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Towards a multiscale crop modelling framework for climate change adaptation assessment

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Predicting the consequences of manipulating genotype (G) and agronomic management (M) on agricultural ecosystem performances under future environmental (E) conditions remains a challenge. Crop modelling has the potential to enable society to assess the efficacy of G × M technologies to mitigate and adapt crop production systems to climate change. Despite recent achievements, dedicated research to develop and improve modelling capabilities from gene to global scales is needed to provide guidance on designing G × M adaptation strategies with full consideration of their impacts on both crop productivity and ecosystem sustainability under varying climatic conditions. Opportunities to advance the multiscale crop modelling framework include representing crop genetic traits, interfacing crop models with large-scale models, improving the representation of physiological responses to climate change and management practices, closing data gaps and harnessing multisource data to improve model predictability and enable identification of emergent relationships. A fundamental challenge in multiscale prediction is the balance between process details required to assess the intervention and predictability of the system at the scales feasible to measure the impact. An advanced multiscale crop modelling framework will enable a gene-to-farm design of resilient and sustainable crop production systems under a changing climate at regional-to-global scales.

Achieving global food security under climate change (CC) is a big challenge facing humanity[1]. Effective adaptation strategies are needed to mitigate the negative CC impacts on crop production and further enhance agricultural resilience. Possible solutions include (1) genetic improvement through plant breeding and genetic engineering of new crops with stress tolerant traits[2,3], and enhanced resource use efficiencies[4,5]; and (2) adaptive crop management practices[6,7]. As CC impacts on crop production will likely vary substantially in space[2,8], environment-specific adaptation strategies may confer advantages[6]. Moreover, CC is very likely to shift the target population of environments in which crop cultivars produced by breeding programs will be grown[9] and may limit the rate of genetic gain through breeding programs alone. Considering both genetic and management improvements can thus expand the opportunities to cope with CC, in which case suitable predictive models that can capture complex interactions among genotype, environment (including climate and edaphic conditions) and management (genetics × environment × management (G × E × M)) in crop development, growth and yield are required[10–12]. Meanwhile, adaptation of crop production to CC should be treated along with environmental sustainability, as the environmental footprint of agriculture may change with adoption of different adaptation strategies over extended areas[13]. Potential genetic and/or management adaptation strategies need to be rigorously assessed for their impacts on both crop production and environmental sustainability in a changing climate (Fig. 1).

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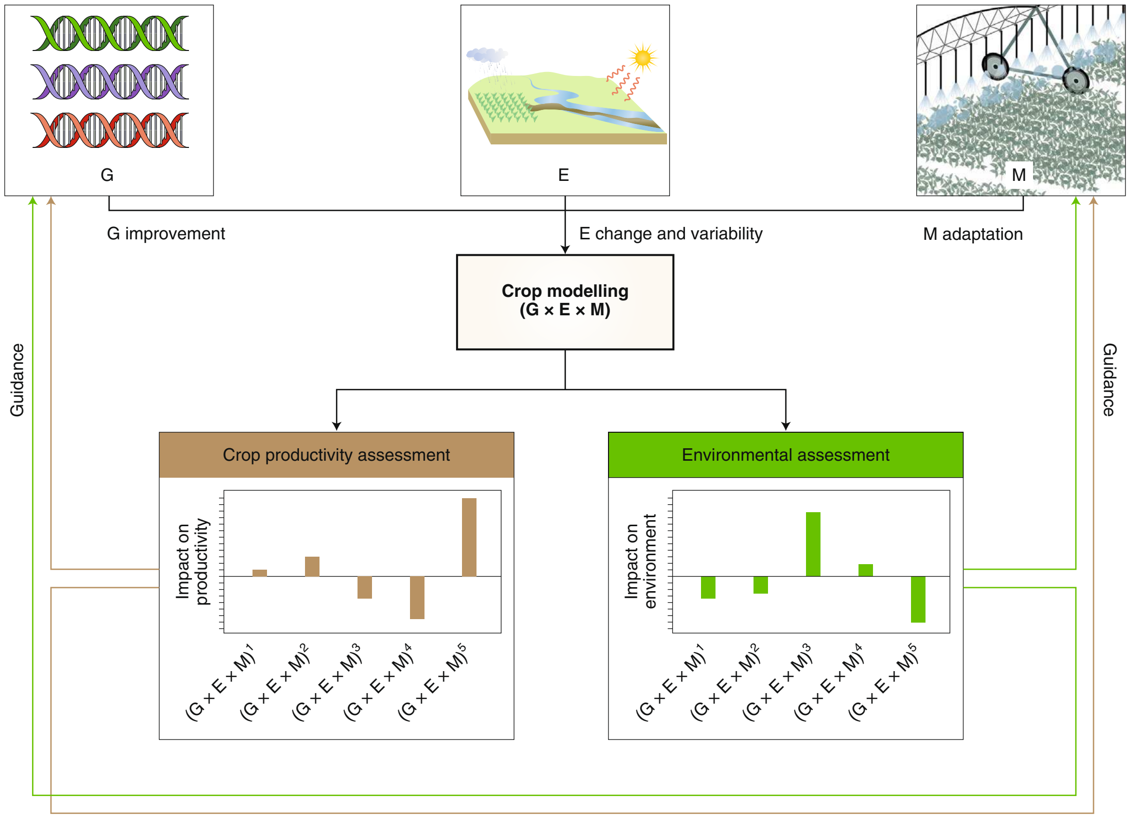

Fig. 1 | Crop modelling plays a central role in assessing agricultural CC adaptation for food security and environmental sustainability. When optimizing existing and designing new agricultural CC adaptation strategies, lessons from both crop productivity and environmental sustainability assessments should be considered. G, genetics; E, environment; M, management.

The need for a multiscale crop modelling framework

Crop modelling can help assess the efficacy of agricultural adaptation strategies to CC (Fig. 1). Complex G × E × M interactions[10–12] affecting crop development, growth and yield, and their nonlinearities present a formidable challenge to designing empirical experiments that adequately sample the G × E × M space. Process-based crop models (CMs) offer a unique way to assess the pros and cons of different adaptation strategies because they integrate physical and biological principles to mechanistically simulate the use and allocation of captured resources[14]. In this way, CMs can help optimize existing strategies and assist the design of new strategies under different environmental scenarios (Fig. 1). For management adaptation, many existing studies used CMs to assess the impacts of different practices on crop production[15,16]. However, their potential impacts on environmental sustainability and feedback to the climate remain under-studied, mainly because current CMs lack the required interfaces with land surface, climate and economic models. Crop modelling is an ideal tool to assess the benefits of various genetic solutions in crop improvement[17]. However, assessments of potential genetic solutions by most existing CMs are restricted due to their limited capabilities to simulate genetic variation and biochemistry[18,19]. Some recent model developments have uncovered opportunities to develop an integrated modelling framework to address questions about genetic improvement under CC. For instance, CMs were improved by considering the variation in relevant adaptive traits to drought in maize[20] as well as the connection between CMs and genomic prediction[21,22]. Although geospatial simulations of the impact of crop genetic improvements on yield exist[23], assessments of their impact on environmental sustainability under current and future climates are still missing. To meet these demands for assessing CC adaptation strategies for both crop productivity and environmental sustainability, and assisting in designing new strategies, a multiscale (from gene to globe) crop modelling framework should be developed using systems approaches. Such a framework can explicitly integrate small-scale mechanisms with multi-sectoral impacts of different adaptation strategies at larger scales (Fig. 2; Table 1).

Going to gene scale

Incorporating the principles of genetics and genomics into CMs will enable genotype-to-phenotype prediction to advance crop breeding and genetic engineering[18,24,25]. Two approaches, referred to as 'top-down' and 'bottom-up' approaches, can be employed to leverage our collective understanding of genetic controls of physiological processes to enhance phenotypic prediction[26–28]. The top-down approach[25,29] follows the philosophy of 'modelling plant hormone action without modelling the hormones'[30], and strives to capture system dynamics and phenotypic consequence from genetic variation at the whole-plant scale, with a relatively coarse granularity but robust prediction accuracy[25]. The simplification made in the top-down approach balances phenotyping capabilities[31], propagation of measurement errors and accuracy, which are required to inform a decision. To effectively connect complex traits (such as yield) with genetic regulation, CMs should include detailed physiological processes[10,29,31,32]. Some cultivar-specific model parameters in CMs are predicted by different mathematical approaches, from simple statistical models based on multiple loci[32–35] to whole genome association prediction using Bayesian and machine learning approaches[21,22,36]. Successful examples of this top-down

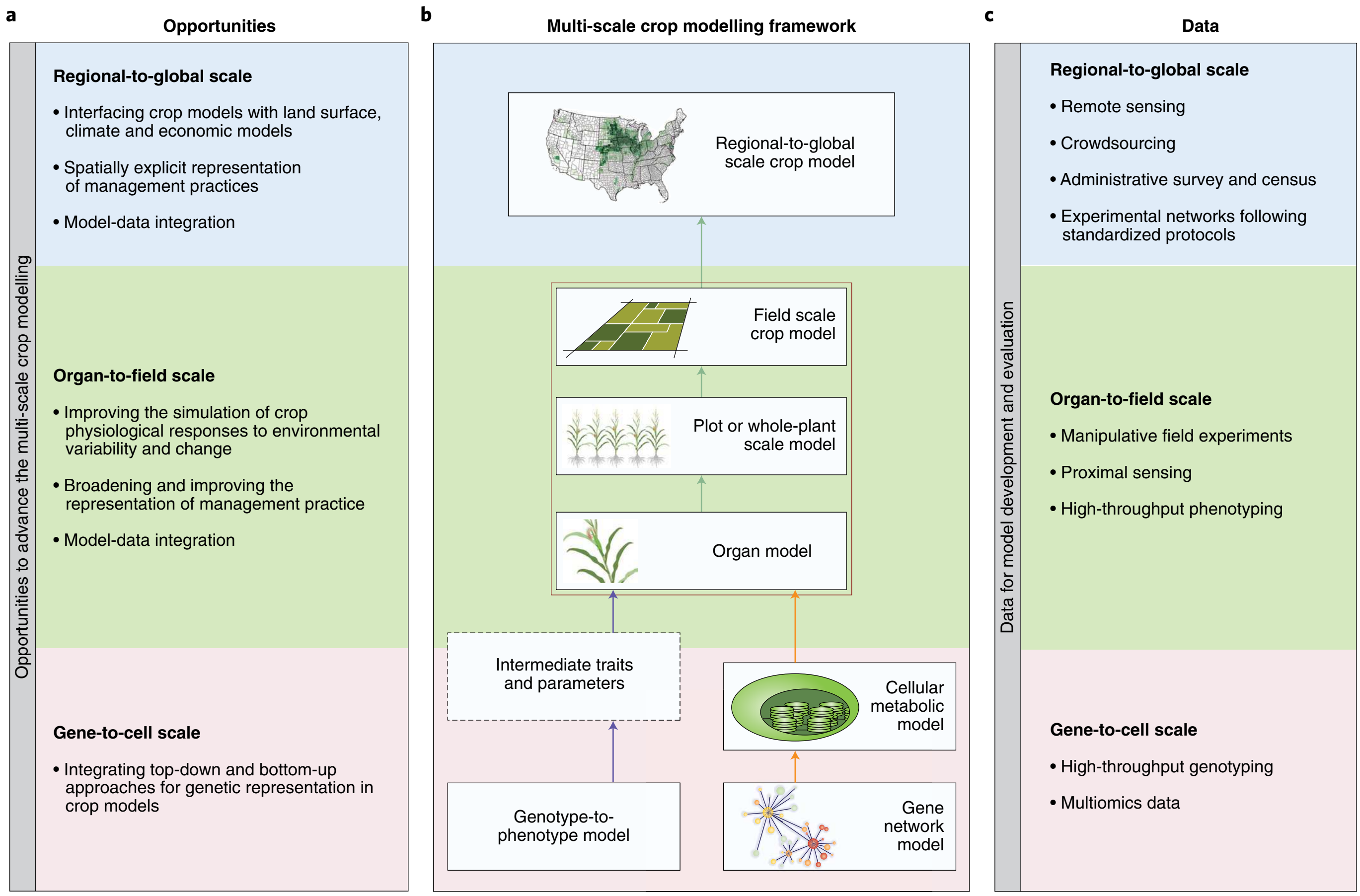

Fig. 2 | A conceptual illustration of the multiscale crop modelling framework. a, Opportunities to advance the multiscale crop modelling. **b**, Models operating at different scales involved in the multiscale crop modeling framework. **c**, Data collection to support model development and evaluation at varied scales.

approach include reasonable predictions with quantitative trait loci models of maize leaf elongation response to soil water deficit and high evaporative demand[33,34], and the transition to reproductive growth in several other crops[32,37]. CMs that incorporated functional relationships between environmental variables and traits for the genetic variation in yield and agronomic performance[22] have been successfully used in breeding drought-tolerant maize hybrids for the US Corn Belt[3].

The bottom-up approach uses systems biology to integrate plant biological processes operating at different temporal and spatial scales[26,38,39]. For example, the *e*-photosynthesis model[40], which simulates individual photosynthesis-related metabolic reactions and their major regulatory mechanisms, is a typical bottom-up model that may potentially link high throughput genomic data with observable macroscopic phenotypes. By explicitly simulating gene network regulation, metabolic reactions and metabolite transport, the bottom-up models, once integrated to the whole-plant scale, could enable testing the impact of genetic manipulation on different proteins (such as photosynthetic enzymes) and identify targets for crop genetic improvements[24]. However, the bottom-up approach is limited to single component processes (for example, photosynthesis)[40,41] or model plants (for example, *Arabidopsis*) that have relatively lower complexity and have been better characterized than conventional crop species[42]. Mechanistic models that include all component processes controlling the forms and functions of crops are being investigated[43]. Although the bottom-up approach can provide a more direct connection with the underpinning of genetic architecture, several key challenges need to be met before scaling up to the whole-plant level. These include how to integrate the component modules and whether the integrated models can give robust phenotypic responses to genetic changes under varied environmental and management conditions, which may be challenging in applications that require a higher prediction accuracy due to error propagation and inabilities to properly phenotype and initialize such models.

Given the different properties of top-down and bottom-up approaches, integrating these two approaches may provide an opportunity to merge their advantages. Such integration will require transdisciplinary cooperation to harness collective knowledge in the form of functional models that capture essential features of the underlying biology while retaining the required predictability. Comparing these two approaches for genotype-to-phenotype prediction under varied environmental conditions will help identify potential model deficiencies and corresponding opportunities for improvement. To make them operationally feasible, the fine-grained bottom-up models must be simplified in mechanistic representations while maintaining predictive capability of system dynamics for large-scale applications[44]. One possibility is to build surrogate models of the bottom-up models which can statistically emulate the behaviours of the latter but with greater computational efficiency. This is critical for some applications requiring many model runs, such as high-resolution simulation over large areas and the Monte Carlo-based parameter estimation. Surrogate models for selected processes could also be combined with top-down models to build a hybrid model to simulate the whole-plant-level impact of crop

Table 1 | A summary of recommended actions to advance multiscale crop modelling

Directions or opportunities	Recommended actions	Process unerstanding	Model development and evaluation	Data collection and model-data integration
Going to gene scale	Comparing top-down and bottom-up approaches for genotype-to-phenotype simulation	✓	✓	✓
	Integrating top-down and bottom-up approaches to represent genetic traits in CMs		✓	✓
Going to global scale	Interfacing CMs with large-scale land surface, climate and economic models	✓	✓	✓
	Scaling the surface heterogeneity from field to regional or global scale		✓	
Better representation of physiological responses to CC	Simulating coupled soil–root–canopy–atmosphere water transfer driven by energy balances	✓	✓	
	Improving the stomatal and intra-leaf diffusional conductance models	✓	✓	
	Improving the simulation of responses of carbon or nitrogen source–sink relationship to stresses	✓	✓	
	Developing mechanistic models for ozone stress	✓	✓	
	Simulating the root growth and metabolism under oxygen deficiency	✓	✓	
Better representation of crop management practices	Simulating coupled carbon–nitrogen–phosphorus cycles in CMs	✓	✓	✓
	Simulating microorganism–root interactions in CMs	✓	✓	✓
	Representing more management practices in large-scale CMs	✓	✓	✓
	Simulating stresses from crop pests and diseases as well as weed competition on crop growth	✓	✓	✓
	Improving simulation of fate and transport of pesticide across landscapes		✓	✓
Closing the data gaps	Collecting more site-level experimental data following standardized protocols			✓
	Conducting multi-dose experiments for observed crop responses to CC factors			✓
	Collecting more soil profile data to improve the gridded soil products			✓
	Enriching management data through working with farmers and government agencies, and using crowdsourcing and remote sensing technologies			✓
Model-data integration	Evaluating CMs using eddy-covariance flux data		✓	✓
	Evaluating CMs in simulating the emergent relationships inferred from data		✓	✓
	Spatially explicit calibrating CMs using remote sensing data as constraints		✓	✓

trait manipulations at finer (gene and metabolic) scales effectively and efficiently. Meanwhile, lessons from the top-down approach may help component integrations in the bottom-up approach, as top-down models provide robust physiological overviews of crop growth and development processes. The top-down approach can also be used in designing better structures for those simplified mechanistic models or surrogate models. Such integration provides a promising approach to represent genetic traits in CMs for breeding and genetic engineering research—a research domain which is still in its infancy[24].

Going to global scale

Reliable large-scale simulations to assess agricultural CC adaptation are needed because decisions about adaptation are usually made at a broader scale, beyond that which the traditional CMs were developed and tested (that is, plot-to-field scale)[45]. Current CMs are mainly designed for yield simulation at the field scale, excluding or implicitly considering processes related to surface fluxes of water, energy, carbon and nutrients. For these reasons, current CMs appear unsuitable for evaluating the environmental impacts of agricultural CC adaptation at large scales. Meanwhile, land surface models (LSMs) and their counterparts in Earth system models (ESMs) focus more on surface and subsurface hydrology, surface energy balance and biogeochemical cycling processes[46]. Many LSMs can be coupled to an atmospheric model, a river model, an ocean model (via the river model) and, occasionally, even to an integrated assessment model. These couplings could enable both assessment of the broader role agriculture plays in the Earth system and studies regarding food security, and environmental quality under socioeconomic development, technological innovations and CC. Although some LSMs have incorporated crop growth and a number of plant physiological mechanisms, such as stomatal and biochemical limitations to photosynthesis and plant hydraulics, crop modelling schemes in ESMs require development of crop-specific processes that are better resolved by field-scale agronomic CMs[47]. Most ESM-based CMs do not incorporate sufficient details describing crop phenology, organ development and their responses to environmental stresses; therefore, they cannot always capture observed variation in crop yields. These inter-model differences occur because field-scale agronomic CMs and LSMs, or ESMs, were originally developed for different goals. LSMs or ESMs can become powerful tools to simulate the 'food–energy–water' nexus[48], the crux of both food security and environmental sustainability, if essential biological functionalities related to both surface energy–water–carbon fluxes and crop growth and yield are included.

Regional-to-global CC adaptation assessment requires a systems approach to understand interactions among different elements of the climate–agriculture–environment system, which can be leveraged to increase overall system efficiency, resilience and sustainability. One possible research pathway is to integrate field-scale crop modelling capabilities with LSMs or ESMs[47,49,50–52] making CMs a sub-module of larger system models. This integration will enable both CMs and the host LSMs to complement and benefit from each other. CMs can take advantage of the more advanced biophysical and biogeochemical representations in LSMs to help improve the simulation of crop growth and yield at regional-to-global scales. Similarly, LSMs can benefit from the explicit and mechanistic representation of crop growth to improve surface energy–water–carbon flux simulation over agricultural land. For regional-to-global scale applications, trade-offs between model complexity and computational efficiency need to be considered[29]. For example, when incorporating genetic models, the coarse-grained top-down approach[33] may be preferred for its better computational efficiency and reliability compared to the fine-grained bottom-up approach. In addition, the three-dimensional representation of leaf anatomy[44] as well as root and canopy architectures[53,54] in structural–functional models[55] may also need to be simplified in LSMs for regional-to-global scale applications[44,56].

One challenge when integrating CMs with large-scale models is scaling the heterogeneity over cropland[45,57]. Most large-scale crop simulations still use field-scale CMs with spatially aggregated input data (soil, weather and management), such as those in the Global Gridded Crop Model Intercomparison[58,59] of the Agricultural Model Intercomparison and Improvement Project (AgMIP; https://agmip.org/)[60]. However, such aggregation may lead to biases in both simulated yield and its variability depending on regional characteristics, CMs and spatial resolution of simulation[45,61]. Finer resolutions could somewhat mitigate the problem but would dramatically increase the computational burden, especially when using ESM-based CMs at regional-to-global scales. Recent advances in representing land surface heterogeneity in ESMs also shed light on the scaling issue in crop modelling. As more data on field-scale elevation, soil, yield and management become available, high-resolution cropland grids (~30 m) can be clustered into several tiles based on the multi-dimensional characteristic space[62]. Simulations over the clustered tiles within one coarse grid can then be mapped back to high-resolution grids through post-processing. Necessary adjustments to model structures may be needed when adding this scaling complexity into CMs, especially for those using a single soil column for all cropland within one coarse grid.

Integrating CMs with large-scale models enables a consistent and systematic assessment of the adaptation impacts on multiple sectors of the Earth system at regional-to-global scales. Possible applications include determining how genetic modifications of crop growth, vigour, stress response or resource use efficiency influence water–energy–carbon cycles at regional-to-global scales and their potential feedback to the climate. These large-scale impacts of possible genetic improvements can be assessed using ESMs with embedded CMs to guide crop breeding, designing sustainable cropping systems and their placement on the landscape. Likewise, adaptive changes in the amount and timing of irrigation[7] as well as nitrogen fertilization[63] in response to CC may have economic and environmental implications that can be assessed with the coupled crop, economic and environmental models[64].

Better representation of physiological responses to CC

Realistic physiological responses to CC in CMs are essential for rigorous CC adaptation assessment[65]. Multi-model intercomparisons, like AgMIP[60], show that current CMs can simulate comparable yields under current climate and management conditions[66–69]. However, those models diverge significantly in predicting future yield under common CC scenarios[67,70,71], mainly due to their diverging assumptions about the underlying physiology of how crop growth will respond to changes in various environmental factors, including carbon dioxide concentration ([CO_2])[67,72,73], temperature[67,73,74], soil water and nutrient availability[68]. The divergence issue becomes more complicated with their significant differences in representing combined effects of different environmental stresses on plant development and biomass production[31,66]. Multi-model ensemble can lead to more robust model predictions with a potentially narrower uncertainty range than an individual model projection[67–69,71,75,76]. However, since most CMs have limited capability to simulate the combined effects of multiple CC factors on crop growth, confidence in such multi-model projections is reduced, especially when considering climate extremes (droughts, heatwaves and flooding) and their interactions.

Higher [CO_2] alone is expected to benefit crop production. Free air CO_2 enrichment (FACE) experiments show that elevated [CO_2] may increase net carbon assimilation and plant growth for C_3 crops and for C_4 crops under water-limited conditions[77,78]. Elevated [CO_2] also reduces stomatal conductance and potentially enhances water use efficiency[79–81]. However, this does not necessarily lower the drought risk, since elevated [CO_2] may stimulate leaf growth and hence lead to more water consumption in some crop species, such as soybean[82,83]. Moreover, reduced canopy cooling associated with lower transpiration rates under elevated [CO_2] could also increase canopy temperature[80]. The magnitudes of these CO_2 effects vary depending on crop species and cultivar[84,85] as well as environmental conditions because the CO_2 effect interacts with temperature, water, nitrogen and ozone stress conditions[79,86–88]. The modelling community has attempted to reconcile model predictions with these observed results, but inconsistencies between model simulation and observations remain[72]. Part of this model-data discrepancy may come from different approaches CMs use to represent plant physiological responses to elevated [CO_2]. For example, CMs may simulate canopy-level assimilation using either radiation use efficiency (RUE)[89] or photosynthetic biochemical limitation approaches[17,90]. In the RUE approach, the CO_2 fertilization effect on assimilation is simulated through a multiplicative modifier to RUE, which is often empirically derived from limited experimental observations[91]. A better understanding of the biochemistry-related responses of leaf-scale stomatal and intra-leaf diffusional conductance, autotrophic respiration to elevated [CO_2] and their scaling to canopy scale is needed for improved model performance[86,92]. Further, long-term effects of elevated [CO_2] on crop growth differ from short-term effects due to photosynthetic acclimation, and current CMs differ in their abilities to translate short-term responses to long-term effects[93]. Coupling CO_2 response to nutrient limitation through product inhibition and understanding the source–sink relationship in carbon and nutrient allocation under varied environmental

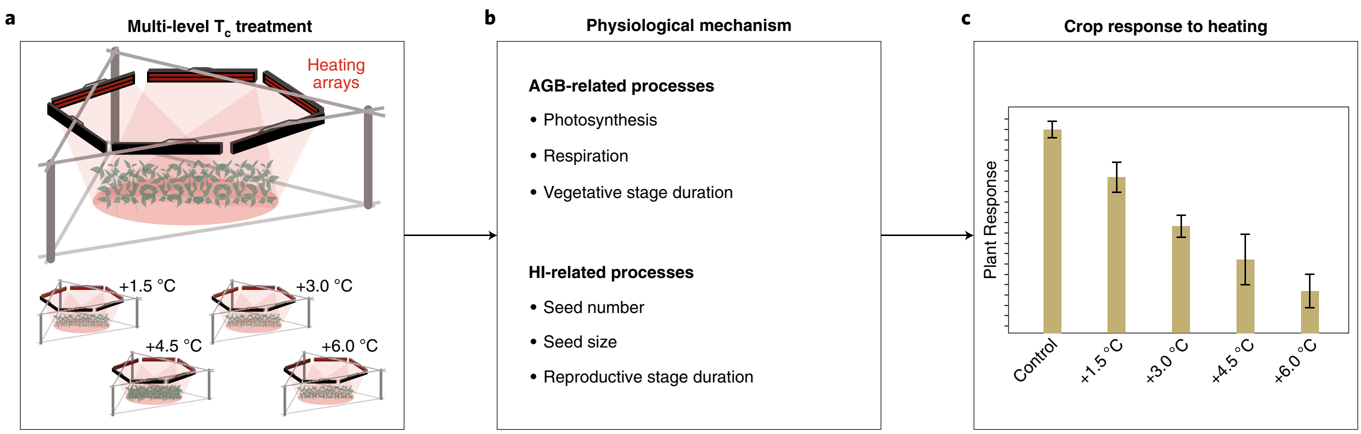

Fig. 3 | Temperature free-air controlled enhancement experiment for soybean in Illinois, USA. a, Experiment design for the multi-level temperature treatment (+1.5 °C, +3.0 °C, +4.5 °C and +6.0 °C). T_c, canopy temperature. **b**, Different physiological mechanisms depicting the responses of soybean growth and yield to higher temperature. AGB, above-ground biomass; HI, harvest index. **c**, A conceptual temperature response function from the field measurement that can be used to constrain CMs, enabling models to reproduce the right yield response with the right mechanism.

conditions are essential for CMs to capture the yield responses to elevated [CO_2][94].

Chronic or acute exposure of crops to tropospheric ozone can decrease photosynthesis, alter carbon allocation and reduce yield quantity and quality[95]. As ozone damage occurs at the cellular level, CMs need to explicitly represent leaf photosynthesis biochemistry, stomatal conductance and daily or sub-daily canopy growth and biomass partitioning to simulate ozone impacts on crop growth, yield and its interaction with other environmental factors. However, current CMs seldom consider these physiological mechanisms of ozone stress on crop growth[96–98], and ozone-induced yield impact assessments at regional-to-global scales mainly rely on empirical or semi-empirical modelling approaches[95]. Future studies should prioritize the development and benchmark of a mechanistic algorithm for ozone stress on crop growth using high-quality data from ozone filtration and fumigation experiments conducted in open top chambers or FACE sites[95,99,100].

Since extreme events, such as heatwaves, droughts and extreme rainfall events, are projected to increase under future climate scenarios[101], representing their impact on crop growth and productivity in CMs is essential for projecting future food security[102]. Heat stress affects grain setting during anthesis and grain size during the grain filling period[103–105], and therefore can directly lead to yield reduction. Asymmetric impacts of high day and night temperatures have been observed for some crop species, particularly rice[106,107]. Drought stress can reduce stomatal conductance, downregulate photosynthesis, slow plant development and growth, cause earlier leaf senescence and reduce yields[103]. The impacts of heat and drought stresses are growth-stage-dependent. For example, greater yield loss is usually observed if crops are stressed from heat and drought during meiosis, anthesis and grain filling stages[108]. Moreover, heat and drought stresses usually occur concurrently and interact with each other, increasing the overall stress for crop growth[109,110]. The crop breeding community has been targeting new cultivars that tolerate both drought and heat stresses over the last two decades. However, current CMs show suboptimal performance in simulating the impacts of drought-heat interacting stresses[111,112], mainly due to complexity in simulating plant physiological responses to such complex abiotic conditions. Deficiencies in model structure can also lead to uncertainty in assessing heat stress impacts on crop yield and understanding the relative importance of drought as compared to heat stress[113,114]. Examples of this problem include using air temperature instead of canopy temperature to quantify heat stress[115,116], and lack of canopy energy budget closure and plant hydraulics in most traditional CMs. Compared with drought and heat stress, negative impacts of excess rainfall or waterlogging on crop growth have received even less attention in current CMs[117,118], although it may lead to comparable yield losses[119]. Root growth and metabolism under oxygen deficiency should be explicitly simulated in CMs to quantify the oxygen limitations on active nutrient uptake and crop growth. Understanding and implementing these physiological responses to changing environmental factors in CMs should be prioritized and would benefit model-assisted design of CC adaptation strategies.

Better representation of crop management practices

Crop management practices are the actions farmers take to ensure crop productivity. Current field-scale CMs generally have specific crop management modules which can simulate parts of the impacts from some management practices. However, opportunities for improvement are abound, especially considering these CMs simulate largely diverged sensitivities of crop yield, soil carbon and nitrogen fluxes to management practices[120,121]. An emerging priority is to improve the model representation of management impacts on soil biogeochemical cycling. Unlike natural ecosystems, biogeochemical cycling in farmland soils is directly affected by crop management practices, and it is a key determinant of crop productivity and CC mitigation potential of agroecosystems. Improved representation of plant–soil–microbial interactions and the impacts of management practices on such interactions could improve simulating coupled carbon–nitrogen–phosphorus cycles in cultivated soil[121]. Recent advancements in soil biogeochemistry and ecosystem modelling could be combined and leveraged[122–125]. Additionally, most previous model-ensemble-based assessments of CC impacts on crop production reinitialize soil water and nutrient conditions in each growing season to solely focus on impacts from climate variability[66,67,126,127]. Only recently have continuous multi-year simulations been used to assess the legacy impacts of management practices on both crop yield and environmental sustainability (such as soil health and greenhouse gas emissions)[128–131]. Inclusion of regionally representative crop management remains a priority for ESM-based CMs[132]. Current ESMs consider a limited number of crop management practices, such as irrigation and nitrogen fertilization[49]. Other crop management practices (such as tillage, crop rotation and cover crops) still need to be implemented. A challenge to implement all of them represents the large data gaps in spatiotemporal characterization of these crop management practices.

Improving pest and disease management simulation in CMs is another priority as crop yield loss from these processes is projected to increase with CC[133–135]. Few CMs simulate the stress from pests and diseases, which, if not well controlled, can be a key determinant of yield gaps. Process-based simulation of crop pest and disease management requires at least three sub-modules: population dynamics, injury and damage, and management action. Population dynamics models have been well developed in the epidemiological community. Linking those population models with crop growth models is the first step to address the complex interactions between crop and pest or pathogen dynamics[14,136]. However, this coupling requires a better understanding of the injuries and damage mechanisms. For example, modelling corn borer injury to xylem vessels, and hence water uptake, requires a hydraulic-driven model of soil–root–canopy–atmosphere water transfer along potential gradients through a series of hydraulic resistances. Pest and disease control actions, such as pesticide use, should be simulated by explicitly considering their impacts on population dynamics and metabolism rates of pests and diseases. Improving the simulation of fate and transport of pesticides in the soil–crop–atmosphere continuum as well as in rivers would benefit environmental sustainability assessment[137,138]. With these advancements, potential benefits in both crop production and environmental sustainability of using genetic mechanisms for protection against pest and disease damage could also be assessed using the multiscale modelling framework.

Closing the data gaps

Observations from individual sites or site networks have been widely used to evaluate and improve field-scale CMs[139]. However, current field experiments have limited coverage of growth conditions (climate, soil and crop management practices). More site-level data collection following standardized protocols for model evaluation and improvement is needed[140]. In addition, current field data generally have limited treatment levels for [CO_2], temperature or [O_3]. Many previous studies have evaluated CMs mainly for their accuracy in simulating target variables such as crop yield, above-ground biomass and leaf area index. Any future projections on crop production should consider that simulating the emergent relationships is as important as, or perhaps more important than, simulating the 'right magnitude' of any particular target variable in CMs[71]. Examples of such emergent relationships are the nonlinear yield response to temperature[141] and kernel number response to plant growth[20]. Focusing on functional relationships could minimize or prevent CMs from predicting right values due to the wrong mechanism[65].

Progress in science and technology is an iterative process whereby experimentation will inform modelling and vice versa. The effectiveness of integrating field research programs with model development and evaluation efforts at the process level across environmental gradients could be increased by designing standardized protocols to collect field data. Future field experiments should be designed to facilitate model development and validation of the 'responses' of CMs to various environmental conditions and stressors. A good example is the multi-level temperature free-air controlled enhancement experiment in Illinois (USA), which collected data for response curves of soybean growth over multiple elevated temperatures (+1.5 °C, +3.0 °C, +4.5 °C and +6.0 °C), instead of a single-dose response value (Fig. 3). Both biometric and leaf gas exchange measurements were collected periodically across multiple growing seasons, providing valuable data for mechanism understanding and model testing.

Data gaps are even larger for crop modelling at regional-to-global scales, especially on soil and crop management characteristics. One major uncertainty is in soil characterization[142]. Though global soil databases exist, their collected soil profiles are insufficient to account for the large heterogeneity in soil characteristics. Moreover, the spatial distribution of soil profiles is largely biased. Traditional soil maps are vector or polygon products linking dominant soil types for different soil horizons in the same soil column as tabular characteristic data without any documented uncertainty. The variability within each soil map unit polygon is largely neglected depending on the map scales[142]. Regional-to-global gridded soil products have recently become available from spatial interpolation with other environmental covariates[143,144], but generalization of the soil-environment prediction models is still poor. Besides, soil parameters from these gridded products are not enough to drive CMs in many regions[145]. As an example, the organic C:N:P ratio is a key attribute currently lacking in those soil products. For large-scale crop modelling, the dominant soil-type approach is still widely used to derive soil parameters, which inevitably introduces uncertainties when either upscaling soil types or applying pedotransfer functions at larger scales[146], sometimes greater than uncertainties from climate aggregation[61]. Moreover, soil characteristics over cultivated areas are actually not static but responsive to CC, land use and management practices[129]. Ignoring this variability may lead to inconsistency in existing soil maps as they are produced from soil surveys conducted at different times. Advancements in new soil sensor development, in situ soil data collection methods and fast soil testing techniques would help collect denser soil datasets with greater frequencies, which will ultimately improve the quality of gridded soil data needed for crop modelling at large scales.

Insufficient agricultural management data at regional-to-global scales also hinders spatiotemporally explicit representation of agricultural management practices in CMs[147]. For example, current global simulation efforts usually use one single reference cultivar or several region-specific cultivars for each crop type without explicit quantification of uncertainties from intra-species variability[58,148]. The spatial distribution and interannual variability in land devoted to specific cultivars of crop species remains poorly quantified. Some of these data gaps are related to strongly held desires for data privacy among farmers. Finding effective ways to work with farmers could be the key to narrow these important data gaps. University extension services and regional farmer groups can play critical roles to facilitate farmer data sharing, research dissemination and farmer benefit from new technologies. Governmental policies on data sharing may also help harness the power of agricultural data collected by public agencies[149]. In addition, crowdsourcing data[150]—for example, crop phenological stages collected by voluntary observer network[151]—can complement such information. Another promising solution is to map agronomic management practices from space. Previous studies have demonstrated the potential of remote sensing in mapping crop species[152], irrigation area and intensity[153], and agronomic conservation practices (for example, cover crops and field tillage)[154,155] at large scales. Important crop phenological states, such as sowing, emergence, anthesis, tasseling and silking (for maize)[156–158] can also be derived from remote sensing, which may assist setting management configurations (for example, sowing or harvesting dates and cultivar maturity groups) in CMs.

Model-data integration

Reconciling model simulations with observations is a natural process to advance model improvements. Besides biomass and yield observations, there is still a largely unrealized opportunity for testing CMs against eddy covariance measurements of water, energy and CO_2 exchange under contrasting environmental conditions. These tests will help identify crop responses to changes in diverse environmental conditions, yet have been largely overlooked by the crop modelling community. A wealth of eddy covariance data has been accumulated at tens of cropland sites and compiled in either regional or global flux networks[159]. It was not until recently that high-frequency eddy covariance observations were used to benchmark simulations of multiple CMs[160]. Besides conventional model-data comparisons, there is a greater need for evaluation and calibration of the response and emergent relationships in model simulations. Experimental response relationships (such as measured temperature responses from experiments in Fig. 3) can be used to evaluate and constrain CMs at site scale[161]. Simulated yield responses to environmental variability at regional scales can further be compared and calibrated using statistical model-inferred yield responses[141,162], and, in turn, the insights from statistical models can help improve process-based CMs for better CC adaptation assessment[163,164]. With these 'responses' as constraints, CMs could be closer to 'delivering right simulations with right mechanisms'. The constrained model would enable identifying bottleneck processes for yield production under current and future climate scenarios at regional-to-global scales, and the resultant assessment can guide crop genetic improvement. Remote sensing observations provide another promising opportunity for spatially explicit calibration of CMs at regional-to-global scales. Complementary information about crop growth and stress across different spectral bands[165], with broad spatial coverage and increasingly finer spatiotemporal resolution of remote sensing data[166], allow explicit incorporation of satellite information to improve regional crop simulation. Satellite-derived crop phenology stages[156–158], leaf area index[167], water use[168] and yield[169] can be used as model constraints[170].

Concluding vision

The research community is actively seeking CC adaptation strategies that can ensure future crop production and environmental sustainability. As conducting trial experiments in all environmental conditions is not feasible and some future environmental conditions do not yet exist, crop modelling is a critical tool for hypothesis testing and scenario analysis under varied environmental conditions. Scenario-based model simulations can potentially guide genetic improvement and management adaptation plans. To fulfil this potential, crop modelling must extend beyond its current scales (organ-to-field scales) to both smaller (gene-to-cell) and larger (regional-to-global) scales. Although not all scales must necessarily be included in a single model for all applications, coherent process representations and standardized interfaces to other scales should be developed to facilitate assembling modelling solutions suitable for specific demands. The development of a multiscale crop modelling framework requires multidisciplinary knowledge, including (but not limited to) genetics, genomics, molecular systems biology, plant physiology, agronomy, soil science, agroecology, hydrology, biogeochemistry, climate, Earth system science, remote sensing and engineering[171]. Transdisciplinary collaboration and convergent research approaches are needed to achieve such a multiscale crop modelling paradigm, which will allow for more robust and useful predictions of crop production under CC along with its environmental implications. Broader collaboration among crop modellers across different communities, and promotion of knowledge exchange, data sharing, open-source coding and community-based model development, benchmarking and intercomparison, are fruitful paths forward to success. Several global partnerships, such as AgMIP[60], Research Program on Climate Change, Agriculture and Food Security (CCAFS) of the Consultative Group for International Agricultural Research (CGIAR)[172] and Crops *in silico* (C*is*)[38,39] serve as guiding examples.

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Author contributions

B.P. and K.G. conceived the research. B.P., K.G. and J.T. wrote the paper; B.P. and K.G. designed the figures. B.P and H.K. produced the figures. B.P. designed and produced the table. E.A.A., S.A., C.J.B., M.C., E.H.D., J.W.E, F.E., R.F.G., D.I.G, G.L.H., J.W.J., Z.J., H.K., D.M.L., Y.L., D.L.L., A.M.C., C.D.M., D.R.O., J.C.S., C.E.V., A.W., X.Y. and W.Z. all contributed to the text.

Competing interests

The authors declare no competing interests.

Additional information

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