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Feature Review

# Contribution of Crop Models to Adaptation in Wheat

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**With world population growing quickly, agriculture needs to produce more with fewer inputs while being environmentally friendly. In a context of changing environments, crop models are useful tools to simulate crop yields. Wheat (*Triticum* spp.) crop models have been evolving since the 1960s to translate processes related to crop growth and development into mathematical equations. These have been used over decades for agronomic purposes, and have more recently incorporated advances in the modeling of environmental footprints, biotic constraints, trait and gene effects, climate change impact, and the upscaling of global change impacts. This review outlines the potential and limitations of modern wheat crop models in assisting agronomists, breeders, and policymakers to address the current and future challenges facing agriculture.**

## Trends

Wheat is the most diversely adapted cereal, with yields ranging from $<1$ t ha$^{-1}$ in arid hot climates to $>15$ t ha$^{-1}$ in cool wet environments.

Modern crop simulation models predict growth, development, and yield as affected by soil, climate, crop management and variety.

Outputs of models facilitate pre-season planning, in-season management decisions, and forecasting of field, regional, and national yields.

In addition to optimizing yield, models are applied to reduce the risks of crop failure, improve grain quality, increase profitability, and/or reduce environmental impacts.

More recent trends in crop modeling are in assisting breeders to improve varieties and in predicting adaptation to climate change up to the global scale.

## Utility of Wheat Crop Models

Agriculture is currently facing great challenges to feed a growing population and to minimize malnutrition [1]. Modern human society largely derives calorific intake from the botanical family of grasses in one form or another – be it rice (*Oryza sativa*), wheat (*Triticum spp*.), maize (*Zea mays* L.), barley (*Hordeum vulgare* L.), sorghum (*Sorghum bicolor* Moench.), millet (*Pennisetum glaucum*), or pasture grasses. Field production of these crops requires the balancing of interacting factors associated with crop **genotype** (see Glossary), the **environment**, and **crop management practices**. Jointly, these factors influence the efficiencies with which solar radiation, water, and nutrients are captured and used by a crop to produce calories and nutritional value.

In the mid-1960s, crop processes began to be viewed quantitatively and were represented by relatively simple mathematical formulations that could be encoded as models into computers [2]. Many developments in **crop models** arose for wheat, which is the most extensively grown commercial crop and provides more than 20% of the human calorie and protein diet (FAOSTAT 2014, Food and Agriculture Organization of the United Nations, http://www.fao.org/faostat/en/#data). Current wheat models depict, with different levels of detail, the timing of the appearance and death of organs, including the leaf surface which intercepts radiation and roots which take up water and nutrients (Box 1). These models further define how plants utilize absorbed energy and chemically reduce $CO_2$ to carbohydrates, how assimilates are partitioned to stems, roots, leaves, ears, and grains, and how physiological processes are moderated in their efficiency and magnitude by excess or deficit of water and nutrients. By integrating crop processes and their response to internal and external cues, crop models are useful tools to improve our understanding of how crops develop, grow, and yield. In addition, they allow the extrapolation of results from a limited number of experiments to a wide range of conditions, and thus they are

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 http://dx.doi.org/10.1016/j.tplants.2017.02.003

### Box 1. Wheat Crop Model

Crop models simulate crop growth and development (outputs) as influenced by climate conditions (typically solar radiation, temperature, and rainfall), soil characteristics (e.g., rooting depth, water holding capacity, nitrogen mineralization capacity) and crop management (e.g., sowing date, plant density, fertilization, irrigation) (inputs) based on mathematical equations and cultivar-specific parameters (inputs). While modern wheat crop models vary in their complexity, most simulate crop growth and development at a daily time-step to ultimately estimate grain yield. Crop processes include phenology driven by temperature and photoperiod, the establishment of the canopy that transpires water and intercepts light to produce the crop biomass, and the partitioning of this biomass into different organs including grains (Figure I). Modeling of soil water and nutrient varies between models, and ranges from simple approaches with no soil description to more complex approaches where soil layers are each described with specific properties. Details on some wheat crop models can be found in [21,136].

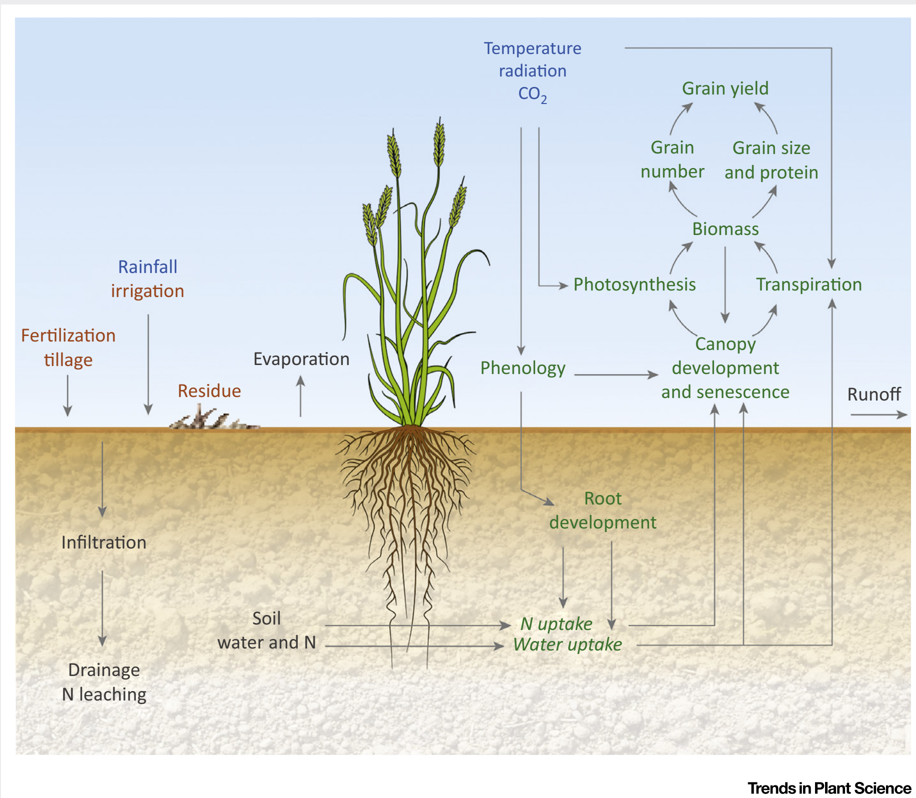


Figure I. Simplified Framework of a Wheat Crop Model. Wheat models typically take daily weather data (blue), crop management practices (brown), and genotypic parameters as inputs. They simulate water and nutrients movements in the soil and atmosphere (grey), and the processes (green) occurring within the crop and in interaction with the environment. Stress impacts related to water, nitrogen (N), or other abiotic factors (e.g., phosphorus, chloride) are not depicted on the figure. Note that only one plant is represented on this schematic, whereas wheat crop models simulate crops at field density.

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valuable for predicting and projecting how internal (e.g., trait, gene) and external factors (e.g., weather, management) impact on crop performance.

In the past decade(s), crop models have evolved to consider (i) integrated cropping systems combining profitability and sustainability, with in particular the development of grower-ready tools and simulations of the production and movements of pollutants, (ii) grain quality, (iii) biotic effects, (iv) gene-to-phenotype effects incorporating physiological processes and their underpinning genetics, and (v) specific responses to new climatic factors (e.g., heat stress, $CO_2$, and $O_3$). Furthermore, in the face of modern agricultural challenges, other new developments have also appeared that (vi) project impacts at the global scale, and (vii) anticipate climate change effects and propose potential adaptations.

This review outlines the potential and limitations of current wheat models for applications ranging across the areas of agronomy, breeding, global impact, and climate change.

## Agronomy

While wheat crops have been cultivated for 8000 years, recent developments in management practices and wheat genetics have led to substantial crop yields of up to 16.5 t $ha^{-1}$ (the 2015 world record, achieved in the UK). In part these improvements have been related to the use of crop models in research over the past 50 years. Nowadays, wheat crop models allow growers, researchers, and policymakers to evaluate potential gains and risks of new agronomic techniques, to predict the outcome of crop expansion into new areas, to investigate the adaptation of new cultivars, and to respond to challenges regarding crop productivity, food quality, and sustainability.

### Adapting Management To Enhance Sustainable Crop Productivity

A common use of wheat crop models has been to determine the factors that limit wheat productivity and quantify the 'yield gap' between achievable and farmers' yields [3]. Multiple studies have assessed management impacts related to, for example, tillage methods [4], weed control [5], planting methods [6], irrigation [7], and fertilization [8] in diverse environments (Figure I in Box 2). Over time, a greater focus on cropping systems has resulted in an emphasis on identifying sets of best-management practices to maximize long-term productivity and profitability [9].

While crop models have been applied either directly or indirectly to assist farmers, consultants, extension specialists, policymakers, and retailers [10], their use in specific commercial applications (e.g., advice for an individual farm) remains potentially costly. To tackle this issue, custom-built tools and communication strategies have been developed [11,12]. For instance, YieldProphet®, a broadly used web application in Australia, exploits wheat simulations to provide timely risk assessments in a digested format to farmers and advisers, and these allow them to manage climate risks and make informed decisions about fertilizer application in their fields [13]. Combining modeling results with socioeconomic information is now typically part of these tools, for example in providing recommendations for best nitrogen and/or irrigation management to maximize sustainability goals [14]. At present, most of these tools operate on a point or field basis, with the necessary data often needing to be manually entered. In the near future, the costs of delivery of this type of knowledge should greatly decrease as commercial providers start to use public and private databases of weather, soils, topography, and field boundaries to prepopulate and conduct simulations for all management zones on a farm.

The impact of agriculture on the environment is a growing concern, and farming system models (which incorporate crop models) can assist in the design of strategies that both increase (or maintain) wheat productivity and profitability while minimizing the environmental footprint [1]. In the past decade, farming system models have been used to assess the long-term impact of agronomic practices such as crop rotation, tillage, residue management, and organic amendments on environmental outcomes such as nitrate leaching [15,16], nitrous oxide emissions [17], and soil carbon retention and losses [17,18]. Economic and environmental impacts of cropping systems have also been assessed in simulation studies, for example by quantifying how forage legumes can reduce runoff and improve drainage while greatly improving wheat yields [19,20].

## Glossary

**Allele:** one of the alternative forms of a gene. A gene typically has several alleles, and different alleles can result in different phenotypes.

**Crop management practice:** farming intervention related to cropping, for example sowing date, planting density, irrigation, and fertilization.

**Crop model:** a model that uses mathematical equations to describe crop growth and development as influenced by environmental conditions and crop management. Crop models typically simulate crop dynamics at a daily time-step and generate outputs such as biomass and yield. They generally consider abiotic factors such as temperature, radiation, water, and nitrogen but do not simulate the influence of weeds, pests, or diseases.

**Data sampling (for spatial upscaling):** selecting a subset of a population; for example considering a subset of locations to represent a wider area.

**Data aggregation (for spatial upscaling):** multipoint representations of spatial variability gathered into homogenous spatial areas within which the variability is considered as relatively small for the processes studied.

**Ecophysiological process:** plant response to an environmental factor.

**Emergent property:** phenotype arising from the interactions of system components.

**Environment:** growing conditions characterized by weather and soil characteristics.

**Gene-to-phenotype model:** model that simulates the effects of genes or genomic regions (e.g., quantitative trait loci) on traits affecting crop growth and development.

**Genotype:** heritable information carried by the genome.

**Genotype × nvironment (Ge × E) and genotype × environment × management (G × E × M) interactions:** interactions between the genotype (G), the environment (E), and the crop management (M) that influence the phenotype. These occur when genotypes respond differently to environmental variations and/or management practices. Note that the effects of the management practices on crops can be viewed as the effect of management practices on the crop environment, in other

With the broadening of model applications, concerns include the reliability of simulation results and their applicability in different conditions. While wheat models have been tested for crop management options in countries around the world (Figure I in Box 2) [21,22], broad-scale applications can be limited [10] given that, for example, most wheat models have rudimentary sub-models of root systems and do not consider soil constraints such as soil acidity [23], salinity, and subsoil toxicities. The range of applications for each specific model depend on the science and the **model parameters** embedded in the model. Under new conditions (e.g., new cultivar, new region), models should be evaluated against experimental data [24]. Reliable **model outputs** require high-quality **model inputs** of local weather, soil, and genotype characteristics (Box 1), with the major uncertainties typically relating to genotype parameters and soil conditions (e.g., soil characteristics, initial soil water, and soil mineral N). While crop models normally portray fields as having homogeneous soil characteristics, the reality may be substantially different; for example, large-field spatial variability can affect the dynamics of water movement in the landscape. To address situations such as this, multiple interconnected subregions may be constructed to simulate these dynamics at the farm [25] or catchment [26] level, albeit with the requirement for detailed field measurements during calibration, testing, and implementation [27].

The scaling of models down to subfield levels underpins the potential of 'precision agriculture' which began in the 1990s with the introduction of geospatial technologies and mobile sensors, typically mounted on tractors. Harvesters with yield monitors, together with imagery from airborne, satellite, and soil-sensor data (e.g., electrical resistivity tomography) allow the capture of spatial variation down to a resolution of a few $m^2$. Crop models can assist in analyzing such spatial variability and in interpreting changes in spatial patterns over time [28]. They are also used to develop prescription maps [29] resulting from simulations of large combinations of inputs and their timing, which aim to increase resource use efficiency by applying the right input at the right place and at the right time. For crops such as maize, sophisticated planters can then be used to vary the plant spacing or type of seed by location, while sprayers can adjust the quantity and type of fertilizer, fungicide, or pesticide by location. The expectation is that high-resolution spectral and thermal imagery, coupled with crop yield models and weather data and forecasts, will allow wheat stakeholders to exploit in-season spatial observations using these 'variable rate technologies' (VRTs). In the near future, such an integrated approach will attempt to provide a prescriptive crop management plan at high spatial resolution comprising automated in-season crop simulations, management recommendations, risk assessments, pest management prescriptions, and accurate harvest recommendations via apps, websites, or smart phones.

### Modeling Grain Quality To Improve Management Decisions

Food quality and nutrition has been identified as one of the great challenges for global food security [30]. Wheat quality encompasses many criteria that depend on the intended market and also change along the grower-to-consumer chain (e.g., grain size, protein concentration, milling performance, baking quality, or nutritional value). For example, high-protein flours are required for leavened bread or pasta, while a low protein content is desirable for biscuits, crackers, cake, or oriental noodles. To deal with these issues, crop models require the ability to simulate year-to-year variation in grain quality aspects across different environments and crop management practices.

Grain protein concentration has a low **heritability** and can vary considerably in response to climate and crop management. Owing to the physiological antagonism between grain protein concentration and yield in wheat, genetic improvement of yield has typically resulted in a decrease in grain protein concentration [31]. In future years, an elevated atmospheric $CO_2$ concentration is expected to further contribute to the negative trend of grain protein

words M can be considered as a sub-component of E. In addition, in utilizing resources (such as soil water and nitrogen) differently over time, genotypes influence some components of their own environment.

**Heritability:** statistical estimate of the proportion of variation in a phenotypic trait that is due to genetic variation rather than to the environment.

**Ideotype:** idealized phenotype of multiple traits that are expected to provide the best adaptation to a given environment and management system.

**Model inputs:** data required to run the model. They typically include soil, weather, management, and cultivar information.

**Model outputs:** data resulting from the model simulations (e.g., flowering date, daily biomass, grain yield, grain protein concentration).

**Model parameters:** quantitative coefficients that define the model. For instance, cultivar-specific parameters typically include sensitivities of development rate to photoperiod and vernalization in wheat.

**Phenotype:** observable characteristics or traits of an organism. A phenotype results from the expression of a genotype as well as from the influence of environmental (including management) factors and interactions between the two.

**Quantitative trait loci (QTLs):** genomic regions that partially correlate with the variation in a quantitative trait (phenotype).

**Target population of environments (TPE):** the ensemble of conditions (including impact from management) that a commercially cultivated crop is likely to experience in a given geographic area.

## Box 2. Impact of Management Practices on Wheat Crops

Crops are sensitive to their environments and management practices, such as sowing dates, irrigation, and fertilization. Sowing a spring wheat crop too early may led to losses due to frost around flowering in some environments [81], while a late sowing may lead to heat and drought stresses [69,113]. Similarly, the timing and intensity of irrigation and fertilization influence crop growth and development, as well as the risk of nutrient leaching. Figure I illustrates how a crop model can predict wheat yield for a large range of management practices across various environments.

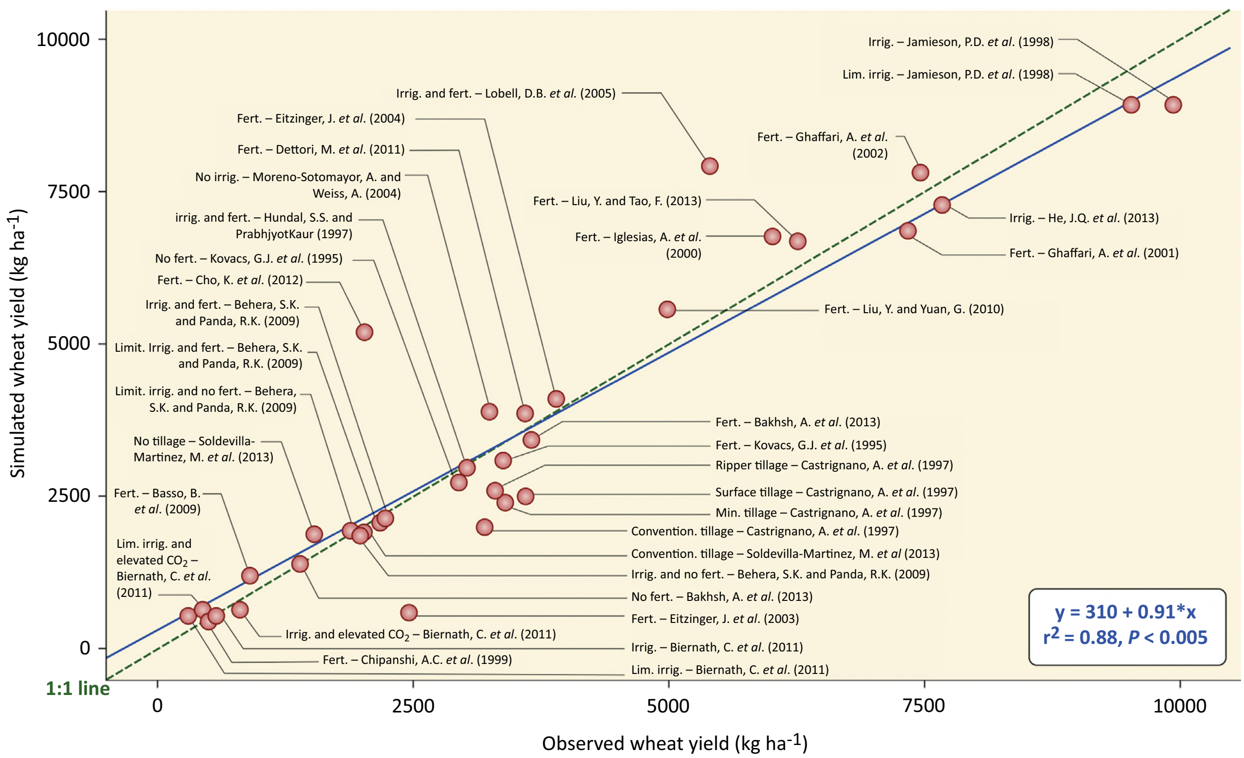


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Figure I. Simulations of Wheat Yields for Contrasting Crop Management Practices in a Broad Range of Environments. The quality of the CERES wheat model was assessed in a meta-analysis using 215 peer-reviewed papers where simulations were compared against field-observed data. Across most testing conditions, the model simulated observed wheat grain yield with a root mean square error of less than 1000 kg ha$^{-1}$. These results demonstrate the ability of modeling to accurately simulate crop growth and development over a wide range of locations and treatments. Data from the literature cited in [20]. Abbreviations: convention., conventional; fert., fertilization; irrig., irrigation; limit., limited; min., minimum.

concentration [32], increasing the urgency to better manage this trait. Several wheat models simulate crop nitrogen (N) status and grain protein concentration [24], but the uncertainty in predicting grain protein concentration is generally high, with an error of up to two percentage points [33]. However, such errors can be overcome by considering the physiological processes leading to grain dry mass and N accumulation in the model. The most advanced models in terms of protein simulations are able to reproduce the effect of environmental factors [34,35] that influence the generally negative relationship between grain yield and protein concentration [36].

In mature wheat grains, the grain storage proteins (gliadin and glutenin) account for 70–80% of total reduced N and greatly influence grain processing and nutritional quality [37]. In wheat, the amount of the different storage protein classes is related through allometric relationships to the total amount of N per grain [38], which has been used to simulate gliadin and glutenin accumulation in developing wheat grain [39,40]. Recently, candidate genes (transcription factors) determining the value of the model parameters were identified [41], and these could be used to simulate the effects of the genetic basis of grain quality.

The high proportion of 'screenings' (suboptimal sized grains) is another quality aspect which has been simulated in a limited number of studies using an empirical relationship [42]. In the future, a more mechanistic approach could potentially capture this effect by using a single-spike sub-model controlling the rate of assimilate deposition into the grains based on their position in the spikelets and florets [43].

Opportunities exist to model other processes related to grain quality in wheat. First, modeling the accumulation of grain sulfur, which influences the composition of protein fractions by regulating the expression of individual storage protein genes [44], would be a step toward simulating dough processing quality [45]. Second, modeling the aggregation of glutenin would be an important step to simulate dough strength because these polymeric proteins give the dough its viscoelastic properties [46]. In addition, modeling the influence of high temperature (above 30 °C) on glutenin aggregation, which causes dough weakening [47], can be seen as a priority for modeling wheat processing quality in the context of global warming. Third, crop models could be improved to simulate grain starch composition because the size distribution of starch granules is an important factor for cereal grain milling yield, rheological properties, and starch digestibility [48]. Such a phenomenological model of the waves of starch granule protrusion and growth could be built based on current knowledge [49], and account for **genotype × environment (G x E) interactions**, notably on starch response to temperature [50]. Finally, grain hardness (endosperm texture) is an important quality attribute in wheat for most markets. However, this trait is mainly determined by well-characterized genes and shows little environmental variation [51]. It has thus not been considered in wheat crop models but could be included if needed.

### Weeds, Pests, and Diseases

Weeds, pests, and diseases currently affect wheat production by ~28% worldwide [52]. The impact of these agents is likely to accelerate with climate change in ways that are not yet predictable [53]. As a result, increasing attention is drawn to the need to model these biotic stresses particularly for less-intensive and lower-yielding production systems, such as in Africa, where the relative importance of these factors in reducing yields is greater [54]. Integrating crop models with weed/pest/disease models is required to assist decision making for farmers both in the short term (e.g., when to spray?) and long term (e.g., rotation strategy), but also for policymakers (e.g., pollution issues, spread of herbicide-resistant weeds).

Historically, crop models and weed/pest/disease models have evolved in parallel, and interactions between these entities have been considered with different levels of complexity. Early simplified modeling approaches based on crop growth represented injuries as reducers of intercepted radiation or of radiation use efficiency [55]. Later, simple crop models have been employed to develop more detailed yield-loss simulation models for pests (e.g., aphids [56], weeds [57], and diseases such as eyespot [58] and brown rust [59]). However, combinations of well-developed crop and weed/pest/disease models remain rare (e.g., with populations of weeds [60] or rust fungal disease [61]). Opportunities exist to extend those new models to other weeds, pests, and diseases, and to upgrade them by developing innovative modeling frameworks related to (i) software engineering, because existing models currently require detailed knowledge of both models, and (ii) more-advanced scientific representation of systems dynamics [62]. In particular, the point-focus of crop models (i.e., field) is a limitation for spatially migratory dynamics of biotic stresses, which can include uncultivated landscape elements (e.g., hedges or roads), other fields, catchments, or regions. Another limitation relates to the instability of the population dynamics of some weeds (seed banks) and pathogens, with growth dynamics often being poorly understood. Therefore, probabilistic approaches, independent from crop dynamics, have generally been favored for weed/pest/disease population models [61]. As crop models and weed/pest/disease models improve in simulating their subsystems, combining these models is opening new opportunities to represent and explore the crop-pest dynamics of cropping systems.

## Breeding

By 2050, the world demand for wheat is expected to increase by 70%, requiring an annual production improvement to increase from its current level of <1% [63] to at least 1.7% [64]. In parts of the world, recent improvements in wheat yields have been modest, partly due to changes in climate counter-acting progress in plant improvement [65]. One of the major factors impacting on yield progress is year-to-year variability in abiotic stresses such as drought and heat. To complicate the task, it takes about 8–12 years to produce a new wheat cultivar, thus highlighting the potential value of crop models to assist wheat breeding in producing varieties adapted to current and future environments in combination with adapted agronomic practices [66,67]. In this context, some wheat models have been enhanced to better serve plant breeding needs. As shown in Figure 1, current and prospective enhancements include the use of crop modeling to (i) characterize the environment that wheat crops experience to better account for environmental variability; (ii) assess the value of physiological traits in targeted environments to focus research on promising traits; (iii) evaluate the potential effects of genetic controls on wheat yield in relevant environmental conditions; (iv) de-convolute G $\times$ E interactions in statistical models; and (v) utilize high-throughput phenotyping to identify 'hidden' traits of interest.

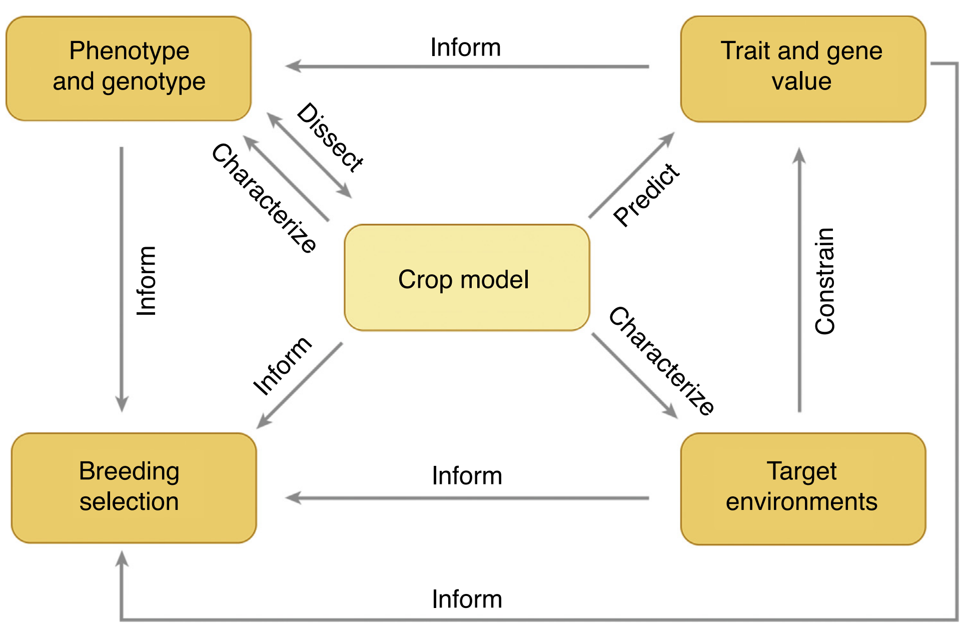
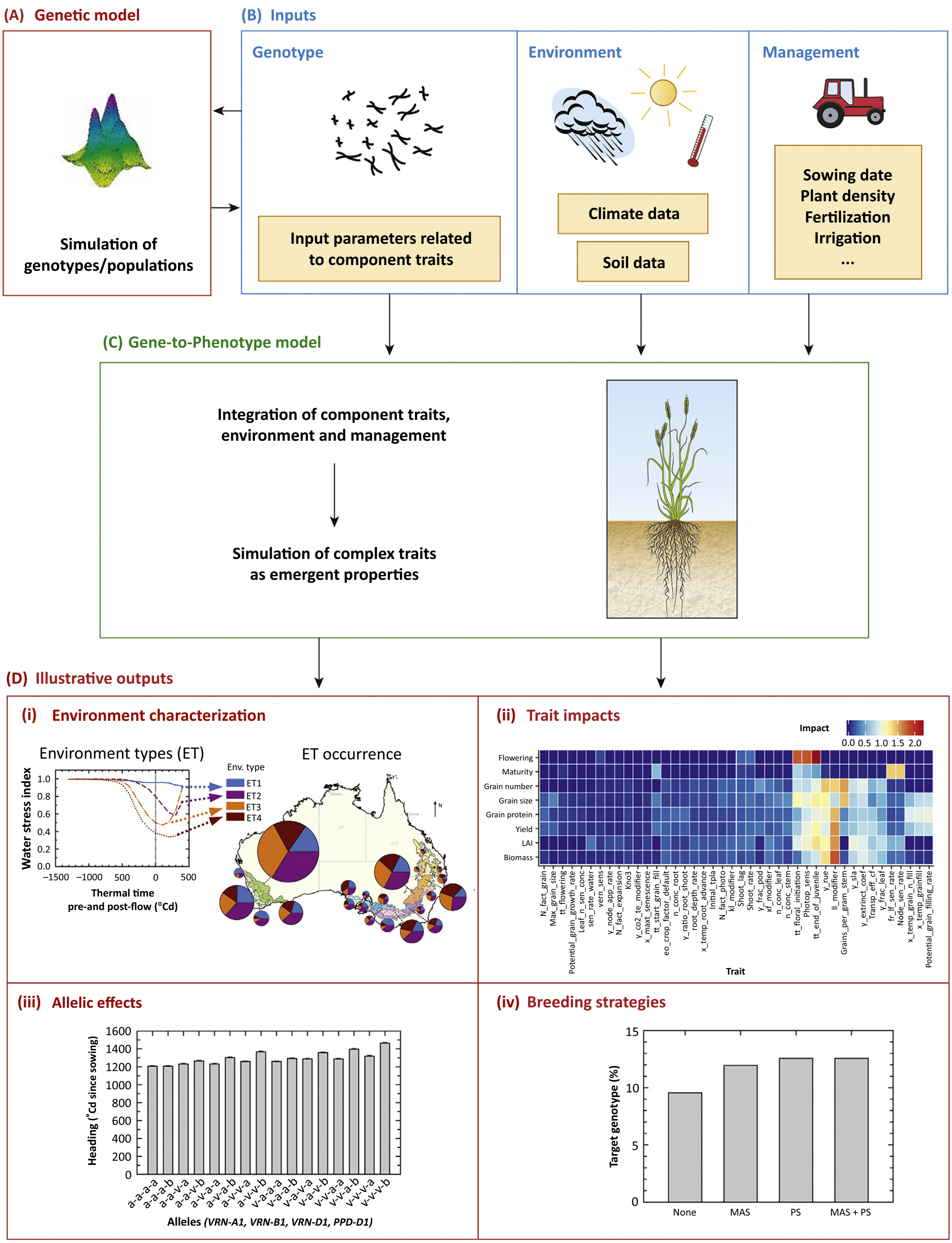



Figure 1. Role of Crop Modeling in Breeding. Crop models can be used to (i) dissect complex traits into simpler components traits, (ii) characterize environments of the target population of environments to identify the main environment types and their frequency, (iii) simulate the impact of traits and genetic controls on end products such as yield, and (iv) inform breeding via integrated analyses with breeding-system models.

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### Environment Characterization

Crop modeling allows the characterization of stress indices that depict the stress a crop is experiencing based on the weather, soil characteristics, and crop status. For instance, for drought stress, crop modeling reflects the impact of stress (Figure 2Di) originating from environmental variations in the timing and amount of water availability [68], from genetic variations (e.g., long-season cultivars are more likely to be affected by late water stress [69]), and/or from nutrient levels or biotic stresses, which interact with water deficits [70]. The use of crop modeling to characterize wheat trials in terms of drought stress [68] or phenology-based indices [71] has been shown to be useful to unravel complex G $\times$ E interactions. Such results open a promising avenue for breeding purposes [66,72], as demonstrated in maize [73].

Environment characterization with modeling can also be performed at a large-scale, over a long-term period, and for both current [69] and future [74] climates (Figure 2Di). Modeling allows comprehensive samplings of environments relevant to the cropping system in oder to define the **target population of environments** (TPE). Such 'big-picture' characterizations inform breeders about environmental spatial and temporal variability, and can assist decisions on the portfolio of cultivars to be delivered to a region, for example where long-season, drought-tolerant cultivars might be needed.

Breeding trials carried out in a single year may diverge from the TPE, potentially causing selection to divert away from the optimum for the TPE. Model-based environment characterization enables breeders to adjust for such deviations by weighting trials according to how well they represent the TPE. This method has been shown as an effective way to increase the value of collected data and improve selection towards elite germplasm with better performance in the TPE of wheat crops [73,75]. It could also be applied to anticipated TPEs associated with future climates.

Finally, modeling of environment characterization has also been applied to wheat pre-breeding programs to simulate the water-stress pattern as the season progresses and to assess the value of alternative irrigation schedules, for example. In this way, dynamic in-season modeling is used to target specific stress patterns of interest to improve the relevance of field phenotyping compared to trials with no control on year-to-year variability [76,77].

### Trait Value

Variations in wheat productivity and nutritional value arise from interactions of physiological traits across the season. To capture these effects, algorithms of physiological processes in crop models are being revised to better account for trait $\times$ trait interactions within a crop and to improve predictions of G $\times$ E interactions. Over the past decade, the impacts of specific physiological traits have been studied in current [78,79] and future [80,81] climate scenarios (e.g., Figure 2Dii). Recently, broad-scale analyses of crop-model parameters have identified potential candidate traits to be considered for wheat improvement in the studied environments [82,83]. Such results are highly valuable to quantify trait values as a function of different **genotype $\times$ environment $\times$ management (G $\times$ E $\times$ M) interactions**, but, together with

Figure 2. Illustration of Using Crop and Gene-to-Phenotype Models To Assist Crop Improvement. Gene-to-phenotype models have genotypic, environmental, and management inputs and can be used in combination with genetic models. Outputs of potential value for crop improvement include (Di) characterization of the environment that the crop experiences (presented here for drought environment types for the Australian wheatbelt [69]), (Dii) assessment of the impact of component traits on more complex traits such as grain yield (presented here for Australia [83]), (Diii) quantification of the effect of genes or quantitative trait loci (presented here for the effect of alleles of phenology genes *VRN-A1*, *VRN-B1*, *VRN-D1*, and *PPD-D1* on heading time across the Australian wheatbelt; based on data from [88]), and (Div) estimation of the value of breeding strategies (presented here for the impact of selection alternatives based on grain yield ('none'), marker-assisted selection ('MAS'), phenotypic selection ('PS') or both ('MAS + PS') on allele frequency of target genotypes [62]). Simulations performed with the APSIM model. Figure adapted from [22,62,69,83,88]. Abbreviations: °Cd, degrees C days; flow., flowering; LAI, leaf area index.

so-called **ideotypes**, they should be considered with caution. For such *in silico* approaches, a comprehensive understanding of the underlying hypotheses is needed because typically (i) variations in the input traits considered may not reflect existing genetic variability (which may not be known); (ii) combinations of trait values considered in such studies may not be physiologically or genetically achievable (e.g., because of pleiotropic trait effects and/or epistatic interactions); and (iii) crop models cannot account for all the interactions occurring among traits. Benefits of ideotype design may thus be conceptual in guiding breeding rather than representing 'absolute' benchmarking of targets [84]. Interpretation of simulation analyses needs to be combined with physiological and genetic knowledge to design trials and selection protocols that best direct resources toward the recombination of promising traits.

The ultimate potential of combining genetic and physiological knowledge via models can be realized via genomic selection, where the projected value of a trait can be used directly by breeders to pre-select germplasm based on their DNA profile measured on single seeds (as has been done for other crops such as maize [73]). This strategy increases the effective throughput and efficiency of breeding resources through the pre-selection of a greater proportion of promising germplasm for field testing.

### Gene-to-Phenotype Modeling

Agronomic traits are typically complex in nature because they depend upon a multitude of genes that often exhibit small individual effects and result in significant G × G (epistatic) and G × E × M interactions. Such traits are thus 'context-dependent' and may be dissected into 'simpler' component traits that are more robust across genetic backgrounds and environments (i.e., 'context-independent' traits) [85,86]. An essential advantage of building models based on robust physiological traits is that (i) their parameters may be more closely linked to **quantitative trait loci** (QTLs) and genes [85,86], and (ii) they allow complex traits to be simulated in a more realistic way as **emergent properties** that arise from the interactions among component traits and with the environment [87]. However, examples remain rare in which we have sufficient quantitative knowledge about the genetic controls on physiological processes. Recently, the effect of genes related to phenology have been modeled in wheat, allowing the simulation of heading dates from 210 spring wheat lines across 190 environments with a root mean square error of 4.3 days (Figure 2Diii) [88]. Further development of **gene-to-phenotype modeling** could be pursued based on (i) promising results for traits such as transpiration rate response to vapor pressure deficit [89], N uptake, root growth and architecture [78,90,91], grain storage protein composition [51], or based on (ii) progress made in other crops such as maize (e.g., impacts of genetic controls associated to leaf elongation [92]).

With the rapid development of genomic selection, new avenues are opening to link modeling with applied breeding. Gene-to-phenotype/crop models are being integrated to genomic selection to increase the accuracy in predicting untested genotypes in untested environments. In maize, such an integrated approach has been demonstrated *in silico* to be more accurate than the classical whole-genome prediction method [93]. With a sufficiently resolved physiological model and appropriate genetic studies, such a strategy could be applied to wheat populations.

When combined with breeding-system models, gene-to-phenotype models can also provide information to breeders with respect to the efficiency of alternative breeding strategies. For instance, they can be used to assess how traits would likely be selected over breeding cycles in different sampling environments (as previously done in sorghum [94]), or which breeding crosses are projected to more quickly increase the frequency of beneficial **alleles** (Figure 2Div) [95]. The combination of genetic and crop model provides a framework to explore the implications of interactions between the genetic architecture of traits, the selection environments, as well as other breeding strategies [66,73,93]. Such an integrated approach also provides hypotheses for further experiments and tests of our current understanding, thus offering a foundation for defining priorities in research (physiology, genetics, and modeling) and for assisting the design of efficient breeding strategies.

## Links to Phenotyping

Physiological dissection and modeling inform the targeting of candidate traits and appropriate environmental conditions. However, the genetic controls underlying candidate traits can be difficult and expensive to phenotype for a large number of genotypes, and proxy traits may be needed to enable high-throughput phenotyping. The recent and fast development of new technologies for high-throughput phenotyping both in controlled environments (for stable, scalable traits) and in the field is now opening new avenues [96,97]. Tighter relationships between modeling and phenotyping approaches are to be encouraged to direct resources

### Box 3. Methods and Uncertainty Related to Upscaling

Because crop models have been developed for field-level studies, scaling up from the field to the globe adds uncertainty to output results. Sources of uncertainty can come from input data (weather, soil characteristics, management, cultivar information), the model itself (structure and parameters), and the chosen upscaling method (Figure I).

Different methods of scaling up crop models are available. They typically concern the manipulation of data (e.g., average of model input or output data), the alteration of model parameters (i.e., adjustment of model parameters for the scale considered), or a change in the model structure (e.g., model simplification by consideration only of processes that matter at the larger scale) [118]. Most commonly applied methods of upscaling refer to **sampling** of representative locations within a larger area (i.e., simulating specific sites) or to **aggregation** of input data (e.g., averaging of site information) before a simulation is carried out.

The errors in simulating, for example, yields at larger areas can be estimated by comparing the results from these methods with simulations at high resolution (Figure II) or with observations [119]. Average deviations (bias) or change in variability between high- and low-resolution estimates inform about the error and likely uncertainty in impact studies. For instance, uncertainty due to data aggregation is particularly high in regions with high spatial variability [106].

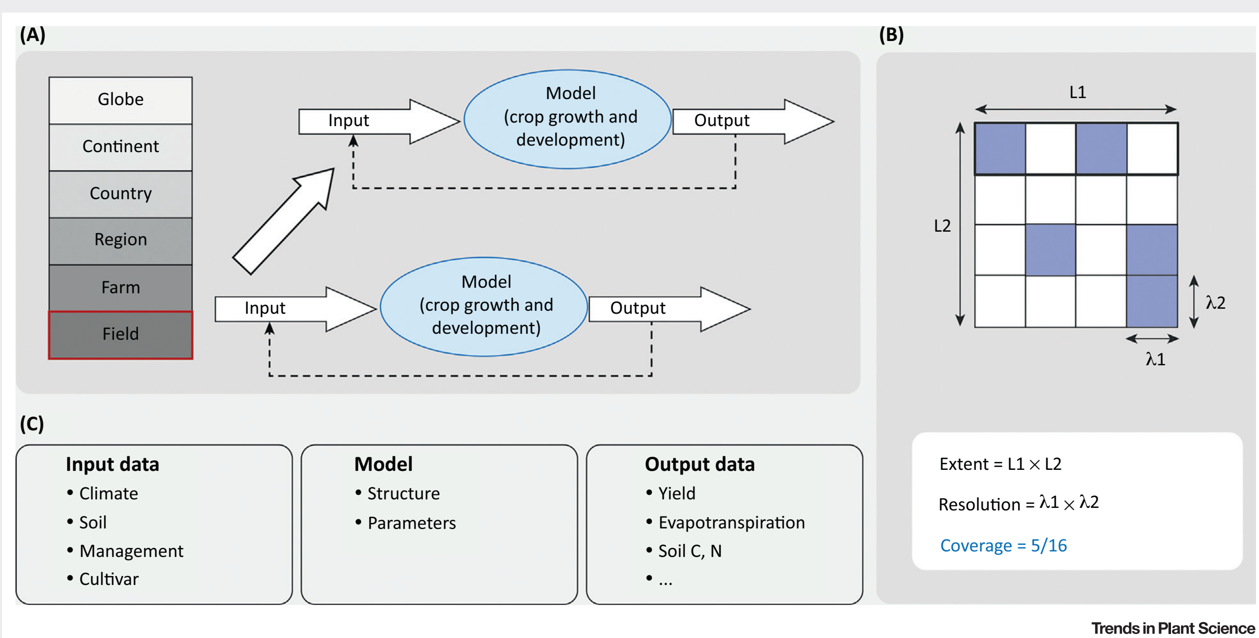


Figure I. Upscaling from the Field to a Larger Area. Upscaling, for example from small regions to the globe (A), results in uncertainty which is related to (B) sampling or aggregation methods (the spatial sampling, the aggregation of an area, or the incomplete spatial information of a grid cell, also referred to as coverage) and to (C) the input data and the model structure and parameters.

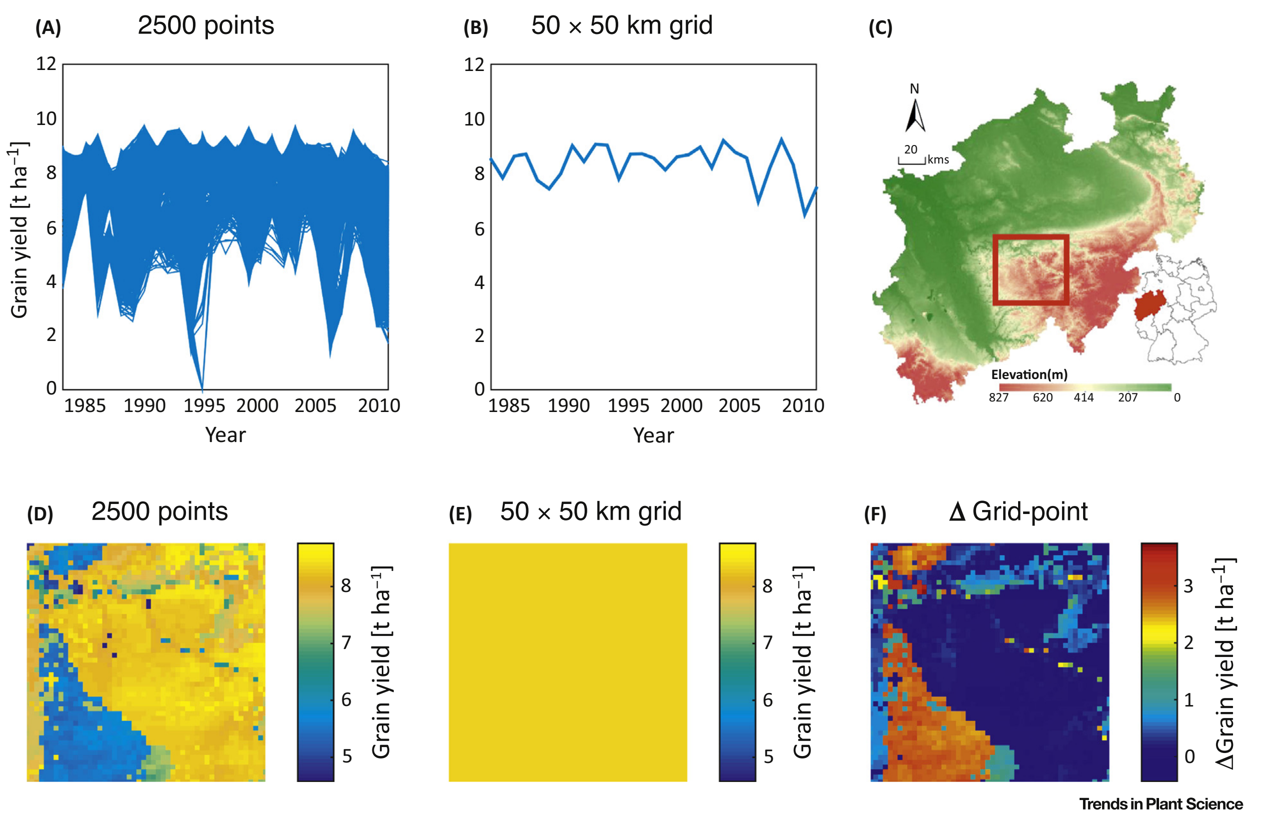


Figure II. Simulations of Winter Wheat with the Simplace LINTUL5 Crop Model for Different Time and Space Resolutions and Associated Errors. Illustration for yield simulations over 30 years for a 1 × 1 km grid at 2500 locations (A,D) or for a large grid at a single point (B,D) for a 50 × 50 km region in Germany (C). Year-to-year variations in yield are presented in (A) and (B), while spatial variations of average yield are presented in (D) and (E). The spatial errors (F) from low-resolution (50 × 50 km) sampling are calculated by comparison to the higher-resolution (2500 points) data ([108,109] for more details).

towards the phenotyping of repeatable 'context-independent' traits rather than the traits that seem easiest to phenotype (e.g., plant dimensions) [76,86,98,99].

Crop modeling can further facilitate phenotyping, for example by using 'inverse modeling' to quantify 'hidden' trait phenotypes. **Ecophysiological** models have been used to estimate traits that could not be measured on a large number of genotypes owing to resource or technical constraints. For instance, inverse modeling allowed the estimation of internal pools of carbon for a diversity panel of rice [100]. Similar model-based phenotyping could be applied in breeding trials to analyze crop growth, phenology [88,101], and stress levels. The development and deployment of such phenotyping-modeling technologies has the potential to increase breeding efficiency by allowing the estimation of component traits that are difficult to measure in large breeding populations, and by allowing the characterization of the environment experienced by individual genotypes (which may explain part of yield variations within a single field experiment).

## Modeling at the Global Scale

The complexity of the issues posed by food security, environmental footprints, and climate change impacts [1] requires global approaches. Accordingly, crop models are increasingly used for large regional to global assessments to explore productivity and sustainability options across diverse environments [102,103]. Applications range from an experimental plot to a field [68,104], farm [105], region [3,106], continent [69], up to the global scale [107].

Because the original scale for crop models corresponds to a plot or homogenous field, any transfer of crop model simulations to larger spatial scales introduces uncertainty in the results (Box 3). The extent of this uncertainty is largely unknown and can be due to incomplete information on input data (climate, soil, crop management, cultivar characteristics), inadequate structure or parameters of the model, or poorly designed upscaling methods (Box 3). Only recently, systematic efforts have been made to better understand these uncertainties [108,109].

Initial results from testing upscaling studies in parts of Europe have suggested that the uncertainty related to manipulation of weather data is relatively small [106,110] compared to the uncertainty related to soil data [111]. However, in these studies, differences in upscaling methods were substantially smaller than differences in using different crop models. Uncertainty also depends on the considered output variable (e.g., yield or evapotranspiration), crop [109], and studied system (e.g., highly heterogeneous geographic region). Much less work has been done to understand the upscaling effects of crop management and crop model parameterization. In particular, the representation of cultivar diversity within a region or country is often largely ignored or is only considered to include basic traits such as phenology [112,113].

In recent years, crop models have increasingly been applied to estimate crop productivity impacts on food security, including the projected effects of future climates. Although the application of crop models to global issues is relatively new, the specific demands for crop modeling have recently been highlighted [102]. These include a better understanding and modeling of G × E × M interactions for large-area applications, and require a more comprehensive representation of factors limiting crop yields, including management and genetic options. Such improvements in the development and deployment of crop models nevertheless depend on the availability of soil, weather, management, and cultivar information that are suitable in detail and coverage to address global issues. This is particularly true for developing countries where data, research, and adaptation resources are typically limited, including in the tropics where climate change is projected to have large impacts [114,115].

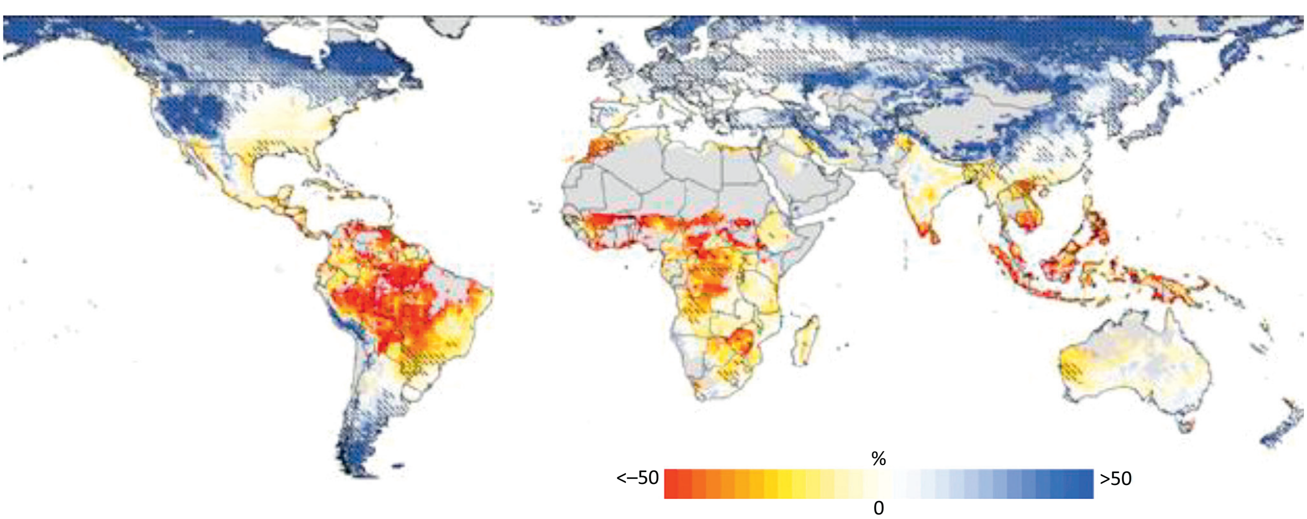


Figure 3. Median Yield Change (%) in Wheat from Seven Global Gridded Crop Models (GGCMs) for 2070–2099 Compared to 1980–2010 for the RCP8.5 Climate Projection Scenario and Five General Circulation Models (GCMs). Simulations are presented for any potential suitable land area (beyond current arable regions) regardless of current or future land use. Hatching indicates areas where more than 70% of the ensemble members agree on the directionality of the impact factor. Grey areas indicate historical areas with little to no yield capacity.
Figure reproduced from [107].

## Climate Change

Reliable estimates of climate change impacts on crop productivity and sustainability are necessary to develop effective adaptation responses for the future [116] (Figure 3). By considering G × E × M interactions, crop models provide a framework to capture impacts of climate which have not yet occurred, and offer an avenue to identify possible adaptations to offset climatic drawbacks on yields [117]. They have been recognized as an essential tool to quantify climate change impacts on wheat production [118].

### Changes in Climate Affecting Wheat Crops, and Implications for Wheat Crop Modeling

Climate change is expected to alter the mean and distribution of climate variables [119]. Although historical weather records show recent changes in $CO_2$, temperature and rainfall patterns [120], further changes are projected by climate models for future conditions [121], including an increase in heat waves [119]. Thus, crop models need to appropriately simulate the impact of such climate factors and to integrate their interaction with processes affecting yield and nutritional value.

Initial wheat crop models were not developed for climate change impact studies, and early applications in this field were mainly site-based to estimate the impacts of unique climate variables (e.g., increase of average temperature or $CO_2$). Recently, climate impact studies have become more elaborate, and explicit attention has been given to issues of adaptation to future climate scenarios [103,118], typically with a focus on sets of climate scenarios to account for inherent climate-projection uncertainties [119].

Wheat crop models typically consider temperature effects on various processes such as phenology, photosynthesis, respiration, and evapotranspiration. However only few models consider heat stress effects (occurring when maximum temperatures surpass critical thresholds) on floret fertility, leaf senescence, and grain development [122–124]. In addition, model improvements are necessary to simulate heat effects on grain quality (e.g., glutenin aggregation; see section on grain quality) [43]. Improvements are also essential to account for the combined effects of different stresses, such as heat and drought stress, which often occur simultaneously.

Another important climate change factor is atmospheric $CO_2$ concentration. Wheat crop models have been tested with elevated $CO_2$ experiments and were recently shown to reproduce $CO_2$ effects on grain yield up to 550 ppm [125]. However, field data are now needed to test and improve how models simulate the interactions of $CO_2$ with other stresses such as high temperature [125,126].

Opportunities exist to integrate in wheat models the effect of other climatic factors or extreme events that could be of importance in the future, such as the level of ozone [127], flooding (i.e., water excess and oxygen deficiency in the root zone), frost [65,81,128], snow, hail, and wind damage. However, predicting the effects of extreme events remains a major challenge because projecting the occurrence and timing of these events is essentially impossible in terms of climate change forecasting.

### Projected Impact and Adaptation

Crop modeling has an increasing role to play in assisting growers and governments to simultaneously adapt to a changing climate and reduce the agricultural footprint, in particular in relation to greenhouse gas emission (see section on agronomy). Until recently, adaptation studies on wheat mainly investigated the shifts in recommended planting dates [113,129]. Lately, wheat crop models have also been applied to consider improved varieties (e.g., longer crop cycle; higher water and N use efficiency) and other management practices (e.g., fertilization and irrigation management) [103,130] as adaptation options to climate change.

While individual crop models are generally able to accurately simulate wheat yields under a wide range of environments, they may not be suited to simulations of future climates. However, across diverse sites, studies on multi-model ensembles have found that median yield simulation from a multi-model ensemble is currently more accurate than simulations from single models, in particular for wheat crops grown under high temperature [33,131]. Now, the challenge is to further reduce such uncertainties by improving temperature relationships in models [132].

## Concluding Remarks and Future Perspectives

Agriculture is facing the challenges of providing food for an expanding human population using lower levels of resource input and reduced environmentally negative effects, while facing an increasingly hostile climate and decreasing area of fertile cropping soils [116]. These considerable challenges have led to new notions such as 'sustainable intensification' of cropping systems and 'climate-smart agriculture'. Sustainable intensification posits a simultaneous increase in primary production and resource use efficiencies of water, nutrients, and solar radiation [133]; climate-smart agriculture aims to minimize greenhouse gas emissions not only per unit area of agriculture but also per unit of harvested yield [134]. While agriculture has outshone many other sectors in decoupling emissions from production by ~40% over the past 40 years [134], greater efforts are needed to ensure that crop models properly simulate sustainable intensification and climate-smart agriculture.

Crop modeling is an essential though insufficient tool to project and upscale our current knowledge to tackle these challenges from the field to the globe. Simulation models, in a plethora of ways from climate to impacts, adaptation, and mitigation, formed the scientific bedrock of the COP21 agreement in Paris in December 2015. Tools based on crop modeling have been developed and deployed to assist agriculture, from individual growers [3] to international policies [119]. Modeling can help to define the target ('ideotype', 'ideosystem'), identify limiting factors, and define strategies to improve agronomy and breeding. Until recently, models have mainly been used for the benefit of local/regional agriculture. Crop models now have a new and important role to play for global risks related to food systems both in the short term (e.g., economic and political impacts of an upcoming staple-food shortfall in major producing regions) and in the longer term (policy regulations).

This review paper has illustrated the ways in which mathematical simulations of crop growth and development can be used to understand crop processes, project the response of wheat genotypes to a variety of environments and management, and be used in prescriptive ways to help policy formation and the design of future crops and cropping systems. Of the three pillars of agronomy (genotype × environment × management), crop models have primarily tackled the response to the environment and management. However, simulating differences across genotypes remains an important challenge, while most models can only simulate genotypic variations related to basic phenotypes such as flowering time. The ~1% of yield increase per annum that wheat breeding contributes to agriculture [63] results from physiological changes that are unknown at the time, hard to capture in models, and typically of smaller magnitude than the uncertainties inherent in simulations. However, while current methods of calibration of cultivars in models are costly and require many experiments, novel methods are emerging to estimate rapidly, and at relatively low cost, genetic parameters that can be incorporated directly into crop models [88]. Currently, success stories are related mainly to crop phenology, generally the largest source of inter-genotypic variability, but the improvements in high-throughput phenotyping is opening new doors to focus on other important physiological traits.

### Outstanding Questions

How will climate change impact on wheat grain yield, functional properties, and nutritional value?

What yield and grain quality could potentially be achieved by 2050 with existing genotypes and current crop management? And when considering the known genetic variability and possible adaptation in crop management?

Can wheat yields be increased with less management inputs? What is the environmental footprint of wheat production? What are the key limiting factors restricting global wheat production? Which crop management and crop traits have the potential to overcome these limitations?

What are the most crucial traits impacting on wheat yield in current and future climates, in different regions, and across the globe? What is the genetic yield potential of wheat as influenced by potential genetic variation for increased biomass production and/or allocation of biomass to grain?

Can wheat yields be increased sustainably on current agricultural land to meet future food demand? Can wheat be expanded sustainably to non-cropping areas, in particular to areas with poor soils, for which most crop models cannot yet be used reliably? What is the potential for sustainable wheat production?

Crop modeling now provides an integrated repository of knowledge and is used across disciplines: linking agronomists, who focus on crop management and environmental impacts; crop physiologists, who dissect physiological processes; geneticists, who interpret the basis of genetic controls; and breeders, who aim to combine the influences of genetics and agronomy to develop high and stable yield and grain quality. Modeling can guide agronomists and physiologists towards promising management and traits, while, vice versa, agronomic and physiological experiments provide sources for model improvement. In addition, interactions between modelers and geneticists are resulting in combinations of well-developed modeling and statistical approaches that are promising for crop improvement [72,93,135]. Crop modeling now has a role to play in the advances that breeding is currently experiencing, and crop simulations have started to assist major breeding programs at different levels [73].

Although crop modeling has increasingly been used for different applications, simulation results are only as good as the model structure, parameters, and inputs. Maintaining good modeling practices, in particular through education of young agronomists and researchers, is essential. Given the new challenges faced by agriculture and globalization, there is also an increasing need for worldwide quality climate data, soil characteristics, proper description of local crop-system practices, trial data (including local daily weather data, soil properties, and status at sowing), and quantitative understanding of elementary process-based mechanism related to crop growth and development. The formulation of crop models requires in-depth knowledge of crop physiology that needs to be molded into logically constructed, justifiable, and measurable representations about how a cropping system functions. Although wheat models are constantly evolving into improved scientific tools, there remain many opportunities to further utilize them to address the massive challenges faced by agriculture.

### Acknowledgments

The authors thank the Wheat Initiative for its financial support of the Expert Working Group on Wheat Plant and Crop Modeling. The development of this review has benefited from many informal discussions between the various authors and many colleagues in wheat modeling and related research.

### Supplemental information

Supplemental information associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.tplants.2017.02.003.

### References

1. Godfray, H.C.J. *et al.* (2011) Linking policy on climate and food. *Science* 331, 1013–1014
2. de Wit, C.T. (1965) *Photosynthesis of Leaf Canopies (Agricultural Research Report 663),* Wageningen Centre for Agricultural Publications and Documentation
3. Hochman, Z. *et al.* (2013) Reprint of 'Quantifying yield gaps in rainfed cropping systems: a case study of wheat in Australia'. *Field Crops Res.* 143, 65–75
4. Basso, B. *et al.* (2006) Simulation of tillage systems impacts on soil biophysical properties using the SALUS model. *Ital. J. Agron.* 4, 677–688
5. Hunt, J.R. and Kirkegaard, J.A. (2011) Re-evaluating the contribution of summer fallow rain to wheat yield in southern Australia. *Crop Pasture Sci.* 62, 915–929
6. Andarzian, B. *et al.* (2015) Determining optimum sowing date of wheat using CSM-CERES-wheat model. *J. Saudi Soc. Agric. Sci.* 14, 189–199
7. Liu, J. *et al.* (2007) Modeling the role of irrigation in winter wheat yield, crop water productivity, and production in China. *Irrig. Sci.* 26, 21–33
8. Dumont, B. *et al.* (2015) Climatic risk assessment to improve nitrogen fertilisation recommendations: a strategic crop model-based approach. *Eur. J. Agron.* 65, 10–17
9. Kirkegaard, J.A. *et al.* (2014) Improving water productivity in the Australian grains industry – a nationally coordinated approach. *Crop Pasture Sci.* 65, 583–601
10. Robertson, M.J. *et al.* (2015) Assessing the place and role of crop simulation modelling in Australia. *Crop Pasture Sci.* 66, 877–893
11. McCown, R.L. *et al.* (2009) Re-inventing model-based decision support with Australian dryland farmers. 1. Changing intervention concepts during 17 years of action research. *Crop Pasture Sci.* 60, 1017–1030
12. Adam, M. *et al.* (2010) CROSPAL, software that uses agronomic expert knowledge to assist modules selection for crop growth simulation. *Environ. Modell. Software* 25, 946–955
13. Hochman, Z. *et al.* (2009) Re-inventing model-based decision support with Australian dryland farmers. 4. Yield Prophet® helps farmers monitor and manage crops in a variable climate. *Crop Pasture Sci.* 60, 1057–1070
14. Basso, B. *et al.* (2013) Wheat yield response to spatially variable nitrogen fertilizer in Mediterranean environment. *Eur. J. of Agron.* 51, 65–70
15. Hasegawa, H. and Denison, R.F. (2005) Model predictions of winter rainfall effects on N dynamics of winter wheat rotation following legume cover crop or fallow. *Field Crops Res.* 91, 251–261

16. Basso, B. *et al.* (2011) A strategic and tactical management approach to select optimal N fertilizer rates for wheat in a spatially variable field. *Eur. J. Agron.* 35, 215–222
17. Huth, N.I. *et al.* (2010) Impacts of fertilisers and legumes on $N_2O$ and $CO_2$ emissions from soils in subtropical agricultural systems: a simulation study. *Agric. Ecosyst. Environ.* 136, 351–357
18. O'Leary, G.J. *et al.* (2016) Modelling soil organic carbon 1. Performance of APSIM crop and pasture modules against long-term experimental data. *Geoderma* 264 (Part A), 227–237
19. Singh, D.K. *et al.* (2009) Validating economic and environmental sustainability of a short-term summer forage legume in dryland wheat cropping systems in south-west Queensland. *Anim. Prod. Sci.* 49, 816–825
20. Basso, B. *et al.* (2016) A comprehensive review of the CERES-wheat, -maize and -rice models' performances. *Advances in Agron.* 136, 27–132
21. Jones, J.W. *et al.* (2003) The DSSAT cropping system model. *Eur. J. Agron.* 18, 235–265
22. Holzworth, D.P. *et al.* (2014) APSIM – evolution towards a new generation of agricultural systems simulation. *Environ. Modell. Software* 62, 327–350
23. Tang, C. *et al.* (2003) Modelling yield losses of aluminium-resistant and aluminium-sensitive wheat due to subsurface soil acidity: effects of rainfall, liming and nitrogen application. *Plant Soil* 254, 349–360
24. Asseng, S. *et al.* (2013) Uncertainty in simulating wheat yields under climate change. *Nat. Clim. Change* 3, 827–832
25. Power, B. *et al.* (2011) A multi-field bio-economic model of irrigated grain–cotton farming systems. *Field Crops Res.* 124, 171–179
26. Paydar, Z. and Gallant, J. (2008) A catchment framework for one-dimensional models: introducing FLUSH and its application. *Hydrol. Processes* 22, 2094–2104
27. Batchelor, W.D. *et al.* (2002) Examples of strategies to analyze spatial and temporal yield variability using crop models. *Eur. J. Agron.* 18, 141–158
28. Basso, B. *et al.* (2007) Analyzing the effects of climate variability on spatial pattern of yield in a maize–wheat–soybean rotation. *Eur. J. Agron.* 26, 82–91
29. Basso, B. *et al.* (2016) Variable rate nitrogen fertilizer response in wheat using remote sensing. *Precis. Agric.* 17, 168–182
30. Shewry, P.R. and Hey, S.J. (2015) The contribution of wheat to human diet and health. *Food Energy Secur.* 4, 178–202
31. Oury, F.X. *et al.* (2003) Yield and grain protein concentration in bread wheat: a review and a study of multi-annual data from a French breeding program. *J. Genet. Breed.* 57, 59–68
32. Myers, S.S. *et al.* (2014) Increasing $CO_2$ threatens human nutrition. *Nature* 510, 139–142
33. Martre, P. *et al.* (2015) Multimodel ensembles of wheat growth: many models are better than one. *Global Change Biol.* 21, 911–925
34. Ferrise, R. *et al.* (2010) Sowing date and nitrogen fertilisation effects on dry matter and nitrogen dynamics for durum wheat: an experimental and simulation study. *Field Crops Res.* 117, 245–257
35. Asseng, S. and Milroy, S.P. (2006) Simulation of environmental and genetic effects on grain protein concentration in wheat. *Eur. J. Agron.* 25, 119–128
36. Triboi, E. *et al.* (2006) Unravelling environmental and genetic relationships between grain yield and nitrogen concentration for wheat. *Eur J. Agron.* 25, 108–118
37. Branlard, G. *et al.* (2001) Genetic diversity of wheat storage proteins and bread wheat quality. *Euphytica* 119, 59–67
38. Landry, J. *et al.* (2002) Effect of the opaque-2 gene on accumulation of protein fractions in maize endosperm. *Maydica* 47, 59–66
39. Martre, P. *et al.* (2003) Modeling grain nitrogen accumulation and protein composition to understand the sink/source regulations of nitrogen remobilization for wheat. *Plant Physiol.* 133, 1959–1967
40. Martre, P. *et al.* (2006) Modelling protein content and composition in relation to crop nitrogen dynamics for wheat. *Eur. J. Agron.* 25, 138–154
41. Plessis, A. *et al.* (2013) Association study of wheat grain protein composition reveals that gliadin and glutenin composition are trans-regulated by different chromosome regions. *J. Exp. Bot.* 64, 3627–3644
42. Asseng, S. *et al.* (2008) Systems analysis of wheat production on low water-holding soils in a Mediterranean-type environment. I. Yield potential and quality. *Field Crops Res.* 105, 97–106
43. Nuttall, J.G. *et al.* (2017) Models of grain quality in wheat – a review. *Field Crops Res.* 202, 136–145
44. Dai, Z. *et al.* (2015) Transcriptional and metabolic alternations rebalance wheat grain storage protein accumulation under variable nitrogen and sulfur supply. *Plant J.* 83, 326–343
45. Zhao, F.J. *et al.* (1999) Responses of breadmaking quality to sulphur in three wheat varieties. *J. Sci. Food Agric.* 79, 1865–1874
46. Don, C. *et al.* (2003) Understanding the link between GMP and dough: from glutenin particles in flour towards developed dough. *J. Cereal Sci.* 38, 157–165
47. Wardlaw, I.F. *et al.* (2002) Contrasting effects of chronic heat stress and heat shock on kernel weight and flour quality in wheat. *Funct. Plant Biol.* 29, 25–34
48. Edwards, M.A. *et al.* (2008) Effect of endosperm starch granule size distribution on milling yield in hard wheat. *J. Cereal Sci.* 48, 180–192
49. Martre, P. *et al.* (2011) Modelling the size and composition of fruit, grain and seed by process-based simulation models. *New Phytol.* 191, 601–618
50. Hurkman, W.J. *et al.* (2003) Effect of temperature on expression of genes encoding enzymes for starch biosynthesis in developing wheat endosperm. *Plant Sci.* 164, 873–881
51. Morris, C.F. (2002) Puroindolines: the molecular genetic basis of wheat grain hardness. *Plant Mol. Biol.* 48, 633–647
52. Oerke, E.-C. (2006) Crop losses to pests. *J. Agric. Sci.* 144, 31–43
53. Chakraborty, S. and Newton, A.C. (2011) Climate change, plant diseases and food security: an overview. *Plant Pathol.* 60, 2–14
54. Webber, H. *et al.* (2014) What role can crop models play in supporting climate change adaptation decisions to enhance food security in Sub-Saharan Africa? *Agric. Syst.* 127, 161–177
55. Johnson, K.B. (1987) Defoliation, disease, and growth: a reply. *Phytopathology* 77, 1495–1497
56. Rossing, W.A.H. (1991) Simulation of damage in winter wheat caused by the grain aphid *Sitobion avenae*. 2. Construction and evaluation of a simulation model. *Neth. J. Plant Pathol.* 97, 25–54
57. Deen, W. *et al.* (2003) An evaluation of four crop:weed competition models using a common data set. *Weed Res.* 43, 116–129
58. Robin, M.-H. *et al.* (2013) Injury profile simulator, a qualitative aggregative modelling framework to predict injury profile as a function of cropping practices, and abiotic and biotic environment. II. Proof of concept: design of IPSIM-wheat-eyespot. *PLoS One* 8, e75829
59. Bregaglio, S. and Donatelli, M. (2015) A set of software components for the simulation of plant airborne diseases. *Environ. Modell. Software* 72, 426–444
60. Thornby, D.F. and Walker, S.R. (2009) Simulating the evolution of glyphosate resistance in grains farming in northern Australia. *Ann. Bot.* 104, 747–756
61. Whish, J.P.M. *et al.* (2015) Integrating pest population models with biophysical crop models to better represent the farming system. *Environ. Modell. Software* 72, 418–425
62. Wang, J.K. *et al.* (2007) Application of population genetic theory and simulation models to efficiently pyramid multiple genes via marker-assisted selection. *Crop Sci.* 47, 582–590
63. Fischer, R.A. and Edmeades, G.O. (2010) Breeding and cereal yield progress. *Crop Sci.* 50 (Suppl. 1), S85–S98
64. Tester, M. and Langridge, P. (2010) Breeding technologies to increase crop production in a changing world. *Science* 327, 818–822

65. Brisson, N. *et al.* (2003) An overview of the crop model STICS. *Eur. J. Agron.* 18, 309–332

66. Chapman, S.C. (2008) Use of crop models to understand genotype by environment interactions for drought in real-world and simulated plant breeding trials. *Euphytica* 161, 195–208

67. Kirkegaard, J.A. and Hunt, J.R. (2010) Increasing productivity by matching farming system management and genotype in water-limited environments. *J. Exp. Bot.* 61, 4129–4143

68. Chenu, K. *et al.* (2011) Environment characterization as an aid to wheat improvement: interpreting genotype–environment interactions by modelling water-deficit patterns in North-Eastern Australia. *J. Exp. Bot.* 62, 1743–1755

69. Chenu, K. *et al.* (2013) Large-scale characterization of drought pattern: a continent-wide modelling approach applied to the Australian wheatbelt spatial and temporal trends. *New Phytol.* 198, 801–820

70. Bänziger, M. and Cooper, M. (2001) Breeding for low input conditions and consequences for participatory plant breeding: examples from tropical maize and wheat. *Euphytica* 122, 503–519

71. Heslot, N. *et al.* (2014) Integrating environmental covariates and crop modeling into the genomic selection framework to predict genotype by environment interactions. *Theor. Appl. Genet.* 127, 463–480

72. Chenu, K. (2015) Characterising the crop environment – mature, significance and applications. In *Crop Physiology: Applications for Genetic Improvement and Agronomy* (Sadras, V.O. and Calderini, D.F., eds), pp. 321–348, Academic Press

73. Cooper, M. *et al.* (2014) Predicting the future of plant breeding: complementing empirical evaluation with genetic prediction. *Crop Pasture Sci.* 65, 311–336

74. Watson, J. *et al.* (2015) Impact of projected climates on drought occurrence in the Australian wheatbelt. In *17th Australian Agronomy Conference*. Hobart, Australia http://www.agronomy2015.com.au/papers/agronomy2015final00411.pdf

75. Podlich, D.W. *et al.* (1999) Computer simulation of a selection strategy to accommodate genotype-by-environment interaction in a wheat recurrent selection program. *Plant Breed.* 118, 17–28

76. Chenu, K. *et al.* (2013) StressMaster: a web application for dynamic modelling of the environment to assist in crop improvement for drought adaptation. In *Proceedings of the 7th International Conference on Functional–Structural Plant Models* (Sievänen, R., ed.), *Proceedings of the 7th International Conference on Functional–Structural Plant Models* 357–359

77. Rebetzke, G.J. *et al.* (2013) A multisite managed environment facility for targeted trait and germplasm phenotyping. *Funct. Plant Biol.* 40, 1–13

78. Manschadi, A.M. *et al.* (2006) The role of root architectural traits in adaptation of wheat to water-limited environments. *Funct. Plant Biol.* 33, 823–837

79. Martre, P. *et al.* (2015) Model-assisted phenotyping and ideotype design. In *Crop Physiology: Applications for Genetic Improvement and Agronomy* (Sadras, V.O. and Calderini, D. F., eds), pp. 349–373, Academic Press

80. Semenov, M.A. and Halford, N.G. (2009) Identifying target traits and molecular mechanisms for wheat breeding under a changing climate. *J. Exp. Bot.* 60, 2791–2804

81. Zheng, B. *et al.* (2015) Frost trends and their estimated impact on yield in the Australian wheatbelt. *J. Exp. Bot.* 66, 3611–3623

82. Martre, P. *et al.* (2015) In silico system analysis of physiological traits determining grain yield and protein concentration for wheat as influenced by climate and crop management. *J. Exp. Bot.* 66, 3581–3598

83. Casadebaig, P. *et al.* (2016) Assessment of the potential impacts of wheat plant traits across environments by combining crop modeling and global sensitivity analysis. *PLoS One* 11, 1–27

84. Hamblin, J. *et al.* (1993) The ideotype concept: useful or outdated? In *International Crop Science I* (Buxton, D.R., ed.), pp. 589–597, CSSA

85. Tardieu, F. (2003) Virtual plants: modelling as a tool for the genomics of tolerance to water deficit. *Trends Plant Sci.* 8, 9–14

86. Hammer, G. *et al.* (2006) Models for navigating biological complexity in breeding improved crop plants. *Trends Plant Science* 11, 587–593

87. Hammer, G.L. *et al.* (2010) Adapting APSIM to model the physiology and genetics of complex adaptive traits in field crops. *J. Exp. Bot.* 61, 2185–2202

88. Zheng, B. *et al.* (2013) Quantification of the effects of VRN1 and Ppd-D1 to predict spring wheat (*Triticum aestivum*) heading time across diverse environments. *J. Exp. Bot.* 64, 3747–3761

89. Schoppach, R. and Sadok, W. (2012) Differential sensitivities of transpiration to evaporative demand and soil water deficit among wheat elite cultivars indicate different strategies for drought tolerance. *Environ. Exp. Bot.* 84, 1–10

90. Laperche, A. *et al.* (2006) A simplified conceptual model of carbon/nitrogen functioning for QTL analysis of winter wheat adaptation to nitrogen deficiency. *Theor. Appl. Genet.* 113, 1131–1146

91. Christopher, J. *et al.* (2013) QTL for root angle and number in a population developed from bread wheats (*Triticum aestivum*) with contrasting adaptation to water-limited environments. *Theor. Appl. Genet.* 126, 1563–1574

92. Chenu, K. *et al.* (2009) Simulating the yield impacts of organ-level quantitative trait loci associated with drought response in maize: a 'gene-to-phenotype' modeling approach. *Genetics* 183, 1507–1523

93. Technow, F. *et al.* (2015) Integrating crop growth models with whole genome prediction through approximate Bayesian computation. *PLoS One* 10, e0130855

94. Chapman, S. *et al.* (2003) Evaluating plant breeding strategies by simulating gene action and dryland environment effects. *Agron. J.* 95, 99–113

95. Li, X. *et al.* (2012) Computer simulation in plant breeding. *Adv. Agron.* 116, 219–264

96. Furbank, R.T. and Tester, M. (2011) Phenomics – technologies to relieve the phenotyping bottleneck. *Trends Plant Sci.* 16, 635–644

97. Fiorani, F. and Schurr, U. (2013) Future scenarios for plant phenotyping. *Ann. Rev. Plant Biol.* 64, 267–291

98. Ghanem, M.E. *et al.* (2015) Physiological phenotyping of plants for crop improvement. *Trends Plant Sci.* 20, 139–144

99. Cabrera-Bosquet, L. *et al.* (2016) High-throughput estimation of incident light, light interception and radiation-use efficiency of thousands of plants in a phenotyping platform. *New Phytol.* 212, 269–281

100. Luquet, D. *et al.* (2012) Functional–structural plant modeling to support complex trait phenotyping: case of rice early vigour and drought tolerance using ecomeristem model. *2012 IEEE Fourth International Symposium on Plant Growth Modeling, Simulation, Visualization and Applications (PMA)* 270–277

101. He, J. *et al.* (2012) Simulation of environmental and genotypic variations of final leaf number and anthesis date for wheat. *Eur. J. Agron.* 42, 22–33

102. Ewert, F. *et al.* (2015) Crop modelling for integrated assessment of risk to food production from climate change. *Environ. Modell. Software* 72, 287–303

103. Zheng, B. *et al.* (2016) Velocity of temperature and flowering time in wheat – assisting breeders to keep pace with climate change. *Global Change Biol.* 22, 921–933

104. Carberry, P.S. *et al.* (2009) Re-inventing model-based decision support with Australian dryland farmers. 3. Relevance of APSIM to commercial crops. *Crop Pasture Sci* 60, 1044–1056

105. Rodriguez, D. *et al.* (2011) The intrinsic plasticity of farm businesses and their resilience to change. An Australian example. *Field Crops Res.* 124, 157–170

106. Zhao, G. *et al.* (2015) Demand for multi-scale weather data for regional crop modeling. *Agric. For. Meteorol.* 200, 156–171

107. Rosenzweig, C. *et al.* (2014) Assessing agricultural risks of climate change in the 21st century in a global gridded crop model intercomparison. *Proc. Natl. Acad. Sci.* 111, 3268–3273

108. Hoffmann, H. *et al.* (2015) Variability of effects of spatial climate data aggregation on regional yield simulation by crop models. *Clim. Res.* 65, 53–69

109. Zhao, G. *et al.* (2015) Effect of weather data aggregation on regional crop simulation for different crops, production conditions, and response variables. *Clim. Res.* 65, 141–157
110. van Bussel, L.G.J. (2015) Simulation of the phenological development of wheat and maize at the global scale. *Global Ecol. Biogeogr.* 24, 1018–1029
111. Hoffmann, H. *et al.* (2016) Impact of spatial soil and climate input data aggregation on regional yield simulations. *PLoS One* 11, e0151782
112. van Bussel, L.G.J. (2011) Effects of data aggregation on simulations of crop phenology. *Agric. Ecosyst. Environ.* 142, 75–84
113. Zheng, B. *et al.* (2012) Breeding for the future: what are the potential impacts of future frost and heat events on sowing and flowering time requirements for Australian bread wheat (*Triticum aestivium*) varieties? *Global Change Biol.* 18, 2899–2914
114. Hertel, T.W. and Lobell, D.B. (2014) Agricultural adaptation to climate change in rich and poor countries: current modeling practice and potential for empirical contributions. *Energy Econ.* 46, 562–575
115. Wing, I.S. and De Cian, E. (2014) Integrated assessment: modelling agricultural adaptation. *Nat. Clim. Change* 4, 535–536
116. Porter, J.R. *et al.* (2014) Food security and food production systems. In *Climate Change 2014: Impacts, Adaptation, and Vulnerability. Part A: Global and Sectoral Aspects* (Field, C.B., ed.), pp. 485–533, Cambridge University Press
117. Martín, M.M.-S. *et al.* (2014) A genotype, environment and management (GxExM) analysis of adaptation in winter wheat to climate change in Denmark. *Agric. For. Meteorol.* 187, 1–13
118. Challinor, A.J. *et al.* (2014) A meta-analysis of crop yield under climate change and adaptation. *Nat. Clim. Change* 4, 287–291
119. Intergovernmental Panel on Climate Change (2014) *Climate Change 2014: Synthesis Report,* IPCC
120. Hartmann, D.L. *et al.* (2013) Observations: atmosphere and surface. In *Climate Change 2013: The Physical Science Basis* (Stocker, T.F., ed.), pp. 159–218, Cambridge University Press
121. Collins, M. *et al.* (2013) Long-term climate change: projections, commitments and irreversibility. In *Climate Change 2013: The Physical Science Basis* (Stocker, T.F., ed.), pp. 1029–1106, Cambridge University Press
122. Lobell, D.B. *et al.* (2015) The shifting influence of drought and heat stress for crops in northeast Australia. *Global Change Biol.* 21, 4115–4127
123. Liu, B. *et al.* (2016) Testing the responses of four wheat crop models to heat stress at anthesis and grain filling. *Global Change Biol.* 22, 1890–1903
124. Asseng, S. *et al.* (2011) The impact of temperature variability on wheat yields. *Global Change Biol.* 17, 997–1012
125. O'Leary, G.J. *et al.* (2015) Response of wheat growth, grain yield and water use to elevated $CO_2$ under a free-air $CO_2$ enrichment (FACE) experiment and modelling in a semi-arid environment. *Global Change Biol.* 21, 2670–2686
126. Batts, G.R. *et al.* (1997) Effects of $CO_2$ and temperature on growth and yield of crops of winter wheat over four seasons. *Eur. J. Agron.* 7, 43–52
127. Ewert, F. and Porter, J.R. (2000) Ozone effects on wheat in relation to $CO_2$: modelling short-term and long-term responses of leaf photosynthesis and leaf duration. *Global Change Biol.* 6, 735–750
128. Bell, L.W. *et al.* (2015) Optimising grain yield and grazing potential of crops across Australia's high-rainfall zone: a simulation analysis. 1. Wheat. *Crop Pasture Sci.* 66, 332–348
129. White, J.W. *et al.* (2011) Methodologies for simulating impacts of climate change on crop production. *Field Crops Res.* 124, 357–368
130. Ludwig, F. and Asseng, S. (2010) Potential benefits of early vigor and changes in phenology in wheat to adapt to warmer and drier climates. *Agric. Syst.* 103, 127–136
131. Asseng, S. *et al.* (2015) Rising temperatures reduce global wheat production. *Nat. Clim. Change* 5, 143–147
132. Rosenzweig, C. *et al.* (2013) The agricultural model intercomparison and improvement project (AgMIP): protocols and pilot studies. *Agric. For. Meteorol.* 170, 166–182
133. Garnett, T. *et al.* (2013) Sustainable intensification in agriculture: premises and policies. *Science* 341, 33–34
134. Bennetzen, E.H. *et al.* (2016) Decoupling of greenhouse gas emissions from global agricultural production: 1970–2050. *Global Change Biol.* 22, 763–781
135. Onogi, A. *et al.* (2016) Toward integration of genomic selection with crop modelling: the development of an integrated approach to predicting rice heading dates. *Theor. Appl. Genet.* 129, 805–817
136. Zheng, B. *et al.* (2014) The APSIM-Wheat Module (7.5 R3008). *Agricultural Production Systems Simulator (APSIM) Initiative*