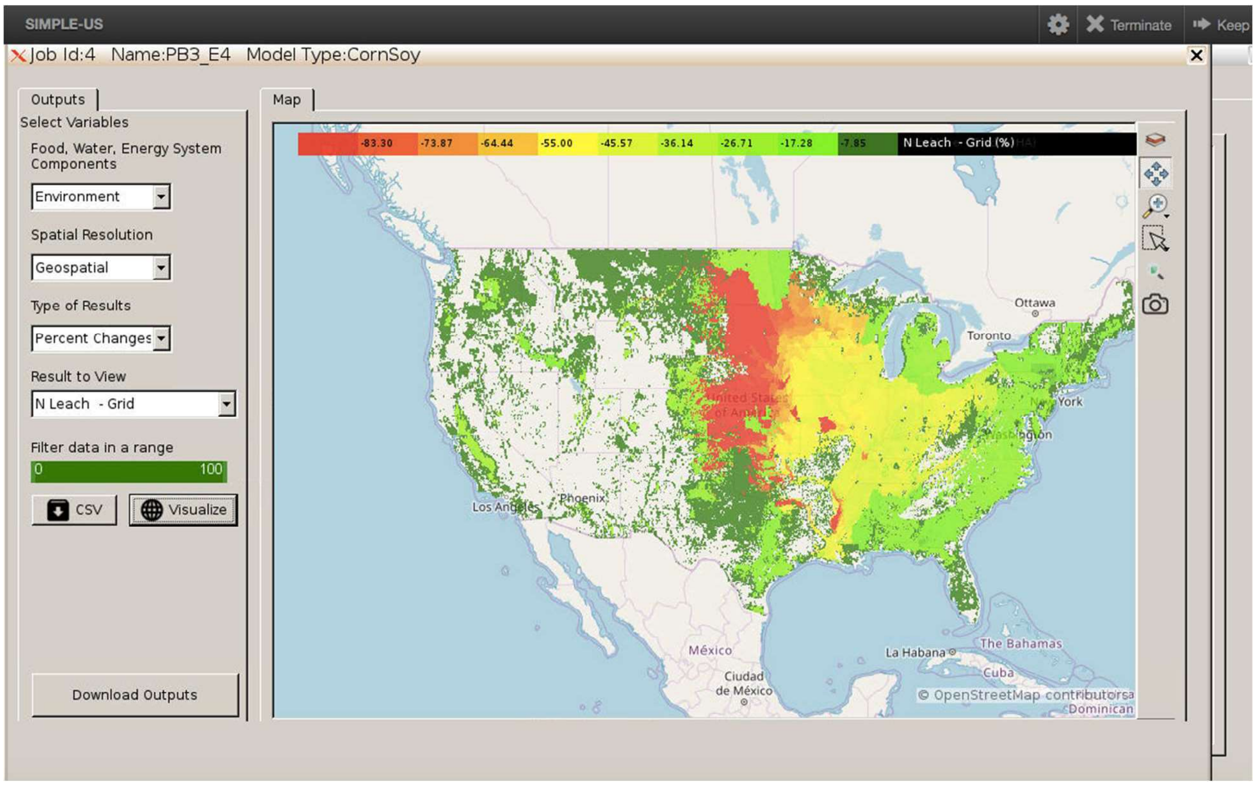
Graphical abstract:



A sample window from web application of SIMPLE-G-US: https://mygeohub.org/tools/simpleus

Outline

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1 INTRODUCTION

The world faces significant sustainability challenges in the decades ahead (United Nations, 2019). Growing populations and rising incomes are placing unprecedented stresses on the planetary boundaries, with the world's land and water resources at growing risk (Steffen et al., 2015). The challenge posed in making such assessments is that the sustainability stresses do not respect disciplinary boundaries. Furthermore, while the stresses are often highly localized, the drivers of these stresses are global, and the local responses can feed back to national and global outcomes. For this reason, assessment of the underlying risks as well as potential solutions, is typically undertaken with a suite of models using complex approaches that often preclude replication and use by researchers outside the core group (Obersteiner et al., 2016; Springmann et al., 2018).

Up to this point, there have been just a few open-source, bottom-up, economic-environmental modelling framework capable of analyzing global sustainability at the resolution of individual grid cells (Lotze-Campen et al., 2008; Valin et al., 2013). There is clearly a tradeoff between complexity and accessibility. Models used in teaching and academic research are generally simpler than those developed by national and international labs and research institutions. Having a relatively simple, global, grid-resolving sustainability framework that can be also run 'in-cloud' will allow wider participation in sustainability discussions and can facilitate greater crowd-sourcing of new ideas, data and parameters to enrich the representation of local stresses, policies and adaptations. This paper introduces such a modelling framework: SIMPLE-G, a Simplified International Model of agricultural Prices, Land use, and the Environment-Gridded version.

The SIMPLE-G framework allows for analysis of the interplay between economic and environmental systems, taking account of the actions of local agricultural producers pertaining to land and water use, within the context of regional and global commodity markets. This model integrates economic theories with environmental sciences to analyze the biophysical and economic impacts at different geospatial scales. The economic supply of land and water takes account of local institutions, biophysical characteristics, sustainability criteria, along with maximum available resources. As a consequence, heterogeneity in local constraints leads to different rates of change in land and water use. On the demand side, growth in income and population lead to changes in food consumption baskets and changes in agricultural trade patterns.

Integrating the human and earth system analysis within a global economic framework is a challenging task and often focuses on one-way linkages, such as those used in down-scaling regional results to a grid cell level (Reilly et al., 2012). It has also been common practice to extrapolate from sophisticated grid-level analysis to national scale by assuming that the share of production or land use is unchanging (Schlenker & Roberts, 2009). Bridging local, national and global scales within a single framework is challenging, yet it is essential if we wish to bring into consideration the behavior of local decision makers within the context of global sustainability analysis. In the SIMPLE-G framework laid out here, these decisions are made endogenously considering local biophysical characteristics and institutions as well as nationally determined input prices and globally determined commodity prices.

Despite computational advances, model solution time remains another major challenge for integrated frameworks – particularly those utilized by individual researchers without access to high performance computing at national labs and major research institutions. With SIMPLE-G, we introduce a solution strategy that dramatically reduces computing time, permitting individuals to solve a version of SIMPLE-G with a million grid cells in a matter of minutes on a desktop computer. Furthermore, by implementing SIMPLE-G on one of the NSF-funded HubZero sites (GeoHub), we have made the model, along with visualization software, readily available to any user with access to a web browser. This greatly expands access to multi-scale modelling of sustainability challenges at the interface of agriculture and the environment. It should also accelerate the development of new and improved data bases and representations of local institutions and other constraints within this framework.

To the versatility of SIMPLE-G in sustainability analysis, we highlight an implementation of this framework wherein the US has been broken out in detail (5 arc minutes), while other regions are aggregated. Previous applications have disaggregated the globe uniformly (30 arc minutes) (Liu et al., 2017). We undertake two experiments aimed at highlighting two different types of analysis that can be undertaken with SIMPLE-G. In the first, we investigate the contribution of global changes in population, technology, and income to change in gridded US water and land use by mid-century. It includes global demand shocks as well as local supply responses. This highlights locations most vulnerable to land and water stresses. Furthermore, we tie these stresses to individual global change drivers, including, for example, population growth in Africa or income growth in Asia. By linking local environmental stresses in the US to global change drivers, we underscore the essence of 21st century global sustainability challenges.

In a second application of the SIMPLE-G framework, we focus on the local-to-global feedbacks associated with sustainability polices. In this case, we begin with the projections made in the first experiment, but now we overlay a location-specific sustainability policy. In particular, we do not allow irrigation withdrawals to increase from the present day in those grid cells where withdrawals currently exceed recharge rates. We then explore how these sustainability restrictions alter global prices, production, consumption and trade.

The remainder of the paper is organized as follows. Section two provides an overview of the model. Section three introduces the diverse information used in the construction of the database and parameters for SIMPLE-G-US. Section four describes the software and implementation of this model. Section five explores the two experiments mentioned above and the final section provides further discussion and conclusions.

2 MODEL

The SIMPLE-G model is based on SIMPLE, a Simplified International Model of agricultural Prices, Land use, and the Environment (Baldos & Hertel, 2013; Hertel & Baldos 2016). This is a partial equilibrium agricultural trade model which has been validated for the study of long run sustainability and food security (Hertel & Baldos 2016; Baldos & Hertel, 2014). We extend the SIMPLE model to include gridded biophysical and economic relationships – hence the name, SIMPLE-G. This model is multi-scale. In other words, it simultaneously solves for outcomes at the level of tens of thousands of grid cells within a region, at the same time global market equilibrium is also enforced. This allows SIMPLE-G to explicitly incorporate local heterogeneity in climate, soils, water and regulatory institutions while also capturing global change drivers and feedbacks for local adaptations to national and international markets.

At each grid cell, land and water resources comprise the linkage to the environment and natural ecosystems. We model economically motivated changes in land use as well as changes in water withdrawals which reflect differential resource availability and constraints. Figure 1 summarizes the main demand and supply components of the SIMPLE-G model. The model solves for equilibrium quantities and prices for land and nonland inputs as well as for irrigation water, and crop outputs. Equilibrium water withdrawals are endogenously determined at each grid cell assuming a grid cell-specific shadow price for water within the grid cell. Crop prices are permitted to vary by region based on the extent of domestic market segmentation from the world market.

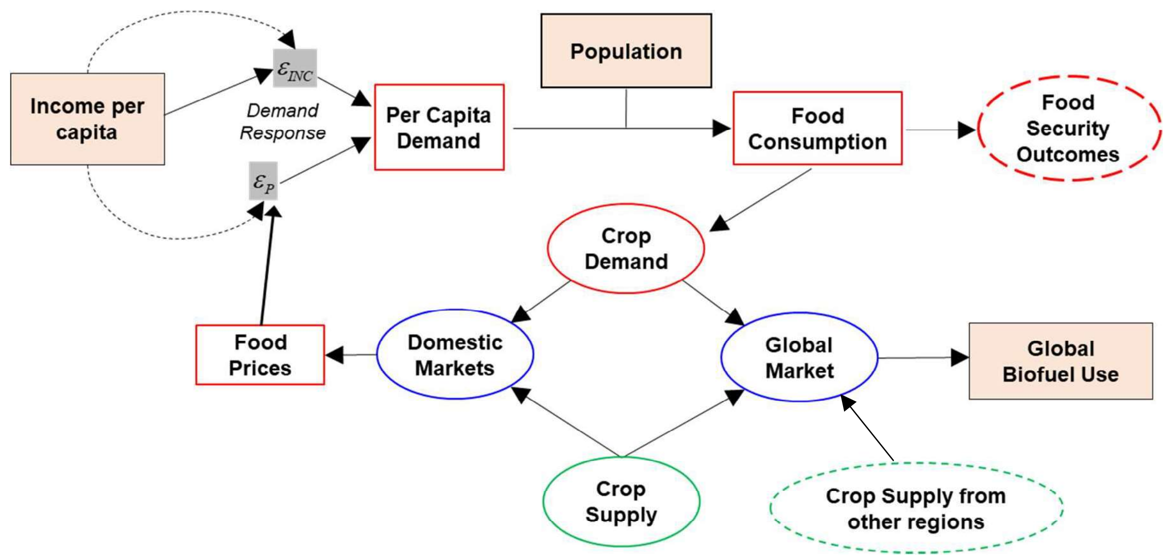


Figure 1. Structure of regional food demand in SIMPLE-G model

2.1 Global socioeconomic determinants of crop demand

At regional scale, the consumption of different commodities is a function of population, income, prices and biofuels. Prices are determined endogenously as a function of supply and demand while population and income changes are exogenous to the model with increases in per capita income driving diet changes. Population, income and biofuels production can be specified to follow long run growth scenarios such as the Shared Socioeconomic Pathways (SSPs) or other global economic projections. Within this framework global food and agricultural markets link the changes in population, income and diets to gridded crop production and associated stresses on land and water resources.

One of the best understood pattern of economic development is Engel's Law, which states that, as per capita income rises, the share of income devoted to food will fall (Clements & Chen, 1996). SIMPLE-G captures this relationship by allowing the income elasticity of demand for food (ε_i^y, the propensity to spend incremental income on food) to evolve with per capita income (Y), based on the estimated parameters, α_i^y and β_i^y, and similarly for the price elasticity of food demand (ε_i^p):

$$(1)\ \varepsilon_i^y = \alpha_i^y + \beta_i^y \ln Y$$

$$(2)\ \varepsilon_i^p = \alpha_i^p + \beta_i^p \ln Y$$

Equations (1) and (2) are indexed by type of food demand (*i*) and SIMPLE-G distinguishes between direct consumption of crops and indirect consumption through either livestock product consumption or processed food consumption. This results in the following equations describing the evolution of per capita demands for each type of food product[1]:

$$(3)\ q_i = \varepsilon_i^p p_i + \varepsilon_i^y y$$

Total demand for crops in a given region is found by first multiplying each per capita demand by population in the region and then summing the total direct demand for crops in final consumption together with the indirect demands in livestock and food processing. To this total we also add the demand for crops in biofuel production – a derived demand that we assume to be exogenously determined by government mandates. The livestock and food processing sector demands for crops are endogenous and modeled using Constant Elasticity of Substitution (CES) production functions that combine the raw crop input with other inputs used in livestock or processed food production. The mathematical representation of these CES functions is developed in the next section.

2.2 Gridded crop production is the result of economic optimization

Crop production is the result of representative producers' maximization of profits, subject to technology, prices, policies and resource constraints. The crop production technologies (both rainfed and irrigated production) in each grid cell allow for substitution between nitrogen fertilizer, water, land, and other inputs (the latter is an aggregate of capital, labor, other chemicals, energy, etc.). The particular mix of inputs employed in a grid cell depends on relative prices, government

[1] The astute reader will ask why there are no cross-price effects in this demand equation. The answer is that SIMPLE-G models only aggregate crop demand. If we were considering disaggregated crop products, we would need to account for cross-price effects. While not 'integrable' into underlying utility or expenditure function, this demand system allows for the evolution of price and income elasticities with per capita income in a manner which has been documented by international cross section studies of food demand (Muhammad et al., 2011). This has proven essential to the long run validation of the SIMPLE model (U.L.C. Baldos & Hertel, 2013).

policies and production possibilities. Output levels expand or contract in order to ensure zero pure economic profits over the long run. Thus, unlike downscaling approaches, the spatial pattern of production is endogenously determined. Crop producers within a given grid-cell are price takers, as they are assumed to have no market power.

The equilibration of supply and demand for crops occurs at the level of market regions. Within the market regions in SIMPLE, crop demands are an aggregate of the four end uses described above. Demands may be satisfied from either from domestic or global markets depending on relative prices. This follows the method of Armington (Armington, 1969) which results in imperfect substitution between domestic and foreign products. Symmetrically, on the supply side, producers transform their products imperfectly between domestic and global markets. This permits us to calibrate the model to the observed data in which similar products are both imported and exported from the same country.

We consider a nested CES structure as shown in Figure 2. In each CES nest, two inputs are combined to produce a composite product using the following specification of technology:

(4) $Q = A(\phi_N Q_N^{-\rho} + \phi_O Q_O^{-\rho})^{-1/\rho}$, where: $\sigma = 1/(1+\rho)$ and $\rho > -1$

Each CES nest comprises three key behavioral equations which result from our assumptions of cost minimization, coupled with free entry and exit from these activities. In keeping with the model condensation and nonlinear solution strategy described in section 4, we write these equations in linearized (percentage change) form (Dixon, 1982). The following three equations pertain to the top-level nest, in which nitrogen fertilizer (N) and other inputs (O) are combined, in variable proportions, to produced aggregate crop output:

(5) $p + a = \sum_j \theta_j (p_j - a_j)$: agricultural entry/exit; zero profits

(6) $q_N + a_N = q - a - \sigma(p_N - a_N - p - a)$: demand for nitrogen fertilizer

(7) $q_O + a_O = q - a - \sigma(p_O - a_O - p - a)$: demand for other inputs

Here, lower case variables denote percentage changes in levels variables, i.e., $p = 100(dP/P)$ is the percentage change in crop price and $a = 100(dA/A)$ is the percentage change in total factor productivity. The variables p_j, q_j, a_j denote the percentage changes in input j's price, quantity and factor-augmenting productivity and θ_j is the share of that input in total costs.

Equation (5) is the consequence of our assumption of unrestricted entry and exit from the crops sector. If output price rises, with unchanged technology and input prices, then there will be excess profits in the sector. This will attract new entrants, or encourage expansion of existing producers, which will drive up input prices and drive down output prices until zero pure economic profits are restored. Manipulation of equations (5) – (7) yields the following, equivalent, quantity-based, expression of this condition (dual to (5)) which we will use in the model to facilitate our condensation strategy described in section 4:

$$(8)\quad q - a = \sum_j \theta_j (q_j + a_j)$$

Equations (6) and (7) are the derived demand conditions for inputs. Thus the percentage change in demand for nitrogen fertilizer – a key source of non-point water pollution from agriculture – depends on changes in technology (α, α_N), changes in total crop output (q) and changes in the price of nitrogen fertilizer (p_N) relative to an index of all input costs (p). In section 3 below, we will discuss how the elasticity of substitution between nitrogen fertilizer and other inputs, σ, can be calibrated to reproduce grid-cell and practice-specific agronomic characteristics of crop production. It is evident from equation (6) that a large substitution elasticity will result in much greater response to (e.g.) a tax on fertilizer use in crop production. Therefore, σ is a key parameter in sustainability analysis.

Returning to the production tree in Figure 2, we see that the 'other inputs' in equation (7) are a composite of water, land and the remaining inputs. Once again, there are three equations, analogous to (5) – (7), describing the substitution possibilities at this level in the production 'tree' (see Appendix). This is followed by a CES nest combining land and irrigation water. If crop output is strictly proportional to irrigation water delivered, then the elasticity of substitution between land and irrigation water is zero. On the other hand, if a reduction in water delivered to the crop does not go hand in hand with a proportionate reduction in output, then this elasticity is greater than zero and it captures the potential for deficit irrigation, i.e., achieving the same output level with less water, but more land.

The next CES nest in Figure 2 combines irrigation water and irrigation capital. The associated elasticity of substitution at the bottom of this production tree describes the potential for conserving irrigation water through investments in (e.g.) drip irrigation to replace sprinkler or canal-based irrigation capital. Once again, this is a key sustainability parameter which will be discussed below in section 3. The final CES nest in Figure 2 combines surface and groundwater to create an irrigation water composite. The rationale for this nest is that surface and groundwater extraction often co-exists in a given grid cell, despite differences in cost. The two sources of water offer farmers different characteristics. Groundwater, for example, is available on demand, and largely independent of current weather conditions.

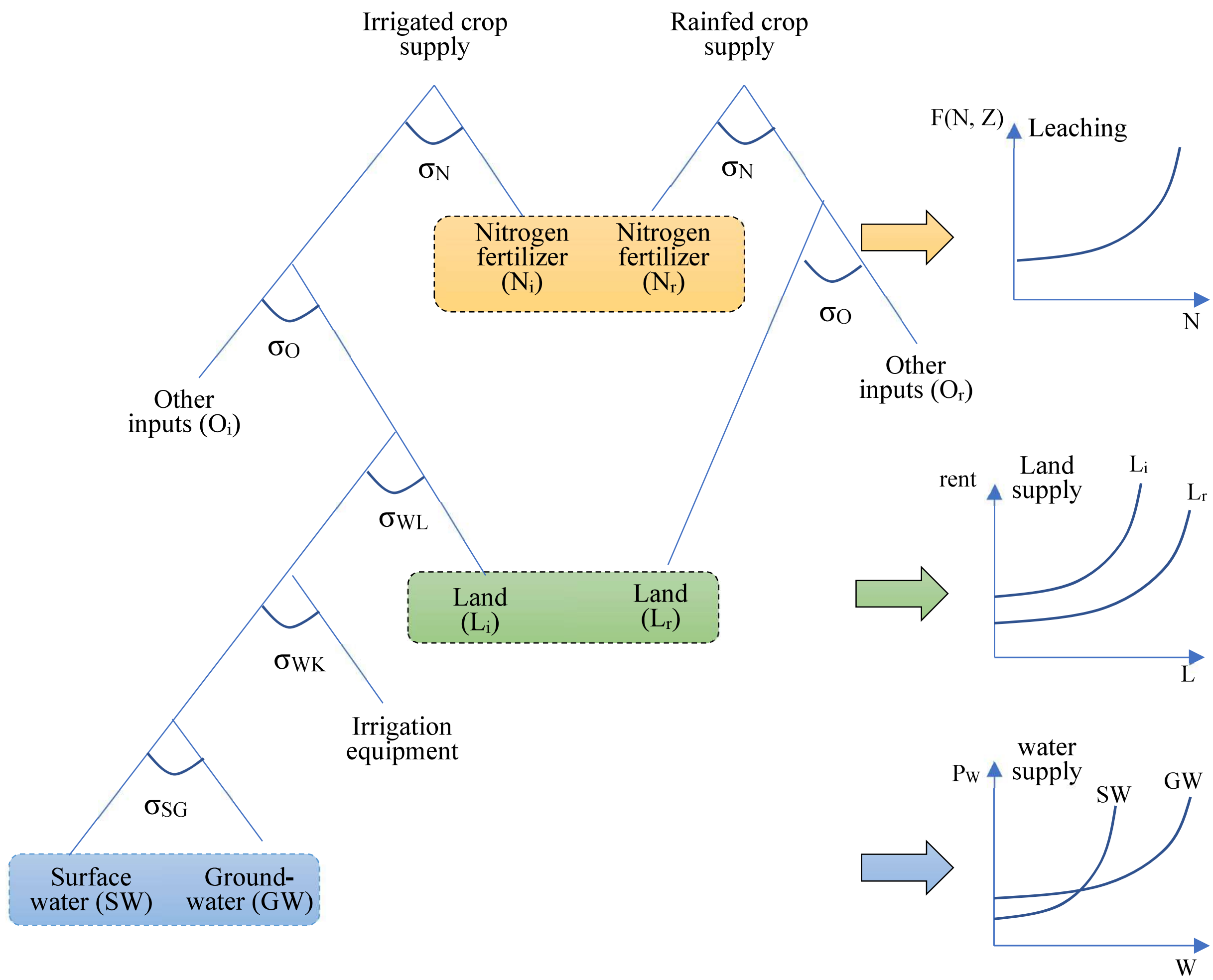


Figure 2. Structure of crop production at each grid cell. Shocks and policy variables are defined for surface water, groundwater, irrigation equipment, land, nitrogen fertilizer, and overall crop production. Elasticity of substitution is shown by σ. The equilibrium quantity and price of land and water are determined at local level. Irrigated and rainfed practices compete for land. Land supply depends on total cropland supply and the elasticity of transformation between irrigated and rainfed. The leaching function is different for irrigated and rainfed crop production.

2.3 Nitrogen fertilizer and nitrate leaching

As noted above, nitrogen fertilizer use is determined endogenously in the model considering relative prices, technology, substitution possibilities and overall output level. The potential for nitrogen-land substitution is grid cell and activity specific and is obtained from agronomic yield functions as described in section 3. The price of nitrogen fertilizer is determined at the regional level through a market clearing condition wherein regional supply equals demand which is, in turn, determined by aggregating nitrogen use across all grid-cells and practices. Nitrate leaching functions are quadratic in form and are practice and grid cell specific (see section 3).

2.4 Local water withdrawals and irrigation

Irrigation water is another focal point of SIMPLE-G. Irrigation water supply and demand are endogenously determined for each grid cell. However, they are linked to exogenous environmental factors. For example, heat stress may increase the water requirement of crops grown in a grid cell; or a drought may reduce the environmental supply of water. Hydrological dynamics are not directly modelled and are treated exogenously. However, SIMPLE-G can be readily paired with a hydrological model to shed light (e.g.) on the economic consequences of changing basin-level water scarcity or inter-basin transfers of water (Liu et al. 2017).

Water withdrawals are endogenously determined through the interaction of supply constraints and irrigation demand for crop production. Demand for water depends on the irrigation area, production levels, technology and relative prices. This includes likely adaptation channels and adjustment mechanisms. We consider change in irrigation extension (Haqiqi & Hertel, 2019) location of crop production, change in irrigation technology, change in water intensity, and trade (Haqiqi & Hertel, 2016). Water supply at each grid cell is limited by hydrological constraints. Figure 3 illustrates two examples. This form of water supply function is slowly increasing at the beginning (up to A) and then rapidly increasing (after B) when approaching the asymptote (C).

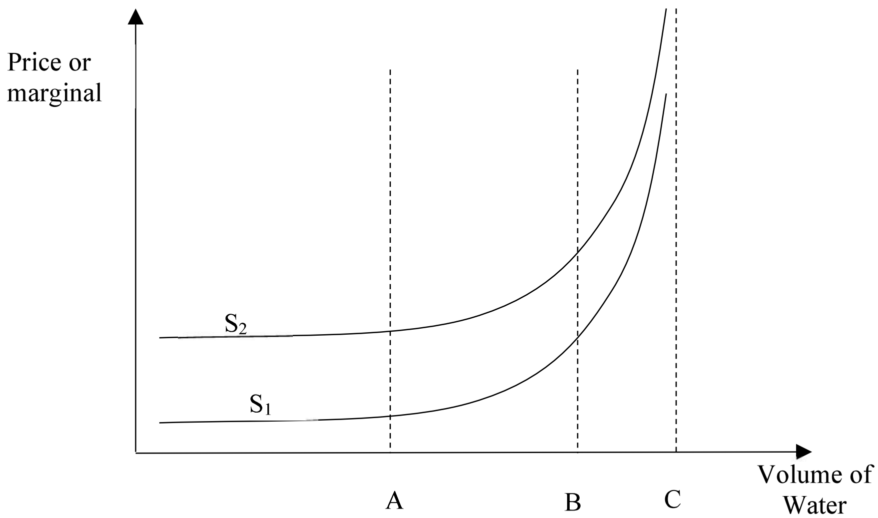


Figure 3. Economic supply for water with maximum availability (asymptote C). The marginal cost of water supply is nearly constant before point A. It starts increasing at a moderate speed up to point B. From B to C the marginal cost increases rapidly. With adverse changes in hydroclimatic conditions, the cost schedule may shift to S_2 (depending on the natural supply of water).

Withdrawal of water is constrained by maximum water available in each grid cell after subtracting non-agricultural water use. The supply elasticity of water, ε^s, varies by grid cell. It depends on the ratio of water extracted, relative to the sustainable extraction level (R) and calibrated parameters ω_1, ω_2, ω_3. We assume a three-parameter Fréchet function for water supply.

(9) $$\varepsilon^s = \omega_1 (R + \omega_2)^{-\omega_3}$$

where, R is calculated as the ratio of annual withdrawal to annual groundwater recharge or as the ratio of annual withdrawal to annual available surface water. We calibrate this supply function separately for surface water and groundwater at each grid cell based on economic and hydrologic information including: the annual water withdrawal for crop irrigation, sustainable extraction level of water by source, and the estimated value of water.

2.5 Gridded land use

Total cropland, divided into rainfed and irrigated practices, and the associated land rents are endogenously determined in the model. Land rents are grid cell-specific and depend on local biophysical characteristics, prices as well as technologies available to each production unit. Allocation of land to rainfed and irrigated production is determined according to their relative returns (land rental). This is determined endogenously for each grid cell assuming a constant elasticity of transformation function (Ahmed et al., 2008). The key parameter in this function is the elasticity of transformation between irrigated and rainfed cropland. This elasticity measures the responsiveness of the rainfed-irrigated crop mix ratio to changes in relative returns. A larger elasticity value indicates easier transformation of cropland between irrigated and rainfed categories. In the case of land conversion from rainfed to irrigated cropping this is heavily influenced by water law which varies by locality in the US.

2.6 Climate

Climate is exogenous in SIMPLE-G. However, the consequences of climate change for land and water use as well as food security may be explored by linking exogenous climate change to key variables in the model. This includes total factor productivity, labor or land productivity, and land and water availability. For example, excess heat stress may affect yields of irrigated and rainfed crops; climate change may affect water availability; global warming may reduce labor capacity, change the water requirements of crops, and alter the suitability of cropland.

3 BENCHMARK DATA AND PARAMETERS

SIMPLE-G requires benchmark gridded data for key economic and biophysical variables describing the crop economy in initial equilibrium. This includes gridded cropland use, crop production, nitrate leaching, and water use. The required data is obtained from global and national products as shown in Figure 4. Here we describe the data for a US-focused version of SIMPLE-G, wherein we utilize gridded data for the US, while employing regional information for other parts of the world. However, there are efforts underway to implement SIMPLE-G for China and Brazil, and the initial application of SIMPLE-G was undertaken at global scale – albeit at coarser resolution (Liu et al., 2017). For SIMPLE-G-US, crop production is at the level of geo-referenced grid-cell units at 5 arc min resolution (squares of side 9.26km at the equator). We add gridded information for US crop production covering both irrigated and non-irrigated practices and including the value and quantity of crop output, land use, nitrogen fertilizer input, water, and aggregated other inputs.

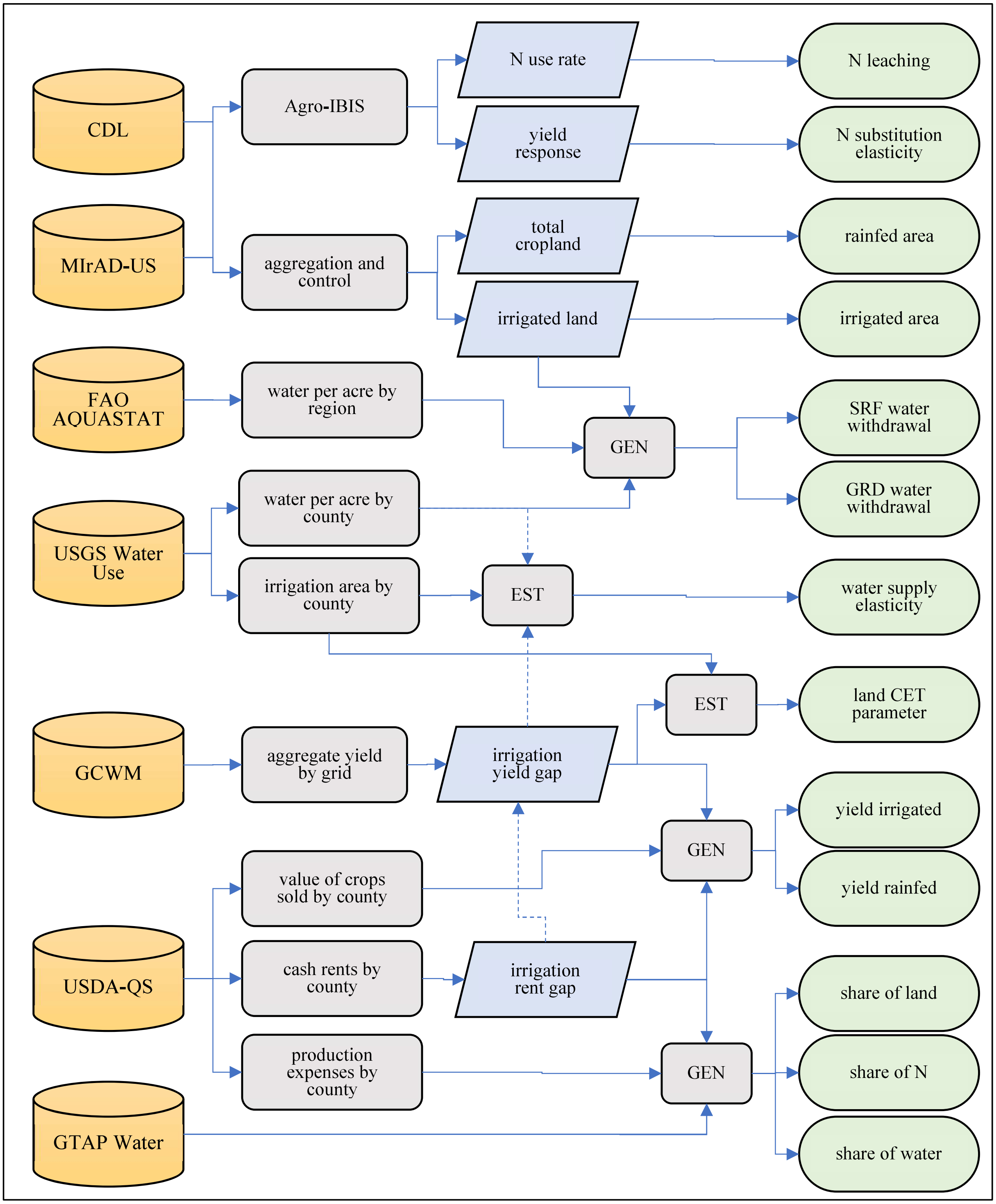


Figure 4: Overview of main data processing for SIMPLE-G-US at global, national, and 5 arcmin. Here, "GEN" represents a computation which does not involves statistical regressions; "EST" is a process which includes statistical estimation. Other versions, (gridded World, gridded China, and gridded Brazil) follow similar flows but employing rich national data sources.

3.1 National and regional data

The benchmark regional data for 2010 is taken from the FAOSTAT (FAO, 2014) and GTAP (Aguiar et al., 2019) global data bases as documented in Hertel and Baldos (2016). This includes regional data on supply and demand for crops, as well as regional cost and sales structures for the crops, livestock and processed food sectors. Consumer demand elasticities are based on the work of Muhammed et al. (2011) who use international cross-section data to estimate food demand systems spanning the full range of national per capita incomes. Estimation of equations (1) and (2) is described in Hertel and Baldos (2016).

3.2 Cropland area

Cropland area is obtained from the USDA Cropland Data Layer (Han et al., 2012) at 30 meter resolution and aggregated to 5 arc min. Irrigated cropland is from the Moderate Resolution Imaging Spectroradiometer (MODIS) Irrigated Agriculture Dataset for the United States (MIrAD-US) provided by USGS at 250 meter resolution (Brown & Pervez, 2014) and aggregated to 5 arc min. This data determines the distribution of irrigated and non-irrigated cropland in the US.

3.3 Cropland supply and transformation parameters

Cropland supply function determines the willingness to supply cropland given the land rents. The main parameter is the supply elasticity which shows the percentage change in cropland supply as a response to a one percent change in cropland average rent. Regional cropland supply elasticities are taken from the SIMPLE model, while gridded land supply elasticities for the US are based on the statistical model developed by Villoria and Liu (2018) using gridded data from the Americas.

A constant elasticity of transformation function determines the allocation of land to irrigated and rainfed. The transformation elasticity parameter determines the percentage change in the ratio of each land type in response to change in relative rents. This parameter shows the flexibility of converting cropland to irrigated or rainfed. In the US, this parameter is estimated following (Jame et al., 2017) considering US water rights. Different water rights can restrict the extension or intensity of irrigation in one location. For this estimation, we employ county level information from USDA including the Cash Rents for irrigated and non-irrigated cropland, as well as total irrigated and non-irrigated cropland area by county. We assume all the grid cells within a county follow the estimated parameter for the county.

3.4 Crop yields and production

Aggregated output at each grid cell is the corn-equivalent total crop output which is calculated as the summation of the value of each crop sold divided by the price of corn in the base year. We take the value of crop sold per acre from USDA-NASS by county (USDA-NASS, 2019) and use GCWM (Siebert & Döll, n.d.) simulated yields to generate gridded yield for all the grid cells in each county. GCWM is aggregated over all crops using USDA/FAO actual prices to calculate corn-equivalent crop output for each grid cell.

We split the base data into irrigated and rainfed crop production employing various satellite data sets, and county level information from USDA and USGS, as well as the simulated yield of irrigated and non-irrigated crops. For yield estimation, we assume that grid cell aggregated yield per hectare is equal to the county average in which the grid cell is located. We split the gridded total production into irrigated and non-irrigated components using total, irrigated, and non-irrigated land as obtained from MIrAD-US and the CDL; and the ratio of rainfed to irrigated yields in a given grid cell as estimated by Siebert and Döll (2010) for 29 crop categories, and aggregated to all crops according to production value weights. Total cropland area from the CDL is matched with USDA county level cropland to ensure consistency of yield and area at the county level.

3.5 Nitrogen fertilizer application and leaching parameters

Nitrogen fertilizer application rates per hectare per year for each grid cell were obtained from either Agro-IBIS for rainfed and irrigated production of major crops (Lark et al., 2020). This product provided high-resolution (8 arc-second) land cover and nutrient application maps across the continental United States (CONUS) for the time period of 1750 to 2017 accounting for the nutrient legacies of historical land use/cover. Their land cover categories are determined based on the vegetation types simulated in Agro-IBIS. This product is also consistent with our land cover data. This is based on several gridded land cover datasets as well as historical county-level USDA Census of Agriculture data. Also, their irrigation maps are created based on the (MIrAD-US) and historical data from the USDA Census of Agriculture. With its reach information, Agro-IBIS helped us to estimate the irrigated versus non-irrigated fertilizer rates.

Thee has been efforts to estimate the leaching parameters from Agro-IBIS to construct a nutrient leaching module for all the grid cells in the SIMPLE-G-US (Liu et al., 2018). This is a non-linear leaching function which shows the nutrient leaching will increase quadratically when the nitrogen application rate increases. The parameters are specific to unique biophysical characteristics of each grid cell including soil type, irrigation, land cover, etc.

3.6 Nitrogen substitution parameters

The substitution elasticity between nitrogen fertilizer and other inputs is an important parameter in the model. It determines the likely changes in nitrogen application rate in response to change in relative price of nitrogen fertilizer. We have estimated this parameter for each grid cell. We follow Liu et al. (2020) to establish a framework for estimating this parameter. This includes obtaining the yield response functions from Agro-IBIS. Then we combined this response function with estimated yields of irrigated and non-irrigated crops to find the substitution elasticity for irrigated and rainfed crop production (Liu et al., 2020).

3.7 Water withdrawal

Irrigation water withdrawal rates are estimated using USGS county level water use data (Maupin et al., 2014). We calculate total water withdrawal per irrigated hectare and split it into ground water and surface water using USGS county level water use by source. The information about groundwater recharge is taken from the Annual Estimate of Recharge (Reitz et al., 2017). Figure 5 depicts the ratio of groundwater withdrawal to local recharge in 2010. The red color shows the locations with a very rapid depletion of groundwater. A ratio equal to ten means the amount of groundwater withdrawal in one year is equal to ten years of groundwater inflow. The High Plains Aquifer, the Central Valley of California, the Snake River Basin and western Washington show dramatic levels of unsustainability, based on this index. The maximum surface water available at each grid cell is calculated after subtracting non-agricultural water use from locally-generated runoff (Wolock, 2003). Maximum available ground water available is determined with groundwater stock (Befus et al., 2017; Gleeson et al., 2016).

3.8 Water supply parameters

We have calibrated the gridded water supply schedules for the continental United States to the benchmark year: 2010. For groundwater, the elasticity of supply is determined based on the ratio of groundwater withdrawal to groundwater recharge (Figure 5). The red areas in this figure have a high ratio of withdrawal to recharge. In these grid cells, the expansion of irrigation is more costly, compared to grid cells with a lower ratio. In other words, given a similar increase in crop prices, expansion is expected to be more rapid in areas with a lower ratio, holding all other factors constant.

For the US grid cells, the water supply elasticity is calculated using the ratio of withdrawal to recharge, and empirically estimated parameters ω_1, ω_2, and ω_3 from equation (9). These are estimated using water withdrawal data from USGS for 2010 and estimated value of water (Haqiqi et al., 2016). Then, we apply the estimated function to all the grid cells to find the unique water supply elasticity for each grid cell.

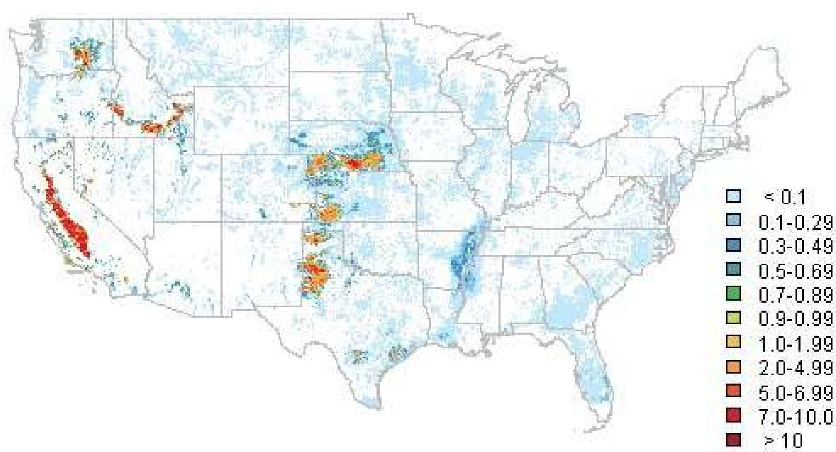


Figure 5. Ratio of groundwater extraction over local groundwater recharge By 5 arc min grid cells for 2010.

4 SOFTWARE

The SIMPLE-G model and database are prepared and solved with the GEMPACK modelling suite (Horridge et al., 2018). This software package is specifically designed for the solution of large-scale economic equilibrium models with numerous markets and agents. The database files can readily store multi-scale and multi-dimensional variables. Other attractive features of this software are discussed below. However, the unique advantage of GEMPACK in the context of multi-scale modelling is the capability to condense the model and later backsolve for key endogenous variables.

4.1 Condensation

Solution times can be substantial for an equilibrium model with many equations and with complex interconnections between the unknown variables (e.g. the market responds to farmer decisions even as the farmers respond to market outcomes). Researchers have designed different algorithms to reduce the solution time. Most algorithms iterate between two phases: a linear algebra phase which solves a first-order approximation to the non-linear equation system; and a 'formula' phase which updates variable values and re-computes coefficients of the linear system. In GEMPACK, solution time for the linear phase rises with the square or cube of the number of equations, while time for the formula phase tends to increase only linearly.

A typical SIMPLE-G application might distinguish 2 million grid cells and 7 regions. For each grid cell, a system of about 20 equations (some shown above) determines crop output of that grid cell, given grid-level exogenous settings and the price of output (which is the same for all cells within a given region). So, these grid level equations may number about 40 million. For each region, other equations add up grid cell output to obtain total crop supply, or inter-relate region level prices and quantities. There might be 100 such equations per region, or 700 in total. Hence the overwhelming majority of equations are at grid cell level.

A linear system of 20 million equations is impossibly slow to solve, and might require enormous amounts of RAM. We need to greatly reduce the number of equations by substitution (a.k.a. condensation).

For example, we could rewrite equation 6 above as (the grid index is omitted):

(6') $q_N = q \quad - a \quad - a_N - \sigma(p_N - a_N - p \quad - a \quad)$: demand for nitrogen fertilizer.

Then, we could replace each occurrence of q_N in *other* equations by

$$q \quad - a \quad - a_N - \sigma(p_N - a_N - p \quad - a \quad)$$

and drop equation (6) from the system, so reducing its size by 2 million equations. After the linear system was solved, we could use equation (6') to recover (or backsolve for) values of q_N.

Such techniques are often used by modelers, who manually perform such substitutions in their model specification file. The drawback is, especially when a number of substitutions are performed, that the necessary algebra is difficult and the remaining equations become extremely complicated and un-transparent. However, GEMPACK is able to do the algebra to perform such substitutions (and the backsolves) automatically, reaping a performance gain while leaving the model specification (TABLO) file in its original, simpler, uncondensed form.

In fact, for SIMPLE-G ***all*** equations at grid level are substituted out leaving a regional level linear system of modest (700) size. Such a system takes very little time to solve. However, the coefficients of the system involve calculations at grid level; the time taken is proportional to the number of grid cells. Hence (see Figure 6) solution time increases only linearly as a function of the number of grid cells.

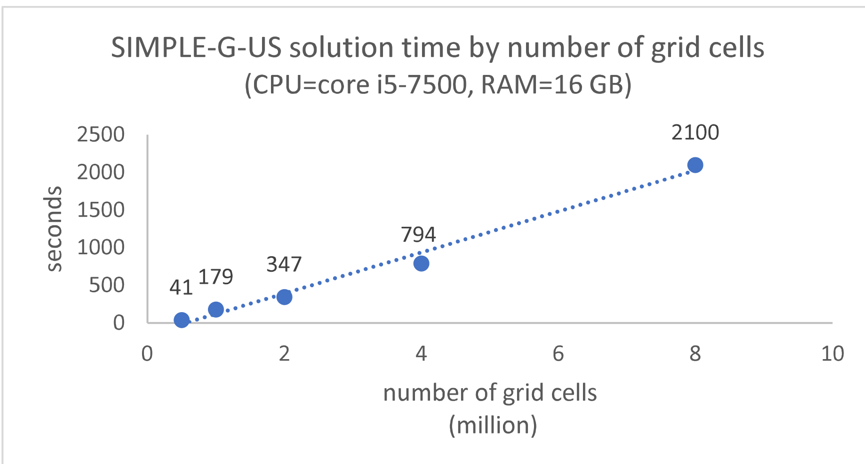


Figure 6. Linear relationship between solution time and number of grid cells. Condensation allows users to solve SIMPLE-G system of equations with one million grid cells (~10 million endogenous variables) on a laptop in a few minutes.

4.2 Linearization

GEMPACK can automatically translate the original equation system into a linearized system (reformulated as a system of first-order partial differential equations). Alternatively, the modeler can specify conveniently interpretable linearized forms of the underlying behavioral equations, as in equations (5) – (7). Clever representation of the model (e.g., using equation (8) in place of (5)) can facilitate condensation as well as more rapid solution of the model. In our case, we substitute out all of the variables with a grid cell index. In SIMPLE-G, all of the cross-grid cell interactions are transmitted through regional market prices. Once we know the regional crop, nitrogen, irrigation capital and other input prices, we can backsolve for crop output, input use, land prices and the shadow price of irrigation water in each grid cell independently.

However, since the model is non-linear (recall equation (1)), the cost shares in equation (5) must be updated at each step in the solution process. Consequently, the model is solved by multistep methods such as the Euler method or Gragg's modified Midpoint method (Pearson, 1991). The solution of a large system of linear equations is accomplished using sparse matrix techniques (Schiffmann & Jerie, 2019). Richardson extrapolation is used to improve accuracy (Pearson, 1991). This linearized approach has proven capable of solving very large, non-linear models (e.g., one data point in Figure 6 is a model with 8 million grid cells).

4.3 Decomposition

In addition to these features, GEMPACK has some extensions which prove invaluable in SIMPLE-G applications. It provides a way to formulate inequality constraints or non-differentiable equations as complementarities (Bach & Pearson, 1996) which can be important in sustainability analyses. It also offers a technique to decompose changes in model variables due to several shocks into components due to each individual shock (Harrison et al., 2000). We will illustrate this in the first application undertaken in the next section of the paper.

4.4 Web-application on GeoHub

The web-app version of SIMPLE-G permits users to simulate, explore and visualize the results of SIMPLE-G without installing the GEMPACK program or any visualization software. (Linux versions of GEMPACK programs run on the GeoHub server.) The GeoHub also includes pre-solved experiments, and demonstrations of how to run the model and analyze results, based on the policy briefs presented at the 2018 Conference on Long Run Sustainability of US Agriculture (https://mygeohub.org/groups/glass/npc2018).

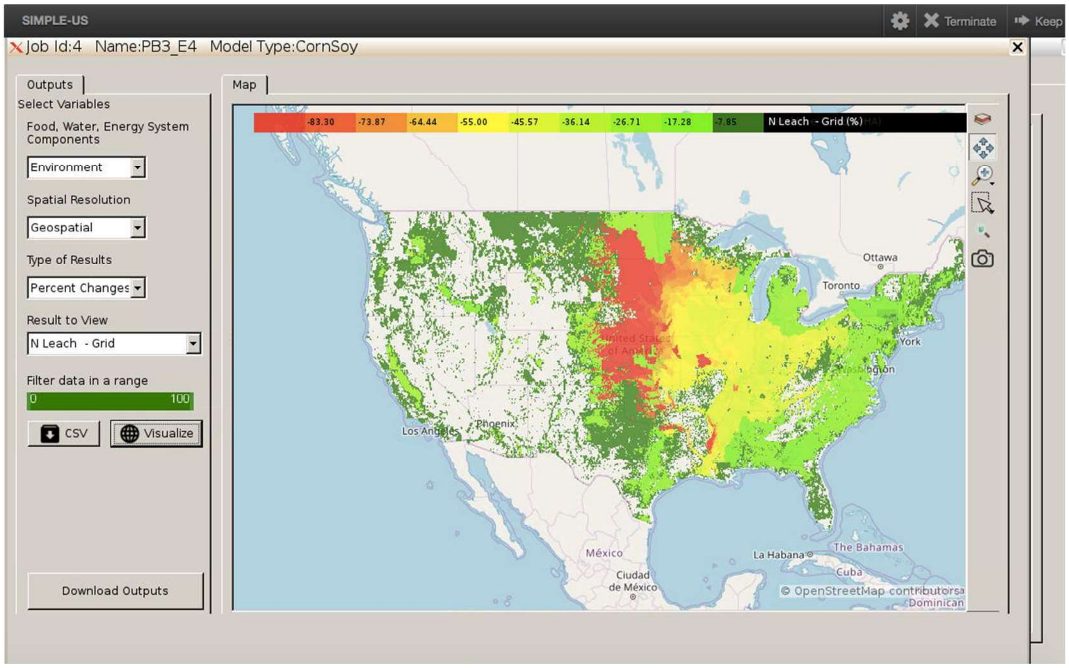


Figure 7. A sample window from web application: https://mygeohub.org/tools/simpleus

5 Two Applications

Here, we illustrate the usefulness of the SIMPLE-G model through two applications. Since we use the US-focused version of SIMPLE-G, these two applications focus on the US. However, similar applications of SIMPLE-G in other regions are underway. The first application evaluates the role of global drivers of local sustainability stresses within the continental US. In the second, we consider the feedback to national and global markets stemming from locally implemented sustainability policies on irrigation water use. Together, these applications demonstrate the capacity of SIMPLE-G to capture global-to-local-to-global interactions.

5.1 Global drivers of local sustainability stresses

In the coming decades, changes in population, income, and technology will alter the pattern of agricultural crop consumption, production and international trade. We expect that productivity growth will lead to higher yields, thereby moderating the demand for scarce land and water resources. On the other hand, we expect the changes in population and income growth will create heightened sustainability pressures. For projecting this footrace between supply and demand forward to mid-century, we take predicted changes in population, income and total factor productivity as in Baldos and Hertel (2014). These are reported in Figure 8 and are based on the 'business as usual' Shared Socioeconomic Pathway (SSP2) (O'Neill et al., 2014). We also assume that historical agricultural productivity growth rates persist to mid-century (Fuglie, 2012). South Asia and China are projected to have the greatest cumulative per capita income growth over this period – rising by 641% and 607% respectively. Sub Saharan Africa is expected to experience the highest rate of population growth: 139%. In contrast, East Europe and Japan and Korea are expected to see declines in their populations by mid-century.

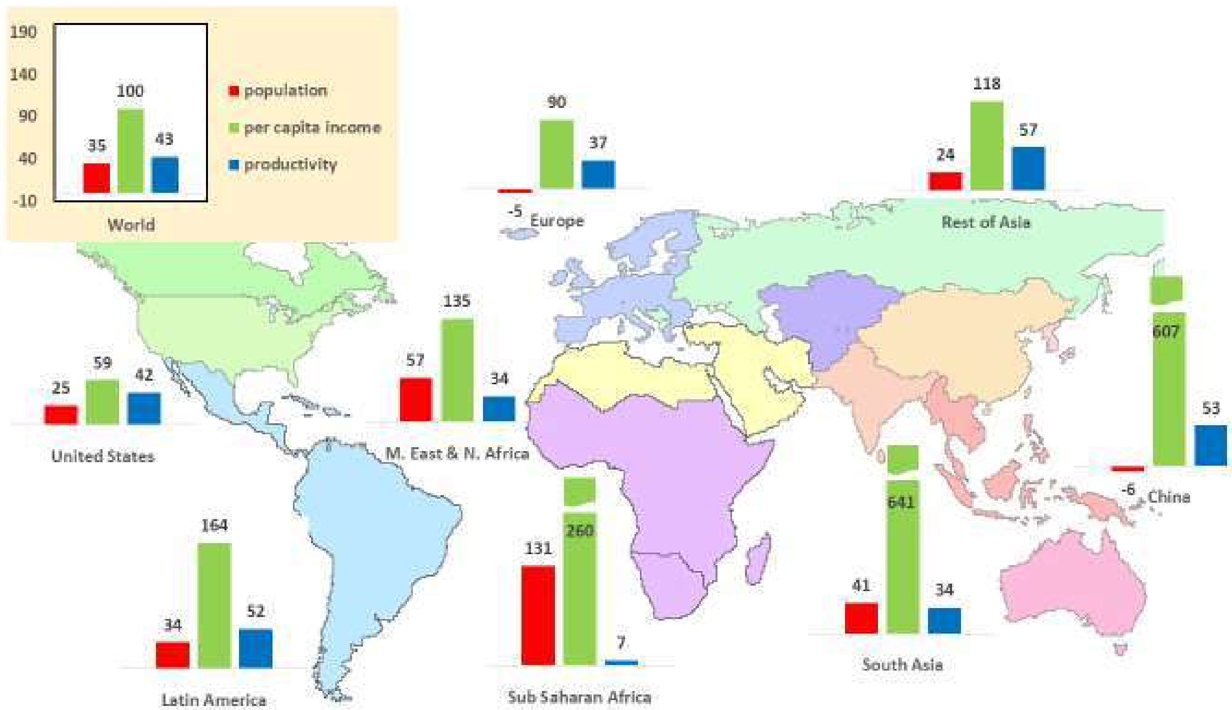


Figure 8. Growth rates for exogenous drivers: 2010-2050. Sources: Changes in population and income is obtained from Baldos and Hertel (2014) aggregated to 16 regions from country level information based on SSP2 *(O'Neill et al., 2014)*. The changes for productivity are calculated based on Fuglie (2012).

The role of global change drivers in projected growth for US crop production by 2050 is shown in Figure 9, exploiting the decomposition feature of GEMPACK (Harrison et al., 2000). This figure shows that that one quarter of the projected US cropland expansion is due to demand growth in South Asia and China alone. Overall, growth in income and population outside the US is far more important in driving US crop production than growth within the US. This is due to higher income growth rates in the developing and emerging economies, coupled with higher income elasticities of demand (1) and higher rates of population growth in Africa and other low-income regions.

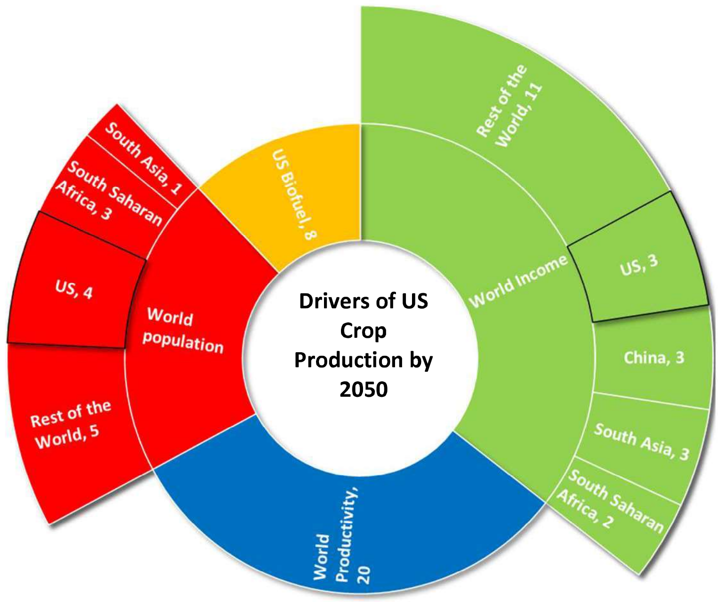


Figure 9. Drivers of US Crop Production: 2010-2050. Decomposition into biofuel demand (US only), productivity growth (worldwide), and regional changes in population and income.

Figure 10 shows the pattern of cropland expansion across the US over the projections period, as a percentage change from 2010. This particular indicator of sustainability stress reveals that, absent any policy interventions, the greatest land use change stresses will arise in the marginal areas on the edges of the Corn Belt. (There is very little remaining land available for expansion in the heart of the Corn Belt.) These marginal regions are often environmentally sensitive and they are also the areas where the largest land use stresses arose during the 2008-2012 biofuels boom period (Lark et al., 2015). These changes are based on the statistically estimated gridded land supply elasticities (Villoria & Liu, 2018).

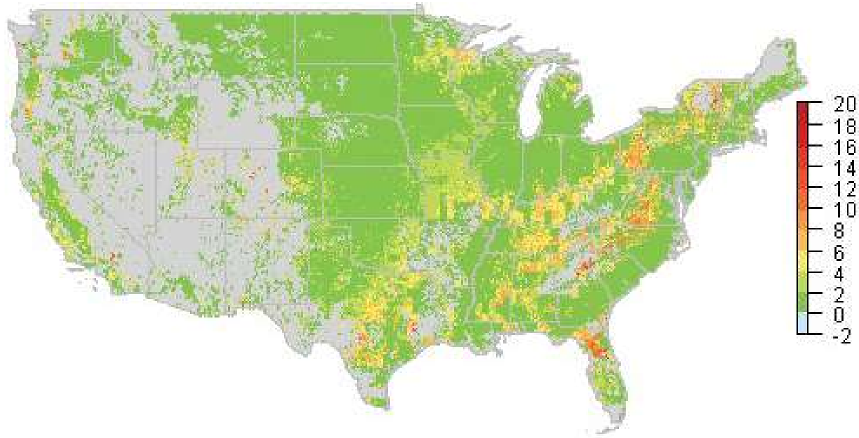
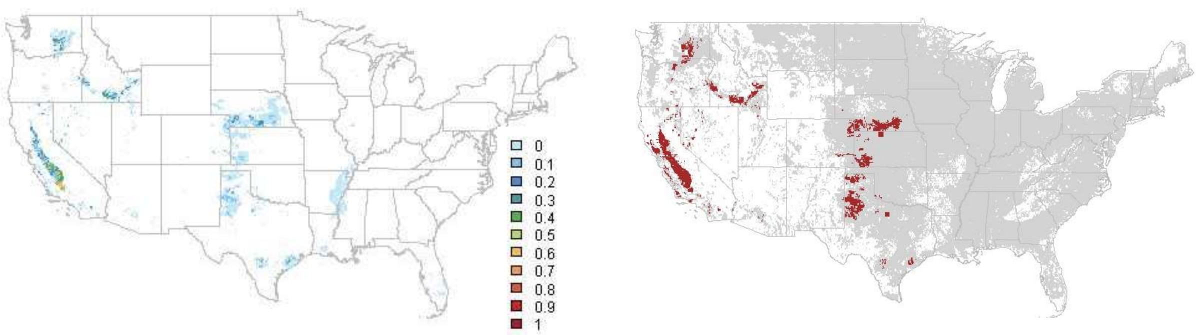


Figure 10. Projected percentage change in US cropland from 2010 to 2050 by 5 min grid cell

5.2 Limiting unsustainable water withdrawals

As seen in Figure 5 above, many locations in the Western US suffer from excess groundwater withdrawals. Despite productivity improvements, our projections suggest that this situation will become even worse under our business as usual baseline, due to global growth in the demand for US crops (Figure 11-a). Here, we examine the impacts of a counterfactual scenario in which we do not allow any increase in water withdrawals in locations showing withdrawals in excess of recharge in the base year of 2010 (Figure 11-b).



(a) (b)

Figure 11. (a) The change in the ratio of water withdrawal to recharge: 2010-2050, business as usual baseline. (b) Grid cells affected by the counterfactual policy shown in red.

Figure 12 shows the impact of this water sustainability policy on irrigated cropland area in the US, as well as global changes in cropland and production owing to this policy. While the aggregate impact of the water withdrawal restriction on US crop production and land use is less than 1%, it nonetheless has a significant impact on the pattern of crop production and the irrigated area. The reduction in US production is partially offset by increased production in other regions of the world, with EU, South America, China, and Sub Saharan Africa, offsetting 19%, 19%, 12%, and 11% of the reduction respectively.

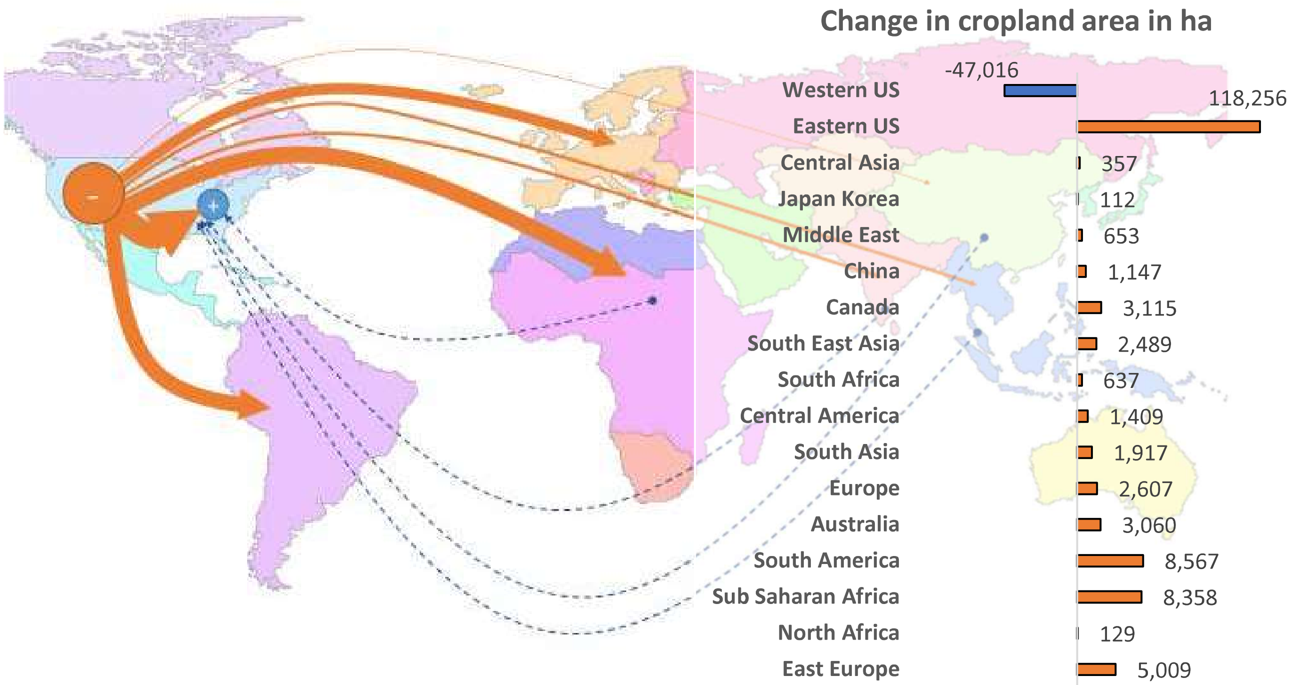


Figure 12. Changes in irrigated area and the relocation of global crop production owing to groundwater sustainability policy in the Western US. This policy does not allow additional water withdrawals in grid cells where withdrawals are already in excess of recharge rates.

Compared to the baseline, US aggregate water withdrawals decrease by 1.82%, irrigated area declines by 0.13% and rainfed area increases by 0.08%. While this figure seems to be very small for the whole country, there are significant impacts on many local communities. Compared to the baseline, irrigated area declines by as much as 17.7% in some grid cells and may increase by up to +5.7% in other grid cells. Rainfed area may also decline by up to 5.7% and may increase by +163.1% in other grid cells. As shown in Figure 13, irrigation is reduced in locations facing the sustainability restriction. In a few grid cells rainfed land is converted to irrigated land in response to water limits which involves improvement in irrigation efficiency. Not allowing the unsustainable grid cells to increase groundwater withdrawal reduces irrigated area by up to 370 ha in some grid cells (each grid cell can have 3500-7000 ha of cropland) (Figure 13).

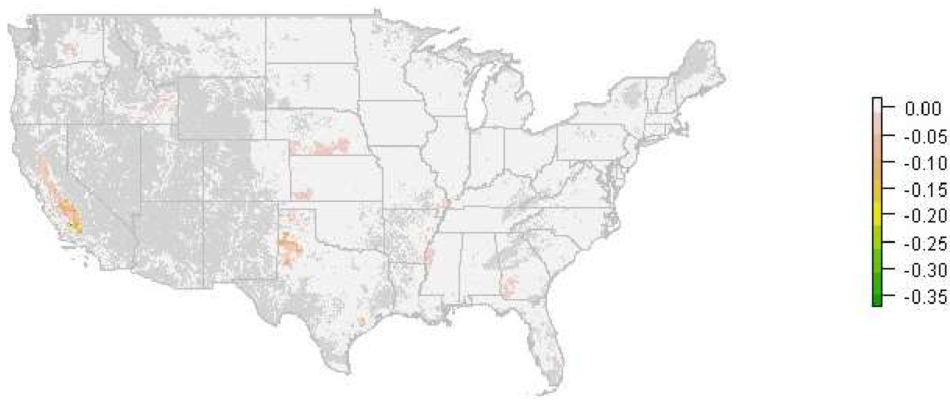


Figure 13: Absolute change in irrigated area (in 1000 ha) can be up to 370 ha per affected grid cell.

While the rainfed cropland is projected to increase in most of the US in response to the water withdrawal restrictions, the highest absolute increase in rainfed land arises in the locations with water withdrawal limits, as land reverts from irrigated to rainfed production. Increases in rainfed land is also projected to be higher in the marginal area as a response to the higher crop prices as shown in Figure 14.

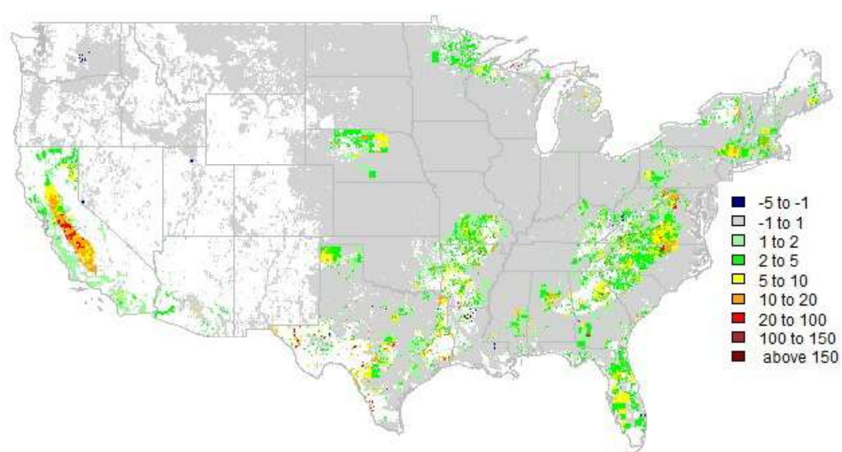


Figure 14: Percentage change in non-irrigated area

5.3 Other applications of SIMPLE-G

While these two applications use the high-resolution US version of SIMPLE-G, there are other applications of this framework designed to address different research questions. These models may have different production structures (Figure 2), different spatial focus, different resolution, different crop coverage, and some employ different modules. In one such application of SIMPLE-G, changes in ecosystem services are linked to land use, as well as the productivity of land. Loduca et al (2020) specify grid-cell specific wetland expansion and habitat conservation measures in SIMPLE-G for the Chesapeake Bay Watershed in the US. Hertel, Ramankutty and Baldos (2014) use the gridded terrestrial carbon data base from West et al. (2010) to deduce changes in terrestrial carbon emissions stemming from an African Green Revolution based on cropland changes in the SIMPLE model.

Given its importance to the sustainability debate, SIMPLE-G has a nutrition module which allows users to assess the impact of changes in price and income on the prevalence and depth of undernutrition in developing countries. It follows the FAO (Neiken, 2003) approach, modelling the distribution of caloric intake in a region using a log-normal distribution. When coupled with information about the mean and standard deviation of consumption, as well as the minimum caloric intake, it is possible to deduce the prevalence of undernutrition as well as the average caloric gap of those who are undernourished. This module allows for assessment of a variety of important questions, such as the impact of climate change on food security (Baldos and Hertel 2014). This nutrition extension of the model links the local resources (mainly land and water) to global food security. The goal is to create opportunities for analyzing the trade-off between global food security goals and local sustainability of land and water resources (Kabir et al., 2019).

One early application of this model has treated the world as a uniformly distributed set of grid cells (Liu et al., 2017). That research focused on the impact of emerging water scarcity at global scale, and was undertaken in conjunction with the global water balance model (Vörösmarty et al., 1998). The global gridded implementation was performed at a coarser resolution (30 arc minute grids), and the economic demands for irrigation and the hydrological supplies (net of non-agricultural uses) were reconciled at the level of nearly 1,000 hydrological sub-basins. This enabled the authors to explore the implications of various adaptations to water scarcity, including inter-basin water transfers as well as increased integration of commodity markets.

Table 1: SIMPLE-G applications and brief description of each version

FEATURES	**SIMPLE-G IMPLMENTATION**		
	SIMPLE-G	**SIMPLE-G US/ China/ Brazil**	**SIMPLE-G-H US**
Application	Land use, irrigation, water scarcity	Local land-water stress from global demand, water pollution and sustainability, irrigation efficiency	Water pollution, wetlands, wildlife habitat conservation
Crop coverage	All-crops	Corn-soy All-crops	All-crops
Gridded scale	30 arc min: global	5 arc min: US/ China/ Brazil	750 meters: US
Sub-national disaggregation	NA.	US production regions	NA.
Market aggregates	15 market regions for production and global demand	16 market regions for production and global demand	One aggregate region for global demand
Land types	Irrigated and rainfed cropland	Irrigated and rainfed cropland	Irrigated and rainfed cropland, and wetlands
Production inputs	Land and nonland	Land, water, fertilizer, and other.	Land, water, fertilizer, and other.
Water	Irrigation extension	Ground water, surface water, and irrigation equipment	Irrigation extension

Another version of the model has been developed for questions regarding sustainability of water resources (Haqiqi et al., 2018). In the agricultural production, it considers not only land use, but also water use, and nitrate fertilizer application. Similar to the model described in this paper, the production is modelled at 5 arc-min grid cells over the US. For the rest of the world, the production is modelled at the level of 16 market regions. In this version, there are two levels of aggregate demand. One aggregation is at sub-national production regions for the US. Then, the global demand is modelled at aggregated regional level. The water withdrawal module is similar to this paper with different functional forms for water supply.

SIMPLE-G is also flexible in terms of crop coverage. While most versions have considered all-crops aggregate, another set of models have focused on corn-soy composite. One application is the analysis of water quality in the Corn Belt of the US (Liu et al., 2018). As a large portion of the water pollution has been related to corn and soy cultivation, it makes sense to focus on the specific responses of these crops. For this application, a nitrate leaching module has been developed with crop-specific yield and nitrate leaching response. This module is parametrized with the outputs of Agro-IBIS agronomic model as described earlier.

The most recent version of SIMPLE-G was developed for high resolution conservation studies. That version of the framework includes a module on potentially restorable wetlands on agricultural lands. The model is solved at a much finer resolution (750-meters) over the continental US. Parametrization of grid cells exploits satellite data as well as reported county level information. This includes a detailed wetland restoration and conservation (Loduca et al., 2020).

These applications illustrate the flexibility of the SIMPLE-G framework. It is not just a single model. Rather, it is a flexible way of looking at the world. Indeed, there are two NSF-funded efforts underway that are building high resolution versions of SIMPLE-G focusing on China and Brazil.

6 DISCUSSION AND CONCLUSIONS

SIMPLE-G is by no means the first attempt to undertake global economic analysis of sustainability challenges at the interface of agriculture and the environment using a grid-resolving approach. To our knowledge the first such model was MAgPIE (Lotze-Campen et al., 2008). This is a global optimization model, with the objective of minimizing the global cost of producing food to meet a pre-specified level of demand. It was developed at the Potsdam Institute for Climate (PIK) and is typically used in conjunction with a gridded dynamic vegetation model to look at issues related to land use change, climate impacts on agriculture, bioenergy and technology change, among other issues. MAgPIE differs fundamentally from the approach developed in this paper. SIMPLE-G is an economic equilibrium model, in which decentralized agents (e.g., irrigated crop producers in a given grid cell, food processors, or consumers in a particular regions of the world) interact through regional and global markets. In the presence of policy distortions and barriers to trade, the global equilibrium determined by SIMPLE-G will not minimize total costs. In this sense, it aims to be predictive, as opposed to normative. Indeed, the presence of market imperfections means that global optimization models such as MAgPIE, must often place artificial constraints on the model in order to allow it to replicate observed patterns of production, consumption and international trade.

More recently, the GLOBIOM model has emerged on the global sustainability scene. It is maintained at the International Institute for Applied Systems Analysis (IIASA). Like MAgPIE, GLOBIOM is a recursive-dynamic optimization model. In addition to 18 major crops, it has a livestock module and, when linked to models of crop growth, bioenergy, forestry and fisheries, it has been used to deal with a wide range of sustainability issues including deforestation, water use and greenhouse gas emissions. There are also regional versions of the model focusing on the EU and Brazil, among others. Due to its large size and complexity, the model is not solved at the individual grid cell level, but rather it is solved for representative groupings of grid cells. In short, it is a very ambitious undertaking involving dozens of researchers and this work represents the cutting edge of global sustainability research with grid cell resolution.

As its name indicates, the SIMPLE-G framework introduced in this paper has more modest aspirations. Rather than continually extending this model to handle new issues, this framework aims to be as simple as possible, while capturing the essence of a given sustainability challenge. If a different set of challenges emerges, the idea is to build a different version of SIMPLE-G, rather than extending the original model to add another feature. At the heart of this simplicity lies the fact that SIMPLE-G always has just one composite crop – albeit produced with different techniques and resource requirements – both within, and across grid cells. In the application presented here, the single crop was a composite of all crops and our analysis focused on the extensive margin of land and water use in agriculture. However, as noted in the preceding section, this crop could also be a single crop, such as maize, or a maize-soy composite such as in Liu et al. (2018). From an economic point of view, this means that, within the crop composite, it is assumed that prices move in tandem – a key economic condition for aggregation of products. This doesn't make sense in the short run, but over decades it is likely the case that substitution – both on the supply and the demand sides – will force crop prices to move together. In part due to this restriction, SIMPLE-G is not run on an annual, recursive basis, unlike the aforementioned models. Rather, it is treated as a 'one-shot', comparative static model, e.g., starting in 2010, one might simulate the global crop economy in 2050, as is done in the application above.

While the restriction to a single (composite) crop and the one-shot comparative static approach may seem like a huge sacrifice, it has yielded one very significant benefit – namely facilitating model parameterization and validation. To date, all of the validation efforts have been conducted using the non-gridded version of SIMPLE which breaks the world into 15 aggregate regions. And these have been quite informative. In the first such paper Baldos and Hertel (2013) found that SIMPLE was able to re-produce global changes in aggregate crop output, cropland area, yield and prices over the 1961-2006 period. This was a significant breakthrough in the global land use change literature and was used as a basis for understanding why many models were likely over-predicting long run land use change in the 21st century (U.L.C. Baldos & Hertel, 2013).

Historical simulation of the SIMPLE model has also revealed significant challenges. In particular, while the first version of SIMPLE closely followed global crop production, it failed to reproduce the regional pattern of production changes over this period. This led the authors to introduce market segmentation, whereby individual consumers and producers in each region have differential access to world markets. At the aggregate level, this results in a constant elasticity of substitution between domestic and international goods on the demand side and a constant elasticity of transformation between domestic and international goods on the supply side. The resulting segmented markets version of SIMPLE (now the default approach) performed much better at the regional level and also resulted in very different consequences for a number of key sustainability policies (Hertel and Baldos 2016). Future work with SIMPLE-G will focus on its ability to reproduce historical patterns of land use change and irrigation intensities at the level of subnational regions and individual grid cells. This will provide the necessary foundation for policy-relevant, multi-scale modelling of future sustainability challenges.

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7 APPENDIX

At each grid cell, the SIMPLE-G explains the changes in crop production, land use, water use, nitrogen fertilizer application, and other production inputs. These changes are linked to the earth and environmental systems via several other modules. Section 7.1.1 summarizes the variables in the gridded production module. The variables are introduced in different categories comprising: value variables, quantity variables, price variables, efficiency (productivity) variables, policy or shock variables, and reporting variables.

7.1 Major variables of the model

Value	
VCROPgl	Value of crops produced by grid cell and land type
VLANDgl	Value of land input in crop production by grid cell and land type
VNLANDgl	Value of the non-land input in crop production by grid cell and land type
VWATERgl	Value of water input in crop production by grid cell and land type
VNITROgl	Value of nitrogen fertilizer input in crop production by grid cell and land type
Quantity	
QCROPgl	Quantity of crops produced by grid cell and land type
QLANDgl	Quantity of land input in crop production by grid cell and land type
QNLANDgl	Quantity of the non-land input in crop production by grid cell and land type
QWATERgl	Quantity of water input in crop production by grid cell and land type
QNITROgl	Quantity of nitrogen fertilizer in crop production by grid cell and land type
Price	
PCROPgl	Price index of crops produced by grid cell and land type
PLANDgl	Price index of land input in crop production by grid cell and land type
PNLANDgl	Price index of the non-land input in crop production by grid cell and land type
PWATERgl	Price index of water input in crop production by grid cell and land type
PNITROgl	Price index of nitrogen fertilizer in crop production by grid cell and land type
Efficiency	
AOCROPgl	Efficiency index of crops produced by grid cell and land type
AFLANDgl	Efficiency index of land input in crop production by grid cell and land type
AFNLANDgl	Efficiency index of the non-land in crop production by grid cell and land type
AFWATERgl	Efficiency index of water input in crop production by grid cell and land type
AFNITROgl	Efficiency index of N fertilizer in crop production by grid cell and land type
Policy and shock	
s_QWATERg	Policy variable for water quantity for crop production by grid cell
s_QNITROgl	Policy variable for N fertilizer in crop production by grid cell and land type
s_QLANDg	Policy variable for cropland extension by grid cell
t_PCROPgl	Policy variable for crop price by grid cell and land type
t_PNITROgl	Policy variable for N fertilizer price in crop production by grid cell and land type

Reports	
YIELDgl	Crop yield by grid cell and land type
WinCROPgl	Water withdrawal per ton of crop produced
WperAREAgl	Water withdrawal per ha of cropland

7.2 Gridded Crop Production Module

Crop production is defined as a function of input uses. All the production inputs are summarized in four major categories including land, nitrogen fertilizer, water, and non-land. Here, water refers to all the inputs related to irrigation. Also, non-land input consists of all other inputs including pesticides, herbicides, other fertilizers, labor, seeds, capital, etc. Depending on the biophysical characteristics of each grid cell and the choice of crop production technology, each location may have a unique composition of these inputs.

We assume a nested CES (constant elasticity of substitution) function allowing for the changes in the composition of the production inputs. This is a widely used functional form in the economics literature and has been proved an appropriate approach to model production. The substitution elasticity is a technical term and refers to a parameter that illustrates the changes in the relative ratio of inputs in response to changes in relative prices of inputs.

Here, we summarize the main equations of the gridded production module for all grid cells and all land types. The grid cells are indexed by *g*, and the land-types are indexed by *l*. Here, the land type refers to production technologies with different input use or production technologies, like irrigated and non-irrigated, or naturally pollinated and artificially pollinated, or organic and non-organic. However, the output of all the practices are similar. For each grid cell and land-type, the revenue from crop sale is assumed to be divided among the inputs according to their contribution. The change in gridded production is determined by:

$$\begin{aligned} p\_QCROPgl_{g,l} \;-\; p\_AOCROP_{g,l} \\ = SHR\_LANDgl_{g,l} * [p\_QLANDgl_{g,l} + p\_AFLAND_{g,l}] \\ + SHR\_NITROgl_{g,l} * [p\_QNITROgl_{g,l} + p\_AFNITRO_{g,l}] \\ + SHR\_NLANDgl_{g,l} * [p\_QNLANDgl_{g,l} + p\_AFNLAND_{g,l}] \\ + SHR\_WATERgl_{g,l} * [p\_QWATSGgl_{g,l} + p\_AFWATER_{g,l}] \qquad \text{Eq-A-1} \end{aligned}$$

where *p_QCROPgl* is the percentage change in the production of crops, and *p_AOCROP* is the percentage change in overall productivity index in crop production. This equation involves four share parameters: *SHR_LANDgl* is the share of land input in crop production, *SHR_NITROgl* is the share of nitrogen fertilizer input in crop production, *SHR_NLANDgl* is the share of the non-land inputs in the crop production, *SHR_WATERgl* is the share of water in crop production. Also, changes in inputs are considered with possibly different rate of productivity change: *p_QLANDgl* is the percentage change in land input, *p_AFLAND* is the change in land productivity index (land-augmented technical change), *p_QNITROgl* is the percentage change in nitrogen fertilizer input, *p_AFNITRO* is the change in nitrogen fertilizer productivity index (nitrogen-augmented technical change), *p_QNLANDgl* is the percentage change in the non-land inputs, *p_AFNLAND* is the change in the non-land inputs productivity, *p_QWATERgl* is the percentage change in water input, and *p_AFWATER* is the percentage change in water productivity.

This equation implies that any increase in the quantity of inputs of production can lead to an increase in crop outputs. Also, it is possible to increase the crop production via improvement in the overall productivity. However, an improvement in productivity of one input alone may have a smaller impact on the overall crop production as it goes through the related share parameter.

Note that the changes in inputs of production are determined endogenously in the model. For each input, the drivers of the change can be summarized in the scale effect and the substitution effect. The scale effect is related to the scale of production. If production increases by α%, in the absence of any substitution effect and technological progress, all the inputs will grow by α% (in economics terms, the production function is homogenous of degree one). However, if the relative prices change, the ratio of inputs will change. We call this the change in production technology. The substitution effect usually involves a relative reduction in one input and a relative increase in another input or a composite input bundle. For example, a shock may increase the application of nitrogen fertilizer but declines the water-land bundle for producing the same level of crop outputs.

Here, we describe the main input bundles in the model. We have two major bundles in the model: land-water bundle shown by *LANDWATER* and land-water-non-land bundle shown by *AUGLAND.* We will refer to the latter as the augmented land. The augmented land includes all the inputs except nitrogen fertilizer. The price index of the land-water composite is defined as:

$$
\begin{aligned}
& p\_PLANDWTRgl_{g,l} \\
& \quad = SHR\_LinLWgl_{g,l} * [p\_PLANDgl_{g,l} - p\_AFLAND_{g,l}] \\
& \quad + SHR\_WinLWgl_{g,l} * [p\_PWATERgl_{g,l} - p\_AFWATER_{g,l}] \qquad \text{Eq-A-2}
\end{aligned}
$$

where *p_PLANDWATER* is the percentage change in the land-water bundle*, SHR_LinLWgl* is the share of land in the land-water bundle, and *SHR_WinLWgl* is the share of water in the land-water bundle. Also, *p_PLANDgl* and *p_PWATERgl* show the percentage change in the price of land and water respectively. The price index for the augmented land bundle is defined as:

$$
\begin{aligned}
& p\_PAUGLANDgl_{g,l} \\
& \quad = SHR\_OinAUGgl_{g,l} * [p\_PNLANDgl_{g,l} - p\_AFNLAND_{g,l}] \\
& \quad + SHR\_LinAUGgl_{g,l} * [p\_PLANDgl_{g,l} - p\_AFLAND_{g,l}] \\
& \quad + SHR\_WinAUGgl_{g,l} * [p\_PWATERgl_{g,l} - p\_AFWATER_{g,l}] \qquad \text{Eq-A-3}
\end{aligned}
$$

where *p_AUGLANDgl* refers to the percentage change in the price index of augmented land bundle. Respectively, *SHR_OinAUGgl*, *SHR_LinAUGgl*, and *SHR_WinAUGgl* are the share of the non-land, land, and water in the augmented land bundle. Also, *p_PNLANDgl* is the percentage change in the price of the non-land input, and *p_AFNLAND* id the productivity index related to the non-land input.

In this framework, SIMPLE-G calculates the changes in individual input use as well as these aggregate bundles. It includes water use, land use, nitrogen fertilizer use, non-land use, land-water bundle, and augmented land bundle. Each equation is obtained by solving the economic optimization problem. Then we linearized all the equations. One of the production inputs that is explicitly considered in the model is nitrogen fertilizer. The demand for nitrogen fertilizer depends on production scale, *QCROPgl*, and price of nitrogen fertilizer, *PNITROgl*, relative to crop prices, *PCROPgl*, as well as productivity parameters. In the percentage change format, the demand for nitrogen fertilizer application is defines as:

$$p\_QNITROgl_{g,l} + p\_AFNITRO_{g,l} = p\_QCROPgl_{g,l} - p\_AOCROP_{g,l} - ECROPgl_{g,l} * [p\_PNITROgl_{g,l} - p\_AFNITRO_{g,l} - p\_PCROPgl_{g,l} - p\_AOCROP_{g,l}] \quad \text{Eq-A-4}$$

where *p_QNITROgl* is the percentage change in demand for nitrogen fertilizer, *p_AFNITRO* is the percentage change in nitrogen fertilizer productivity index, *p_QCROPgl* is the percentage change in the scale of crop production, p_AOCROP is the percentage change in the overall crop productivity index, and *p_PNIROGL* is the percentage change in the price of nitrogen fertilizer. Here, *ECROPgl* is the grid-cell specific elasticity of substitution between nitrogen fertilizer and the augmented land bundle. In other words, this parameter governs the ratio of nitrogen fertilizer application over all other inputs (For the SIMPLE-G-US-CS, this parameter is calibrated based on agronomic characteristics of AgroIBIS model). The demand for all other inputs is summarized in the augmented land equation:

$$p\_QAUGLANDgl_{g,l} = p\_QCROPgl_{g,l} - p\_AOCROP_{g,l} - ECROPgl_{g,l} * [p\_PAUGLANDgl_{g,l} - p\_PCROPgl_{g,l} - p\_AOCROP_{g,l}] \quad \text{Eq-A-5}$$

where *p_QAUGLANDgl* is the percentage change in the augmented land input bundle, and *p_PLAUGLANDgl* is the percentage change in the price index of the augmented land input bundle as defined in Eq-5. The augmented land consists of two other components: the land-water bundle and the non-land component, an aggregate index of chemicals, labor, capital, seeds, etc. In linearized form, the demand for the non-land input is defined as:

$$p\_QNLANDgl_{g,l} = p\_QAUGLANDgl_{g,l} - p\_AFNLAND_{g,l} - EAUGLANDgl_{g,l} * [p\_PNLANDgl_{g,l} - p\_AFNLAND_{g,l} - p\_PAUGLANDgl_{g,l}] \quad \text{Eq-A-6}$$

where *p_QNLANDgl* is the percentage change in the non-land input, *p_PNLANDgl* is the percentage change in the price index on the non-land input, and *p_AFNLANDgl* is the percentage change in the productivity index on the non-land input. Note that *EAUGLANDgl* is the substitution elasticity between the non-land input and the land-water bundle. The demand for land-water bundle is expressed similarly as:

$$p\_QLANDWTRgl_{g,l} = p\_QAUGLANDgl_{g,l} - EAUGLANDgl_{g,l} * [p\_PLANDWTRgl_{g,l} - p\_PAUGLANDgl_{g,l}] \quad \text{Eq-A-7}$$

where $p\_QLANDWATERgl$ is the percentage change in the land-water bundle, $p\_PLANDWATERgl$ is the price index of the land-water bundle as defined in the Eq-xx. Here, $EAUGLANDgl$ parameter governs the substitution between the land-water and non-land input. For example, it shows the increase in the non-land input (capital, seed, chemicals, etc.) when facing a relatively more expensive land-water bundle.

An important decision in crop production is the combination of water and land . The land use decision is not separated from water use decision. Considering the relative costs of land and water as well as their benefits, certain combination of land-water is economically optimum. The demand for land is derived considering these production possibilities. The linearized for of land demand in crop production is:

$$\begin{aligned} p\_QLANDgl_{g,l} &\\ = p\_QLANDWTRgl_{g,l} &- p\_AFLAND_{g,l} \\ - EIRRIGgl_{g,l} &* [p\_PLANDgl_{g,l} - p\_AFLAND_{g,l} - p\_PLANDWTRgl_{g,l}] \end{aligned} \quad \text{Eq-A-8}$$

where $p\_QLANDgl$ shows the percentage change in the land use, p_AFLAND is the percentage change in the productivity index of land, and $EIRRIGgl$ is the substitution elasticity between water and land. We already introduced $QLANDWATER$ and $PLANDWATER$ which are composite indices of water and land for crop production. Finally, the decision about water applied per area depends on the price of water relative to the price of land. Thus, the demand for water for crop production is determined by:

$$\begin{aligned} p\_QWATERgl_{g,l} &\\ = p\_QLANDWTRgl_{g,l} &- p\_AFWATER_{g,l} \\ - EIRRIGgl_{g,l} &* [p\_PWATERgl_{g,l} - p\_AFWATER_{g,l} - p\_PLANDWTRgl_{g,l}] \end{aligned} \quad \text{Eq-A-9}$$

where $p\_QWATERgl$ is the percentage change in overall irrigation demand, $p\_QLANDWATERgl$ is the percentage change in the water-land composite, $EIRRIGgl$ is the substitution elasticity between water and land, and $p\_PLANDWATER$ is the percentage change in the price index of composite land-water.

The water module includes three main decisions at the grid cell level about 1) the level of water withdrawal, 2) water conservation technology, and 3) water applied per area. These decisions are made in markets based on demand and supply forces and prices. The benchmark value of water is implied following Haqiqi et al. (2016).

The changes in the price of water applied is modeled by considering changes in the costs of water withdrawal and the changes in the price of water conservation technology, mainly capital equipment. Here capital equipment is considered as a substitute to water and thus helping to conserve water (for example, a decline in equipment prices may lead to lower water applied per area). Percentage change in water price is:

$$\begin{aligned} p\_PWATERgl_{g,l} \\ &= SHR\_WWinWgl_{g,l} * [p\_PWATSGgl_{g,l} - p\_AFWATSG_{g,l}] \\ &+ SHR\_WKinWgl_{g,l} * [p\_PWEQPTgl_{g,l} - p\_AFWEQPT_{g,l}] \end{aligned} \quad \text{Eq-A-10}$$

where *p_PWATERgl* is the percentage change in local price of water, *SHR_WWinWgl* is share of water withdrawal in irrigation costs, *SHR_WKinWgl* is the share of water conservation technology in irrigation costs, *p_PWATSGgl* is the percentage change in aggregate water (groundwater and surface water) price, *p_AFWATSG* is the efficiency index of aggregate water, *p_PWEQPTgl* shows the change in the price of water conservation technology, and *p_AFWEQPT* is the efficiency index for water conservation technology.

Changes in local water price and local water withdrawal is determined according to demand and supply forces. The water supply schedule reperesents the costs of water withdrawal. The linearized version of the water supply to each grid cell is:

$$p\_QWATSGgl_{g,l} = EWATSGgl_{g,l} * p\_PWATSGgl_{g,l} + s\_QWATERg_g \quad \text{Eq-A-11}$$

where *p_QWATSGgl* is the percentage change in total water withdrawal (surface water and groundwater), *EWATSGgl* is the supply elasticity of water, *p_PWATSGgl* is the percentage change in the price of water, and *s_QWATERg* is the slack variable for policy or shocks. Similarly, the supply of water conservation technology is determined by:

$$p\_QWEQPTgl_{g,l} = EWATKLr_g * p\_PWEQPTgl_{g,l} + s\_QWEQPTg_g \quad \text{Eq-A-12}$$

where *p_QWEQPTgl* is the percentage change in water conservation technology equipment, *EWATKLgl* is the supply elasticity of water conservation technology equipment, *p_PWEQPTgl* is the percentage change in the price of water conservation technology, and *s_QWEQPTg* is the slack variable for policy or shocks.

The decision about water withdrawal depends on water withdrawal cost (price) relative to the costs of water conserving technology and the benefits of irrigation. The linearized version of the demand for water withdrawal is:

$$p\_QWATSGgl_{g,l} = p\_QWATERgl_{g,l} - p\_AFWATSG_{g,l} - ESUB\_WKgl_{g,l} * [p\_PWATSGgl_{g,l} - p\_AFWATSG_{g,l} - p\_PWATERgl_{g,l}] \qquad \text{Eq-A-13}$$

where *p_QWATSGgl* is the percentage change in total water withdrawal (surface water and groundwater), *p_QWATERgl* is the overall irrigation demand, *ESUB_WKgl* is the substitution elasticity between water withdrawal and conservation technology, *p_PWATSGgl* is the percentage change in the price (cost) of water withdrawal, *p_AFWATSG* is the efficiency index of aggregate water, and *p_PWATERgl* is the aggregate irrigation water cost (including conservation technology).

Similarly, the decision about water conservation depends on water withdrawal cost (price) relative to the costs of water conserving technology and the benefits of irrigation. The linearized version of the demand for water withdrawal is:

$$p\_QWEQPTgl_{g,l} = p\_QWATERgl_{g,l} - p\_AFWEQPT_{g,l} - ESUB\_WKgl_{g,l} * [p\_PWEQPTgl_{g,l} - p\_AFWEQPT_{g,l} - p\_PWATERgl_{g,l}] \qquad \text{Eq-A-14}$$

where *p_QWEQPTgl* is the percentage change in water conserving technology, *p_QWATERgl* is the overall irrigation demand *ESUB_WKgl* is the substitution elasticity between water withdrawal and conservation technology, *p_PWEQPTgl* is the percentage change in the price (cost) of water conserving technology, *p_AFWEQPT* is the efficiency index of aggregate water, and *p_PWATERgl* is the aggregate irrigation water cost (including conservation technology).

Declaration of interests

☒ The authors, *U. L. C. Baldos, I. Haqiqi, T. Hertel, M. Horridge, & J. Liu*, declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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