

# Modelling plants across scales of biological organisation for guiding crop improvement

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**Handling Editor:**

Rana Munns

**Received:** 10 January 2023

**Accepted:** 6 April 2023

**Published:** 28 April 2023

**Cite this:**

Wu A (2023)  
*Functional Plant Biology*, **50**(6), 435–454.  
doi:[10.1071/FP23010](https://doi.org/10.1071/FP23010)

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**ABSTRACT**

Grain yield improvement in globally important staple crops is critical in the coming decades if production is to keep pace with growing demand; so there is increasing interest in understanding and manipulating plant growth and developmental traits for better crop productivity. However, this is confounded by complex cross-scale feedback regulations and a limited ability to evaluate the consequences of manipulation on crop production. Plant/crop modelling could hold the key to deepening our understanding of dynamic trait–crop–environment interactions and predictive capabilities for supporting genetic manipulation. Using photosynthesis and crop growth as an example, this review summarises past and present experimental and modelling work, bringing about a model-guided crop improvement thrust, encompassing research into: (1) advancing cross-scale plant/crop modelling that connects across biological scales of organisation using a trait dissection–integration modelling principle; (2) improving the reliability of predicted molecular–trait–crop–environment system dynamics with experimental validation; and (3) innovative model application in synergy with cross-scale experimentation to evaluate  $G \times M \times E$  and predict yield outcomes of genetic intervention (or lack of it) for strategising further molecular and breeding efforts. The possible future roles of cross-scale plant/crop modelling in maximising crop improvement are discussed.

**Keywords:** APSIM, crop dynamics, cross-scale modelling,  $G \times M \times E$ , genetic engineering, photosynthesis, plant/crop physiology, trait dissection, yield improvement.

**Introduction**

Genetic improvements in crop yield performance through cycles of selective breeding have contributed to year-on-year increases in grain yield per land area for major cereals. However, current approaches are unlikely to meet the increasing demand from a growing human population, shifts in diet, and the use of crops for fuel production (Ray *et al.* 2013). This serious deficit will occur amid the negative impacts of climate change on crop yield (Lobell *et al.* 2015). There is growing interest in using our wealth of fundamental understanding of plant growth and development mechanisms and processes to devise yield enhancement strategies. The dominant approach focuses on deepening molecular and pathway understanding and manipulation of aspects of plant growth and development, which are often then extrapolated to seasonal crop yield performance. For example, this has led to the common perception that demonstrating enhancement in instantaneous leaf  $\text{CO}_2$  assimilation rate would simply translate to increased plant/crop biomass growth, therefore increasing yield at harvest (Long *et al.* 2015; Simkin *et al.* 2019). While such a ‘bottom-up’ appraisal of genetic manipulation is attractive, interactions of emerging traits at the plant/crop-scale with the environment could feedback on the performance of processes at smaller scales, which can complicate crop performance assessment (Wu *et al.* 2016).

Field crop experiments show that if increased crop biomass growth is at the expense of increased transpiration and faster depletion of soil water, such growth can increase terminal (flowering–grain filling period) water stress and reduce final grain yield (Herwaarden *et al.* 1998). Theoretical analysis predicts that faster biomass accumulation

and more water use are disadvantageous in water-limited conditions (van Oosterom *et al.* 2021). An extensive survey of free-air CO<sub>2</sub> enrichment studies have found that nitrogen deficiency diminishes yield benefit of elevated CO<sub>2</sub>-induced photosynthesis and growth (Ainsworth and Long 2021). Theoretical analysis also predicts that molecular enhancement of photosynthesis diminishes at higher biological scales of organisation, and fails to increase yield if N accumulation is not also increased (Sinclair *et al.* 2004, 2019). These cross-scale feedback regulations are often not considered in molecular manipulation studies and can confound yield improvement efforts.

A method is to conduct empirical phenotypic assessment, which typically measure final crop yield per land area of plant genotypes. This is routinely applied in plant-breeding operations to inform genotype ranking and selection (Hammer *et al.* 2019a). This ideally requires yield information from across all land areas intended for crop production, over many years. Location × year combinations make up the target population of environments (TPEs) (Chenu *et al.* 2011). In practice, researchers and plant breeders estimate crop performance using multi-environment trials (METs) and managed stress environments (MSEs) based on sampling of the TPEs. The same empirical assessment approach can be followed for mechanism- and process-based crop improvement. In a remarkable effort over some 20 years of molecular breeding, Simmons *et al.* (2021) created a vast number of maize genotypes with genetic perturbations in growth and development processes, measuring the yield outcomes of the transgenics using METs and MSEs and synthesising important lessons for decision making in molecular breeding.

However, METs and MSEs are inherently large scale and costly, which poses a significant challenge in testing an ever-growing number of transgenic materials. While transgenic testing has largely been confined to pot experiments (Simkin *et al.* 2019), there have been some examples of field testing of photosynthetic manipulations. For instance, a transgenic tobacco (*Nicotiana tabacum*) plants altered in the glycolate metabolism pathway reported biomass increase of >40% (South *et al.* 2019). However, this increase could not be explained by the reported advantages in canopy photosynthesis, which was generally less than 10%. As pointed out in the eLetter by Tony Fisher, Richard Richards, and Victor Sadras in response to the work, the faster growth of transgenic plants was likely biased from advantages in light interception due to non-standard planting configuration – factors beyond intrinsic leaf photosynthetic enhancement. Another study of soy beans (*Glycine max*) tested transgenic plants, using hastened leaf non-photochemical quenching relaxation in the field and found that grain yield increased by up to 33% (De Souza *et al.* 2022). However, in a subsequent field trial, against expectations no yield change was observed. These results confound crop improvement decision making and highlight the need for improved field-testing standards to validate the understanding of the relationship between underlying mechanisms and

processes with crop-scale performance and demonstrate the benefits of genetic engineering on crop yield.

It has been broadly proposed to use plant/crop models to predict the yield outcomes of trait manipulation to inform molecular breeding (Evans and Lawson 2020; Furbank *et al.* 2020; Paul *et al.* 2020; Roell and Zurbruggen 2020; Zhu *et al.* 2020). Coupled with advances in our knowledge of complex networks of component traits that underpin crop yield and the development of a multitude of crop-growth models (CGMs) with origins dating back to the 1960s and 1970s (Jones *et al.* 2017; Hammer *et al.* 2019b), our ability to predict crop performance has advanced significantly. CGMs typically model macroscale traits (e.g. crop resource capture, conversion, and partitioning) as exemplified by classic textbooks such as *Physiological Determinants of Crop Growth* by Charles-Edwards *et al.* (1986); *Crop Ecology* by Connor, Loomis, and Cassman; and the broader crop science literature (e.g. Hammer *et al.* 2019b). These authors consider plant growth and development at organ–plant–crop spatial scales on a per unit ground basis, and timescales from hourly to daily to seasonal. Model formulation is based on crop ecophysiological insights. Daily crop biomass growth per unit ground, for example, is linearly related to the solar radiation intercepted by the canopy in water and N non-limiting conditions; the slope of the relationship is radiation use efficiency (RUE) (Sinclair and Muchow 1999). Crop yield per land area is in fact a complex function of the genetic/biology (G) of component traits, agronomic management of the plants as field crops (M), and weather and soil environments (E). CGMs have reached sufficient maturity with proven ability in predicting emergent consequences of G × M × E and crop yield outcomes, and their value for crop improvement decision making is recognised by researchers, plant breeders, and agronomists (Hammer *et al.* 2019a, 2019b). But are CGMs the means to fulfil the widening phenotypic assessment gap as we pursue mechanism- and process-based crop improvement?

A barrier to using organ–plant–crop-scale CGMs to predict the effect of bioengineering is that model parameters and equations may not have clear links to molecular and pathway manipulations. For example, the RUE (a crop-scale trait underpinned by the collective photosynthetic CO<sub>2</sub> assimilation capacity of all leaves in the canopy and the efficiency of dry-matter synthesis from assimilated carbon) cannot be easily determined *a priori* to simulate such factors as changes in the leaf CO<sub>2</sub> assimilation rate arising from manipulation of Rubisco catalytic properties (e.g. Salesse-Smith *et al.* 2018). Plant modelling at molecular and pathway scales can provide the ability to model specific enzymatic manipulations (Zhu *et al.* 2013). Models with greater molecular details are perceived as more realistic and are often more appealing to fundamental plant experimentalists (Kromdijk *et al.* 2016; South *et al.* 2019). But the trade-off in using these models is that their predictive capabilities are largely limited to molecular and pathway scales, and typical timescales of sub-seconds to minutes. Without spatial–temporal upscaling,

molecular models do not have the means to capture the organ–plant–crop-scale growth and development dynamics and  $G \times M \times E$  interactions necessary for crop yield prediction.

Given the variety of plant/crop models that are available, how can we best use them to support plant-science research and crop-improvement decision-making? It is clear that we need models to adequately capture both (1) bioengineering effects at lower biological scales, and (2) crop ecophysiological knowledge for predicting crop growth and development dynamics,  $G \times M \times E$  interactions, and yield across TPEs. Given the amount of photosynthesis research globally and its role in crop biomass and yield growth, I now discuss a model-enabled strategy using photosynthesis and crop yield as a case study, but the approach is general for all plant traits. Specifically I will:

- survey plant/crop modelling at multiple scales of biological organisation, and their utilities and limitations;
- describe an emerging model-guided crop improvement strategy and its benefits for genetic engineering and breeding selection; and
- discuss opportunities related to advancing plant/crop modelling and crop improvement.

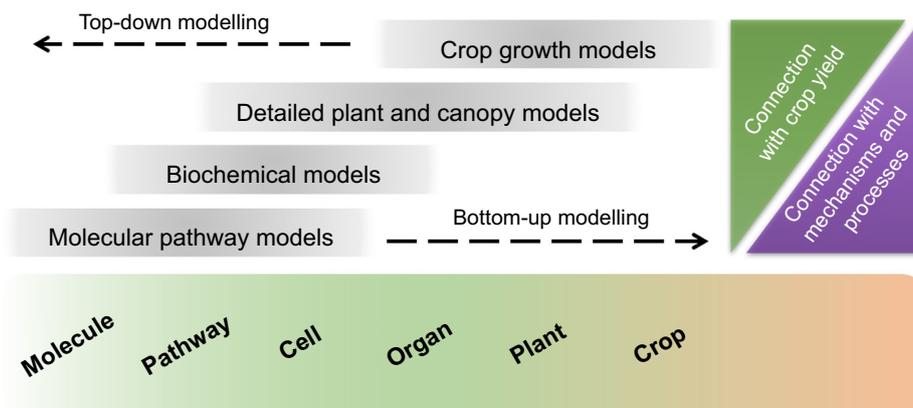
### Trait–crop–environment modelling at multiple scales of biological organisation and utility

The process of mathematically modelling plant data/information is arguably becoming a plant-science research topic in its own right. Modelling is the most effective means for developing a holistic understanding of the networks of interacting mechanisms and processes drawing from a wide range of research areas; providing the means to study the dynamics of these systems, which may be difficult to grasp

with experiments. These make modelling more than an exercise in hindsight: it can work synergistically with plant science discovery. Naturally, modelling approaches that focus on specific biological questions emphasise particular aspects of plant/crop biology, using their own scales, biological variables, and abstractions, leading to divergent model structures and parameterisations. Using photosynthesis, plant growth, and yield as an example, categories of modelling thrusts at different biological scales of organisation are presented (Fig. 1). Their potential (or lack of it) for supporting photosynthesis and crop yield improvement are now discussed.

### Molecular and biochemical models of photosynthesis

Photosynthesis is the primary process that drives plant and crop growth, which involves a large number of enzymes and metabolites, and is one of the most well studied traits. Our knowledge of photosynthesis has been captured in the three types of photosynthesis models: (1) molecular pathway models (metabolic models), which explicitly include many enzymes and metabolites of the Calvin–Benson cycle, and the electron transport chain by using systems of differential equations (e.g. Laisk *et al.* 2006; Zhu *et al.* 2013; Bellasio 2019); (2) the coarse-grained biochemical models of steady-state photosynthesis, which elegantly reduces the many photosynthetic steps to the carboxylation- and electron transport-limited states, controlled by the catalytical properties of Rubisco via Michaelis–Menten kinetics and electron transport chain (Farquhar *et al.* 1980; von Caemmerer and Furbank 1999); and (3) empirical models of steady-state leaf photosynthetic  $CO_2$  and light response, using linear, hyperbolic, and exponential equations (e.g. Thornley 1976). The degrees of coarse-graining and empiricism in the model influence the relationship between model parameters and intended



**Fig. 1.** Plant/crop models and their emphasis on biological scales of organisation. The models are discussed in the next subsection. The dashed arrows indicate major modelling principles to achieve connections across biological scales of organisation. The triangles indicate the trade-offs between connections with specific plant mechanisms and processes vs crop yield.

enzymatic actions. These models cover the molecule–organ scales of biological organisation (Fig. 1).

The biochemical models of steady-state leaf photosynthesis are widely used to simulate leaf CO<sub>2</sub> assimilation rates under various CO<sub>2</sub>, light, and temperature conditions. They require input of a few key photosynthetic parameters with biological meanings: maximum carboxylation ( $V_{\text{cmax}}$ ) and maximum electron transport ( $J_{\text{max}}$ ) rates, Rubisco catalytic properties, the light–electron transport rate relationship, and the temperature response of those photosynthetic parameters (von Caemmerer 2000). Model parameter values for different species are becoming available (Bernacchi *et al.* 2002; Silva-Pérez *et al.* 2017; Sonawane *et al.* 2017). The biochemical models can be used to infer changes in biochemical attributes, given measured photosynthetic CO<sub>2</sub>- and light-response curves (von Caemmerer and Farquhar 1981) and in transgenic plants (von Caemmerer 2000). The models can predict CO<sub>2</sub>- and light-response curves with photosynthetic manipulation if the effects of genetic manipulation on model parameters can be *a priori* determined (e.g. von Caemmerer 2000), but this may not be straightforward. Molecular pathway models with explicit links to enzymes could offer the means to predict, but using such models would require assumptions in equations and parameterisation of all modelled enzymes for CO<sub>2</sub>, light, and temperature, which is challenging to fully validate experimentally. Nonetheless, Kannan *et al.* (2019) calibrated a model of molecular pathways for simulating the effects of elevated plant growth CO<sub>2</sub> on the steady-state leaf photosynthetic CO<sub>2</sub> response curve; Zhao *et al.* (2021a) used similar models to predict the CO<sub>2</sub> assimilation rate with changing individual enzymatic activity in the Calvin–Benson cycle.

### Detailed plant and canopy models

An intuitive approach for modelling aboveground canopy photosynthesis involves calculating the CO<sub>2</sub> assimilation rate for every photosynthetic organ (predominantly leaves) within the volume of a canopy, which also requires canopy microclimate and photosynthetic attributes of the plant materials. This includes levels of light, CO<sub>2</sub>, and temperature, and vapour pressure deficit, canopy architecture, and any required parameters of the photosynthesis model used. Song *et al.* (2017) calculated the heterogeneity of one environmental factor, light, by parameterising a 3D plant architecture model after measuring tiller number and leaf number, base height, length, width, angle, and curvature, and inferring leaf optical properties combined with ray-tracing algorithms. Such modelling of plant structure is commonly referred to as functional–structural plant modelling (Vos *et al.* 2010; Soualiou *et al.* 2021). The concept can be applied to leaf-scale modelling (Earles *et al.* 2019). For the belowground, there are 3D modelling of root system architecture and solute (water and nutrient) transport in the soil such as OpenSimRoot (Postma *et al.* 2017). In the aboveground

canopy, modelling of environmental factors other than light in such detail remains to be seen. Validating 3D model outputs by measuring the photosynthetic rates of every photosynthetic organ is not feasible; a common practice is to test predicted whole-canopy CO<sub>2</sub> uptake rates against canopy-scale gas-exchange chamber measurement (Song *et al.* 2016; Chang *et al.* 2022).

Combining molecular pathway models with a detailed canopy upscaling approach presents a means for highly detailed canopy modelling that can explicitly simulate the effects of photosynthetic bioengineering on canopy CO<sub>2</sub> uptake rates. Model parameterisation and perhaps simulation runtime can be challenging, and in some circumstances model simplification was made by switching to biochemical and empirical models of leaf photosynthesis (Song *et al.* 2017; Chang *et al.* 2022). While the capacity to simulate the entire crop cycle is theoretically sound, the requirement to predict 3D canopy architecture (including time-series plant architectural, leaf morphological, and physiological attributes, and parameterisation of all photosynthetic model parameters) and canopy micro-environment remain major barriers.

A greater number of upscaling techniques have been explored for the coarse-grained biochemical and empirical models of leaf photosynthesis. More abstract upscaling approaches such as the big-leaf and sun-shade (single or multiple layers) models (Hikosaka *et al.* 2016) use pre-defined angle of leaf surfaces relative to the angle of incoming solar radiation. This provides a simple means for simulating realistic light intensities intercepted by different layers of the canopy, without incorporating explicit 3D canopy models or inputting plant organ morphological features (Duncan *et al.* 1967). Complexity is further reduced by grouping leaf surface areas into a small number of entities, allowing calculation of their averaged light interception, temperature, leaf nitrogen, photosynthetic parameter values, and CO<sub>2</sub> assimilation rates.

There is, however, a balance between the simplification and reliability of a model. Sun-shade models are more complex than big-leaf models, which assumes the canopy is a slab of photosynthetic medium; but sun-shade models are more reliable because grouping leaf surfaces in a canopy into either sunlit or shaded fractions accounts for most within-canopy light heterogeneity without relying on empirical corrections (de Pury and Farquhar 1997). Sun-shade modelling has been shown to accurately predict canopy CO<sub>2</sub> assimilation rates measured at various incoming light intensities in the field (de Pury and Farquhar 1997). The approach is widely used for upscaling to canopy photosynthesis and much of sun-shade modelling papers reference studies by de Pury and Farquhar (1997) and Leuning *et al.* (1998). Wu *et al.* (2018) used a sun-shade canopy modelling approach to predict the effects of photosynthetic manipulation on canopy-scale CO<sub>2</sub> assimilation and biomass growth rates. Abstract upscaling approaches capture canopy architecture and leaf morphology effects on canopy CO<sub>2</sub> assimilation rates, using the aggregated parameters that describes light extinction through the

canopy; but parameterisation is challenging due to our lack of knowledge of how specific architectural and morphological traits can affect the aggregated parameters. However, a spherical leaf angle distribution approximation is typically sufficient for field-crop canopies due to their relative heterogeneity (de Pury and Farquhar 1997). Current detailed plant and canopy models operating in isolation cannot predict crop-scale outcomes, since such models cannot simulate the dynamics of crop growth and development. For example, total leaf area per ground area (the leaf area index) changes over a crop cycle, but needs to be prescribed to allow canopy photosynthesis calculations. Most detailed plant and canopy models cover scales of biological organisation from pathway to (static) plant/canopy (Fig. 1).

### Crop growth models

Crop growth and development are the two major determinants influencing yield performance. Growth is the daily aboveground biomass increment considered on a per ground area basis, and accumulation of dry matter in leaves, stems, roots, and grains; plant/crop development concerns the timing of the formation of new leaves, tillers, roots, flowering, and grains. Grain yield is a complex emergent property of growth and development dynamics, agronomic management, and environment (soil and weather). These soil–crop–environment ecophysiological insights have been incorporated into crop physiological determinant networks (including environmental factors, traits, and biological input parameters) that underpin CGMs such as those in Agricultural Production System sIMulator (APSIM) and Decision Support System for Agrotechnology Transfer (DSSAT) platforms (Holzworth *et al.* 2014; Jones *et al.* 2017). Fig. 2 showcases the networks of the APSIM–sorghum crop model. Typical CGMs link the organ–crop scales of biological organisation (Fig. 1).

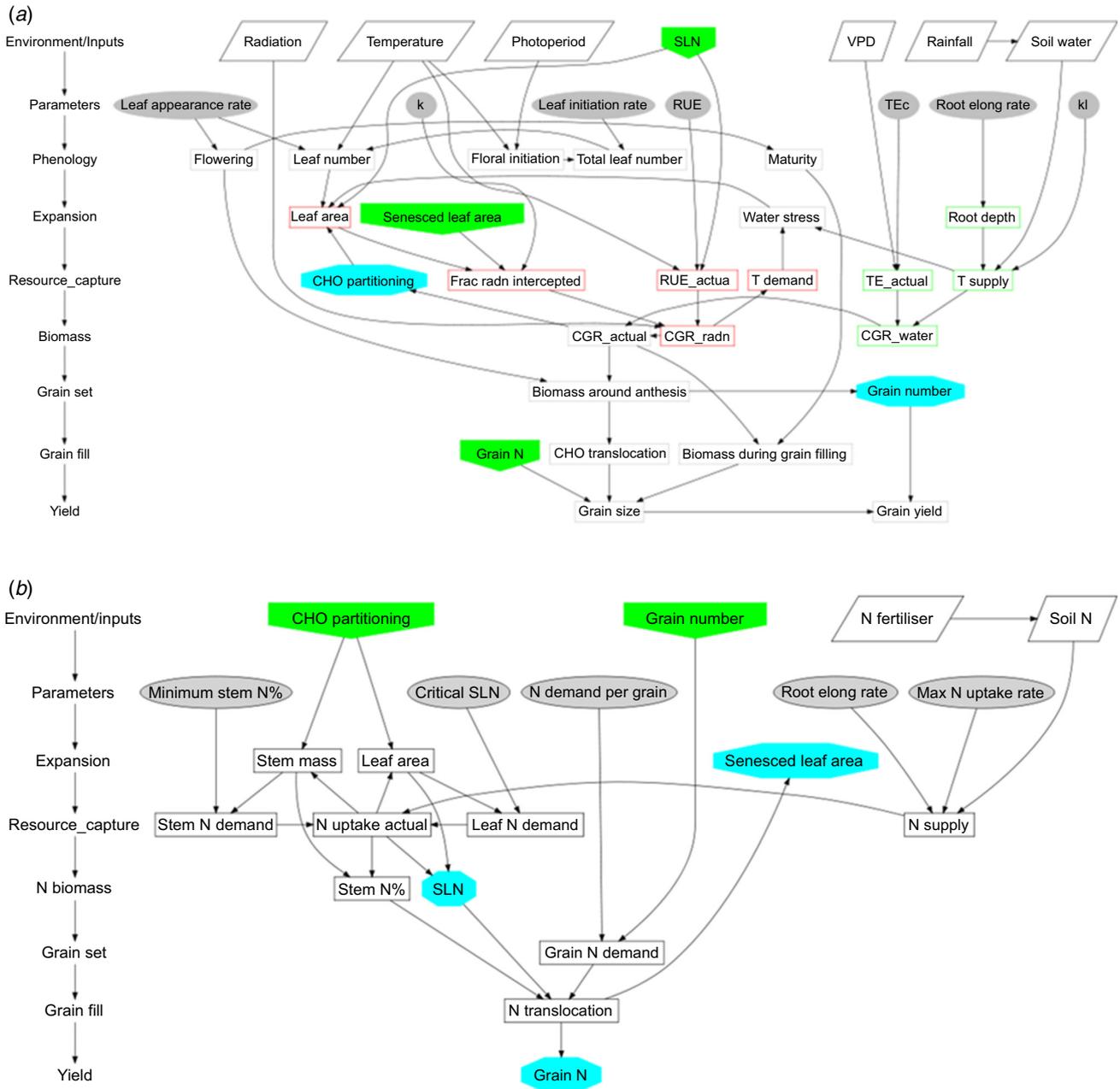
Modelling of plant/crop developmental rate in CGMs typically uses a thermal time approach factoring in the growth temperature and photoperiod (Hammer *et al.* 2010). Actual growth rate in N abundant conditions is the minimum of either the potential growth rate when water is not limiting and the water-limited rate. The potential rate is calculated by the RUE equation where canopy-intercepted radiation is the driver (described above). This also establishes crop water demand by dividing the accumulated biomass by the crop's transpiration efficiency (TE, g biomass kg<sup>-1</sup> water). RUE and leaf area expansion are reduced by low specific leaf N (SLN, g N m<sup>-2</sup> leaf) when N is limited. The SLN is predicted using a crop N dynamics network in leading models such as the APSIM–sorghum crop model (Fig. 2b). If water demand is not met by the uptake of soil water by the roots (supply), water-limited growth rate calculated by multiplying the reduced water supply and the TE. Together the RUE and TE equations capture the efficiency with which a canopy produces biomass from intercepted radiation and allowable transpiration. Biomass accumulation in plant organs (leaf,

stem, grains, roots) is determined by development-stage-sensitive partitioning rules and the supply and demand of C by the growing organs, and is modulated by N and water stress. Grain number is determined by crop biomass at anthesis; grain size increase is fuelled by biomass growth during the grain-filling period, C translocation, and is modulated by N. Crop nitrogen dynamics – involving leaf, stem, and grains – follow the supply–demand in the biomass growth modelling described above (Fig. 2b).

CGM has been widely used to interpret and predict the seasonal dynamics of soil–crop–environment systems, G × M × E interactions, and crop yield. They help to improve the interpretation of empirical yield information via dissection and explanation of yield in relation to the underlying physiological networks of component traits (Fig. 2). The interpretative nature of the APSIM–sorghum crop model helped to explain that the well-documented sorghum stay-green phenotype – the ability to retain green leaf area late in the crop cycle, benefiting yield in drought-prone environments – is mainly ascribed to seasonal timescale shifts in water use patterns toward the reproductive phase of the crop (Hammer *et al.* 2019b). Progress in maize (*Zea mays*) drought tolerance improvement had been aided by crop modelling, which revealed that the rate and patterns of water use during crop growth and development were important components, contributing to the higher yield of some maize hybrids under important field drought conditions within the TPE (Cooper *et al.* 2014a; Hammer *et al.* 2019a). The predictive potential of CGMs set up the capacity to simulate seasonal crop dynamics, G × M × E interactions, and the consequences of component traits on grain yield across the TPEs, which is valuable for identifying phenotyping strategy and supporting breeding selection (Cooper *et al.* 2014a; van Oosterom *et al.* 2021).

### Contextualising model utilities and limitations

Mathematical models that represent our understanding of actual biological systems have emerged at many scales of biological organisation (Fig. 1), but the phenotypic prediction capabilities necessary for facilitating mechanism- and process-based crop improvement are beyond any one model can offer. The modelling approach that enables connections across biological scales of organisation have emerged as a natural solution to address the prediction gap, and are now at the frontier of plant/crop modelling (Wu *et al.* 2016; Chew *et al.* 2017; Marshall-Colon *et al.* 2017; Xiao *et al.* 2017; Yin *et al.* 2018; Hammer *et al.* 2019a; Zhu *et al.* 2022). This can take the form of either (1) a bottom-up modelling approach, starting with molecules/pathways and progressive spatial and temporal upscaling, or (2) a top-down modelling approach, beginning with macroscale component traits and dissection of traits to their underpinning mechanisms and processes (Fig. 1).



**Fig. 2.** (a) Crop growth and development and (b) crop nitrogen dynamic networks used in the Agricultural Production System simulator (APSIM)-sorghum crop model. The blue and green boxes show connection points between (a) and (b). CGR, crop growth rate ( $\text{g biomass m}^{-2} \text{ day}^{-1}$ );  $k$ , crop canopy light extinction coefficient;  $kl$ , soil water extraction decay constant; RUE, radiation use efficiency ( $\text{g biomass MJ}^{-1}$  intercepted solar energy); SLN, specific leaf nitrogen ( $\text{g N m}^{-2}$  leaf); TE, transpiration efficiency ( $\text{g biomass kg}^{-1}$  water); VPD, vapour pressure deficit (kPa). Adapted from (Hammer *et al.* 2010) permitted by John Wiley and Sons (publisher).

The bottom-up approach typically aims for elaborate descriptions of plant/canopy morphology and architecture, then adapt molecular pathway models to each part of the simulated plant, resulting in a large number of input parameters that are needed to simulate all model mechanisms and processes under each specific set of environmental conditions. Extending bottom-up plant/canopy models temporally to simulate growth dynamics requires parameterisation of

changes in morphological and architectural features. Current method for reliably quantify time series canopy architectures is to rely on experimental measurements throughout the growth (e.g. Chang *et al.* 2022). Both spatial and temporal parameterisation requirements of bottom-up models hinder prediction of seasonal timescale dynamics of soil-crop-environment systems,  $G \times M \times E$  interactions, and crop yield.

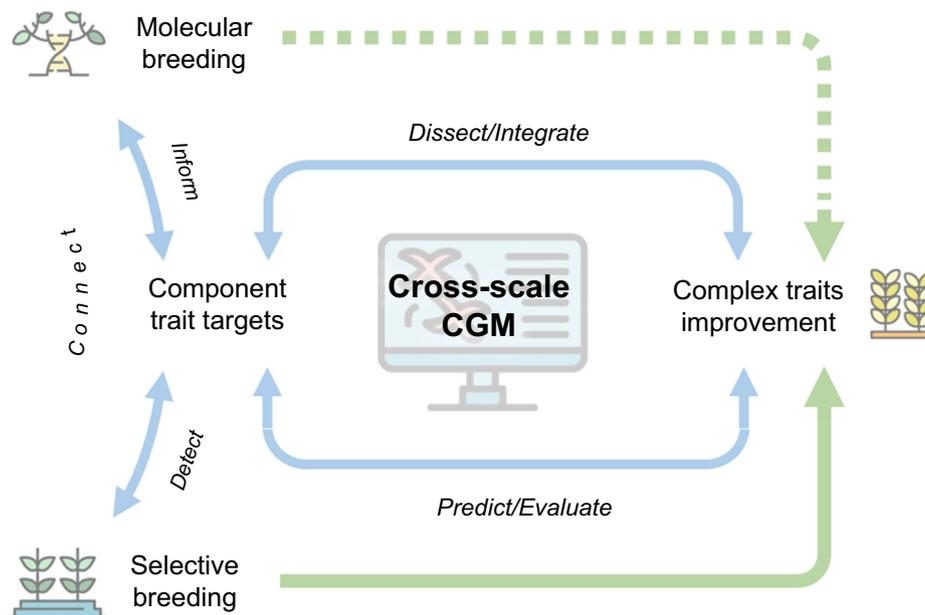
In contrast, the emphasis in the top-down approach is to capture primary physiological-component traits to allow simulation of crop growth and development dynamics (Fig. 2). But the details of mechanisms and processes are typically traded off (Fig. 1). An example is the use of the RUE equation to simulate aboveground biomass growth to represent the molecular pathways underpinning leaf photosynthesis and the 3D canopy architecture that influence canopy microclimate and leaf photosynthesis. The resulting lack of explicit links to molecular/enzymatic actions hinder use of top-down models to simulate molecular manipulation effects on crop performance.

A modelling strategy put forward by Wu *et al.* (2016) and Hammer *et al.* (2019a) emphasises the need to combine modelling principles from both top-down and bottom-up perspectives for effective and efficient model development. Existing top-down frameworks at the organ–plant–crop scale with capacity for  $G \times M \times E$  and yield predict are useful foundations. But this means the frameworks need to readily accommodate variations in the representation of biological mechanisms and processes – capabilities that can be found in current CGMs such as those in the APSIM platform (Hammer *et al.* 2010, 2019b; Brown *et al.* 2014; Holzworth *et al.* 2014). An effective way of integrating models across biological scales of organisation is to follow a trait dissection principle that progressively incorporates biological complexities into the top-down frameworks by

including elaborate models of mechanisms and processes at lower biological scales. These need to have structure and parameters with improved links to bioengineering targets, and from which model parameter values can be easily obtained via experimental or model simulation means to function in the top-down framework. Importantly such composite models would need to be evaluated for their phenotypic prediction performance. With these modelling ambitions, the following section describes principles for forming cross-scale models (also referred to as multiscale or plant/crop systems modelling), trait–crop–environment system dynamics generated by cross-scale models, and how such models can be used to facilitate model-guided crop improvement.

### Prospects for model-guided crop improvement strategies

With growing interest in mechanism- and process-driven crop improvement, how can we maximise translation of fundamental discovery science into more grain yield per land area? And where does this sit with ongoing selective breeding? Can plant/crop modelling unlock new integrated pathways for plant science and crop improvement? I now discuss such prospects by summarising past and present experimental and modelling work that jointly point to a model-guided framework for crop improvement (Fig. 3). Research topics



**Fig. 3.** Model-guided crop improvement framework, defining the potential role of cross-scale crop growth modelling (CGM) in unlocking new avenues for tapping into fundamental plant science research and molecular breeding, and enhancing selective breeding (blue arrows). Selective breeding has been supporting historical gains in complex traits, e.g. crop yield (green solid arrow), but there are growing interests in using genetic engineering to improve crop yield (green dashed arrow).

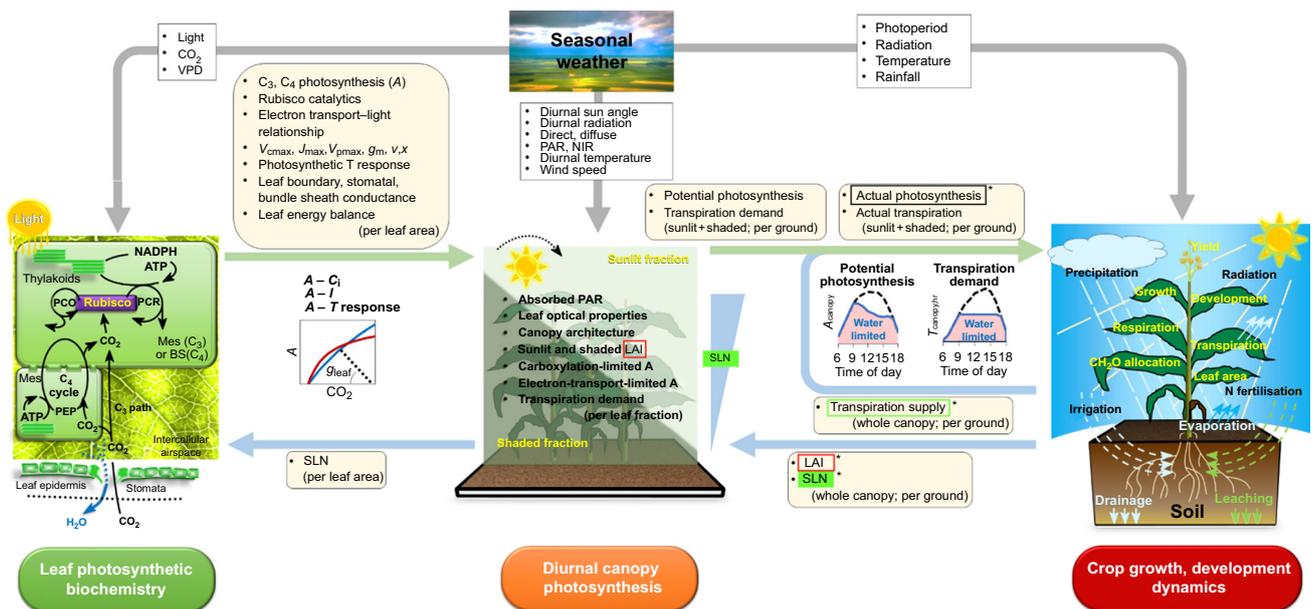
can be grouped into three main areas. The first is modelling plants across multiple scales of biological organisation. This develops the plant/crop modelling science that connects molecular- and pathway-scale mechanisms and processes with the integrated crop scale; and adds biological details into organ-plant-crop-scale ecophysiology. The second is developing an understanding of time-series soil-crop-environment system dynamics through the predictive ability of plant/crop models. Combining this with targeted experiments aids integrative understanding across scales of biological organisation and model validation. The third is applications of model-guided crop improvement strategies for supporting genetic engineering and selective breeding efforts.

### Modelling of plant across biological scales of organisation using cross-scale modelling principles

As seen in the previous section, modelling can be at multiple scales of biological organisation (Fig. 1), and many models have matured sufficiently to adequately reflect the biological systems they set out to address. But do we have the necessary modelling tools for guiding translation of plant growth and development knowledge to crop yield improvement? Achieving this effectively and efficiently will be unlikely if

models continue to evolve in silos. Cross-scale modelling principles first involve identifying a useful foundational framework of soil-crop-environment systems that reflect field crop production. This foundation should be capable of simulating dynamic plant/crop growth and development processes over a crop cycle to predict yields under given agronomic management and seasonal environmental conditions. The crop physiological determinant network used by the APSIM-sorghum growth model (Fig. 2) can serve as one such foundational framework. Additional mechanism and process models are then selected to replace elements of the network via a trait dissection approach and by ensuring the overall crop physiological determinant network remains as functional as the original models.

This idea was explored in a cross-scale modelling study by Wu *et al.* (2016), who proposed the dissection of crop-scale biomass growth rates in both radiation- and water-limited situations into the biochemical processes of leaf photosynthesis and stomatal conductance (Wu *et al.* 2018, 2019) (Fig. 4). This requires photosynthesis models to predict leaf CO<sub>2</sub> assimilation rates according to light, CO<sub>2</sub>, and temperature conditions and canopy upscaling. Wu *et al.* (2019) found that upscaling coarse-grained biochemical models of steady-state leaf photosynthesis with the relatively abstract sun-shade canopy modelling was an effective and efficient strategy



**Fig. 4.** An advanced cross-scale crop physiological determinant network showing the two-way connections between mechanisms and processes smaller and larger biological scales of organisation. Trait dissection expands biological details on the radiation- and water-limited growth-rate component in the conventional crop growth and development network (the far-right image and expanded in Fig. 2) to include processes in leaf photosynthesis, stomatal conductance, and a sun-shade canopy upscaling model. Component trait connection is an important aspect of cross-scale modelling, here it involves upscaling of the leaf photosynthetic biochemistry to the crop scale through a canopy model (left-right green arrows), as well as crop ecophysiological regulation on leaf- and canopy-scale photosynthesis and transpiration (right-left blue arrows). The blue triangle indicates a reduction in SLN going down the canopy. The asterisked component traits are linked to the conventional physiological determinant network in Fig. 2. Environmental factors affect processes throughout biological scales (grey arrows). Adapted from (Wu *et al.* 2019) under Springer Nature journal authors' rights.

for representing radiation- and water-limited growth rates. And such parsimonious models can be effectively integrated with crop growth and development dynamics for robust yield prediction with negligible changes in predicting performance (Wu *et al.* 2019). The alternative bottom-up canopy modelling approach has also generated models that upscale photosynthesis with elaborate 3D canopy models to simulate the canopy CO<sub>2</sub> assimilation rate (Wang *et al.* 2020); but using such models to simulate crop dynamics across a seasonal timescale remains challenging due to the need for accurate canopy architecture spatial and temporal parameterisation. Parsimonious plant/crop models contribute significantly to linking mechanisms and processes across biological scales (Yin and Struik 2017; Hammer *et al.* 2019a; Matthews *et al.* 2022).

Trait dissection modelling concerns not just incorporation of elaborate mechanisms and processes into existing plant/crop modelling frameworks: the science on how component traits are connected is also important if models are to realistically reflect soil–crop–environment systems. But this aspect of multiscale modelling is rarely detailed and often overshadowed by seeking to model elaborate molecular pathways and plant/canopy architecture. Wu *et al.* (2019) presents one of the few modelling studies to improve component trait connections, enabling simulation of crop growth, development dynamics, and yield prediction across TPEs. For crop biomass growth, since leaf CO<sub>2</sub> assimilation allows carbon gain, and biomass growth depends on photosynthesis of a whole canopy, modelling this involves the connection between leaf CO<sub>2</sub> assimilation, respiration rates, and crop growth via modelling of canopy upscaling (Fig. 4). This aspect is common to all plant/crop models that aim to predict biomass growth. Canopy leaf area index (LAI, m<sup>2</sup> leaf m<sup>-2</sup> ground) is an input to the canopy model, together with canopy architecture: both determine the available leaf area for photosynthesis and heterogeneous light on leaves throughout a canopy. Plants partition N into their leaves (Fig. 2b) and use it to synthesise photosynthetic machinery. Leaf N is represented as SLN and can vary depending on leaf position on the plant and the N requirements of competing organs. SLN is used to drive leaf photosynthetic parameters using the relationships between SLN, the maximum carboxylation rate ( $V_{\text{cmax}}$ ), and the maximum electron transport rate ( $J_{\text{max}}$ ) (Evans 1983, 1989; Silva-Pérez *et al.* 2020).

On the water side, canopy transpiration demand arises from stomata on leaves that are open to allowing photosynthesis; this needs a combination of the biochemical models of leaf photosynthesis and leaf-energy balance and transpiration calculations, upscaled to canopy level (Wu *et al.* 2019). Crop water supply is determined by soil water content, root distribution in soil layers, and water extraction by roots. Actual biomass growth is driven by potential canopy CO<sub>2</sub> assimilation and modulated by water limitation, which restricts stomatal conductance and leaf photosynthesis (Fig. 4). These present a trait dissection–integration modelling

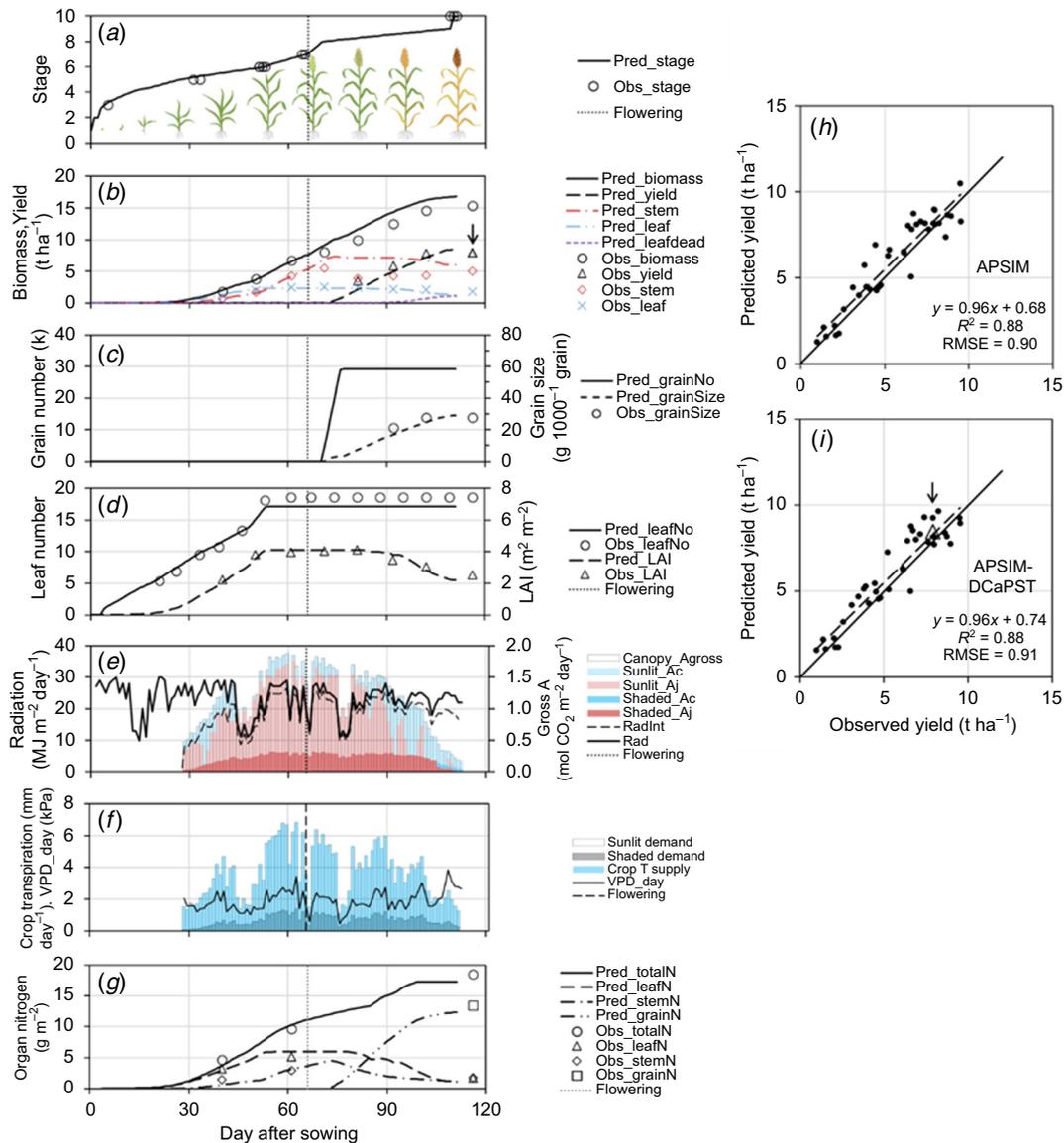
principal used to connect component traits in advanced plant/crop models (Wu *et al.* 2019). I now consider the effectiveness of this approach in capturing the complex biological system spanning multiple scales of biological organisation from leaf photosynthetic biochemistry to crop-scale growth.

## Evaluating reliability of predicted molecular–trait–crop–environment system dynamics

Plant/crop modelling research is a fast-evolving plant-science topic, and the variety of tools, including those discussed earlier, can be overwhelming. How do we appraise model reliability? In discussing the credibility of models Hammer (2020) proposed three criteria. They must: (1) predict phenotypic outcomes for experiments with high-quality plant/crop data; (2) generate known quantitative responses to key factors that influence crop yield (solar radiation, CO<sub>2</sub>, temperature, water, N, crop maturity, and crop configuration); and (3) predict emergent phenotypes and interactions associated with key traits. Below I apply them on cross-scale CGMs.

High-quality data for analysing CGM credibility should contain key environmental drivers and crop attributes for yield determination. Nowadays environmental data can be automatically collected with a temporal resolution from minutes to days. Fig. 4e, f show daily incoming solar radiation and air vapour pressure deficit – the main environmental drivers of canopy photosynthesis/biomass growth and canopy transpiration (Fig. 2a). Many crop attributes can be measured from field experiments, but should consider data requirements for CGM validation, which can be guided by crop physiological determinant networks (Figs 2, 4). A number of first-order crop growth and development attributes important for validating yield prediction are shown in Fig. 5a–d, g. This includes timeseries crop phenological stage, biomass (by plant organs) and yield growth, grain number and size, leaf number, canopy leaf area index, and the amount of N in plant organs. This field experiment was sown on 27 November 1997 at Hermitage, Australia, with non-limiting water and N, using a sorghum genotype close to the elite commercial variety (Buster), and grown in solid configuration with plant density of 10 m<sup>-2</sup> and row spacing of 0.5 m, representing intensive management of the environment (data: Hammer *et al.* 2010, sourced from the APSIM Initiative: <https://tinyurl.com/mtcpuze6>). Most of the attributes were collected on a per-ground-area basis for calculation of grain yield per land area. A unique quality of this high-quality dataset is time-series observations of the key field crop attributes, which is of great value for validating the capability of models in simulating growth and development dynamics over the crop cycle, and significantly deepens our understanding of complex soil–crop–environment systems over time.

Expanding model validation to assess key factors encountered by field crops can increase model robustness for a wider range of G × M × E conditions. This includes combinations of



**Fig. 5.** Predicted sorghum crop growth and development dynamics and high-quality field experiment data. Time series of: (a) phenological stages and the time of flowering, indicated by the vertical dotted line; (b) growth of the crop biomass, and leaf, stem, and grain components; (c) grain number and grain size (weight of 1000 grains); (d) plant leaf number and canopy-leaf area indices; (e) daily incoming solar radiation and that intercepted by the canopy, and detailed simulation of instantaneous photosynthetic CO<sub>2</sub> assimilation with either the carboxylation or electron-transport-limited state by the sunlit and shaded leaf fractions of the canopy, but aggregated to daily results; (f) observed daily representative vapour pressure deficit (VPD) and predicted transpiration demand and supply of the sunlit and shaded leaf fractions (the empty and grey bars are filled indicating that all demand was met in this case); (g) the amount of N in leaves, stems, and grains (per ground area basis); (h) observed final sorghum yield across various solar radiation, temperature, water, and N conditions vs predicted yield using the standard APSIM–sorghum model (Hammer *et al.* 2010); (i) predicted vs observed using the APSIM cross-scale sorghum model (Wu *et al.* 2019). The diamond-shaped data point indicated by the arrow is the predicted yield outcomes in (b). See text for details of experimental data. Daily representative VPD is calculated by subtracting the saturated vapour pressure at daily minimum temperature from that of the daily maximum temperature, multiplied by a correction factor of 0.75 (Lobell *et al.* 2015). (h) and (i) are reproduced from Wu *et al.* (2019), under Springer Nature journal authors' rights.

sowing location, sowing date (giving contrasting seasonal patterns of radiation and temperature), water and N treatments,

and crop management. But this requires considerable commitment in synergistic experimental–modelling research. The

APSIM Initiative ([www.apsim.info](http://www.apsim.info)) is a leading example of such enduring effort: its CGMs are leading the crop modelling space (Hammer *et al.* 2010; Brown *et al.* 2014; Holzworth *et al.* 2014). The APSIM–sorghum crop model shows good performance in predicting sorghum crop dynamics and yield across a wide range of experimental conditions (Fig. 5h; the APSIM–wheat crop model equivalent can be found in Brown *et al.* 2014). These experimental–modelling studies are foundational to model robustness in quantifying crop dynamic response to key environmental factors, and permit reliable outscaling of models to wider agricultural situations.

Models need to predict crop dynamics and emergent phenotypes associated with perturbations in key crop improvement traits for assessing genetic engineering. Wu *et al.* (2019) developed a state-of-the-art APSIM cross-scale modelling framework with which daily crop biomass growth rates are predicted by integrating (1) the two limiting states of photosynthesis and stomatal conductance at any instance, (2) the emergent consequence of collective photosynthetic CO<sub>2</sub> assimilation and transpiration contributed by the sunlit and shaded leaf fractions of a canopy leaf area, and (3) crop growth and development dynamics (Fig. 4). Simulated biomass accumulation over the crop cycle agreed with the field data adequately (Fig. 5b), with good agreement between the observed time-series data for the key crop growth and development attributes (Fig. 5a–d, g). This supports the simulated photosynthesis data (Fig. 5e), despite the absence of field data equivalent. Wu *et al.* (2019) further showed that the cross-scale model can predict sorghum crop dynamics and yield across a wide range of experimental conditions (Fig. 5g; the wheat simulation equivalent is in Wu *et al.* 2019), making it the most extensively validated photosynthesis–plant–crop-scale CGM.

Given our increased understanding of plant growth and development, CGMs are being increasingly sought for predicting crop-scale outcomes from manipulating plant growth and developmental traits. Photosynthetic enhancement is a research area that has integrated well with CGM use, generating predicted yield outcomes of biochemical/leaf-scale manipulations (Yin and Struik 2017; Hammer *et al.* 2019a; Leakey *et al.* 2019; Wu *et al.* 2019, 2023; Harbinson and Yin 2023). But how do we know that the models have got it right? Without actual data, the best approach requires painstaking analysis of model outputs through the biological scales of organisation to support results at the integrated scale. This can involve assessing the reliability of simulated leaf A–C<sub>i</sub>, diurnal canopy photosynthesis, crop growth, and development dynamics over a crop cycle, across a range of production environments (more in the section below). This important aspect of plant/crop modelling research is only beginning to be comprehensively explored (Wu *et al.* 2019, 2023), which needs to be presented in future modelling studies. Beyond model simulation analysis, we need synergetic field experiments with transgenics that can generate improved cross-scale data (from molecular to whole-crop) to interrogate and validate model predictions.

## Model-guided genetic engineering: evaluating molecular manipulation target

Despite the promises of genetic manipulation for crop yield improvement, there has not yet been a significant improvement in yield. The major reason is that enhancements at lower biological scales of organisation often diminish with increasing biological scales (Sinclair *et al.* 2004; Wu *et al.* 2018, 2023; Hammer *et al.* 2019a). Experimental evidence related to major strategies of photosynthetic manipulation and their consequences on plant/crop performance is mostly confined to the leaf- and single-plant scale (Table 1). Only a few studies have reported transgenic field experiments (e.g. South *et al.* 2019; De Souza *et al.* 2022), but until more robust field tests are carried out their asserted biomass and yield benefits remain speculative, hampering decision making for crop improvement. Cross-scale plant/crop modelling offers a means for *a priori* probing of the effects of genetic manipulation across scales of biological organisation by predicting and evaluating molecular–trait–crop–environment dynamics and yield (Fig. 3). Table 1 summarises model predictions related to major strategies of photosynthetic manipulation and their consequences at the leaf, plant, and crop scales, providing insights into the likely yield enhancement or lack thereof for supporting molecular breeding efforts (Fig. 6a).

One intriguing finding from comparing predictions from different work is that predicted enhancement (or lack of it) at leaf, canopy, and crop scales varies dramatically (Table 1). This can confound the decision support aspirations of plant/crop models. A key issue is that simulated growth advantage and yield by some measure are often presented without adequate elaboration on photosynthesis–plant–crop dynamics for appraising the predicted results. This stresses the need for modelling studies to give greater weight to unpack predicted emergent phenotypes, crop dynamics, and feedback regulations between key traits and the environment. Wu *et al.* (2023) addressed this issue by comprehensive comparisons of changes across leaf, canopy, and crop scales, with and without introduction of parameter change representing photosynthetic manipulation.

A seasonal sorghum crop simulation reported by Wu *et al.* (2023) is reviewed here with an informative comparison approach (Fig. 6). This analysis compares theorised effects of leaf photosynthetic enhancement by a combination of improved Rubisco catalytic properties, increased Riseke FeS, and mesophyll conductance. At the leaf scale A–C<sub>i</sub> curve was predicted to increase; e.g. a 7% increase in leaf CO<sub>2</sub> assimilation rate at an ambient C<sub>i</sub>, and high-light condition (Fig. 6b). Fig. 6c–h shows the baseline simulation of the dynamics of key crop-scale growth and development attributes, capturing effects of the leaf photosynthetic enhancement at the canopy/crop level. This simulation predicted that with the given leaf photosynthetic enhancement there would be no change to the developmental rate of sorghum plants over

**Table 1.** Summary of observed and predicted photosynthetic manipulation effects in C<sub>3</sub> and C<sub>4</sub> model/crop species across the different scales of biological organisation.

Manipulation			Leaf scale effect	Canopy scale effect	Crop biomass/ yield effect	Observed and predicted effects	References
Carboxylation	Enhanced Rubisco catalytic properties	Exp.	15%	–	–	Measured high-light leaf CO <sub>2</sub> assimilation rate ( $A_{leaf}$ ) in Rubisco subunits and RUBISCO ASSEMBLY FACTOR 1 OE maize.	Salesse-Smith <i>et al.</i> (2018)
		Model	–	–8% to 27%	–	Predicted single-day canopy CO <sub>2</sub> assimilation rate ( $A_{canopy}$ ) using a sun-shade canopy photosynthesis model combined with the biochemical model of C <sub>3</sub> photosynthesis. Various Rubisco sources with different $K_c$ and specificity were simulated.	Zhu <i>et al.</i> (2004)
			15%	4%	0% to 4%	Predicted ambient-C <sub>i</sub> -high-light $A_{leaf}$ in wheat using the biochemical model of C <sub>3</sub> photosynthesis (reflecting an A–C <sub>i</sub> curve with improved $k_{cat}^c$ and CE based on (Sharwood <i>et al.</i> 2016a) and (Sharwood <i>et al.</i> 2016b) and a +20% $S_{c/o}$ ). Predicted CO <sub>2</sub> assimilation rate ( $A$ ) by the collective sunlit leaf area of the wheat canopy ( $A_{sunlit}$ ) on a sunny day. Predicted wheat grain yield outcomes over 720 seasons in dryland cropping situations across the whole of Australia with realistic weather, soil and nitrogen input using a cross-scale model.	Wu <i>et al.</i> (2023)
			1%	2%	1% to 3%	Analogous to the above for C <sub>4</sub> photosynthesis (reflecting an A–C <sub>i</sub> curve with improved +20% in $V_{cmax}$ and $K_c$ based on (Salesse-Smith <i>et al.</i> 2018) and (von Caemmerer and Furbank 2016)), a sorghum canopy, and sorghum grain yield outcomes over 480 seasons in dryland cropping situations across the sorghum producing regions of Australia.	Wu <i>et al.</i> (2023)
	Reducing photorespiration	Exp.	30%	–	–30% to 40%	Measured ambient-C <sub>i</sub> $A_{leaf}$ in soybean with alternative glycolate metabolism pathways. Field plant biomass were from 2 years of experiment where plants were grown in a four-by-four configuration surrounded by wide-type plants; the variability was a result of different transgenic event.	South <i>et al.</i> (2019)
		Model	26%	–	20%	Predicted $A_{leaf}$ loss at air CO <sub>2</sub> of 350 ppm, predicted yield increase with minimal photorespiration by assuming no O <sub>2</sub> in the air in the simulation using a multilayer canopy–soil–root systems model.	Walker <i>et al.</i> (2016)
			30%	–	5%	Predicted ambient-C <sub>i</sub> , high-light $A_{leaf}$ in wheat using the biochemical model of photosynthesis (reflecting a transgenic plant A–C <sub>i</sub> curve from South <i>et al.</i> 2019). Predicted average wheat grain yield outcomes over 120 seasons in dryland cropping situations at Dalby, Australia across the whole Australia with realistic weather, soil and abundant nitrogen input using a cross-scale model.	Hammer <i>et al.</i> (2019a)
CO <sub>2</sub> delivery	Increased mesophyll conductance	Exp.	n.s.	–	–	Measured high-C <sub>i</sub> , high-light $A_{leaf}$ in <i>Setaria viridis</i> with overexpressed plasma membrane intrinsic aquaporins and higher mesophyll conductance	Ermakova <i>et al.</i> (2021)
		Model	5%	–	–	Predicted ambient-C <sub>i</sub> , high-light $A_{leaf}$ in tobacco by doubling of mesophyll conductance to 1 mol m <sup>-2</sup> s <sup>-1</sup> bar <sup>-1</sup> .	Clarke <i>et al.</i> (2022)
			3%	2%	0% to 1%	Predicted ambient-C <sub>i</sub> , high-light $A_{leaf}$ in wheat using the biochemical model of C <sub>3</sub> photosynthesis (reflecting an A–C <sub>i</sub> curve with +20% $g_m$ ). Predicted $A_{sunlit}$ of the wheat canopy on a sunny day. Predicted wheat grain yield outcomes over 720 seasons in dryland cropping situations across the whole of Australia with realistic weather, soil and nitrogen input using a cross-scale model.	Wu <i>et al.</i> (2023)

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Table 1. (Continued).

Manipulation		Leaf scale effect	Canopy scale effect	Crop biomass/ yield effect	Observed and predicted effects	References
		0%	0%	0%	Analogous to the above for C <sub>4</sub> photosynthesis (reflecting an A–C <sub>i</sub> curve with +20% g <sub>m</sub> ), a sorghum canopy, and sorghum grain yield outcomes over 480 seasons in dryland cropping situations across the sorghum producing regions of Australia.	Wu <i>et al.</i> (2023)
Cyanobacterial CO <sub>2</sub> concentrating mechanism	Exp.	–	–	–	–	–
	Model	60%	–	–	Predicted high-light A <sub>leaf</sub> using a detailed leaf scale CCM model.	McGrath and Long (2014)
		48%	27%	0% to 8%	Predicted ambient-C <sub>i</sub> , high-light A <sub>leaf</sub> in wheat using a CCM version of the biochemical model of C <sub>4</sub> photosynthesis (see Wu <i>et al.</i> (2023) for model parameterisation details). Predicted A <sub>sunlit</sub> of the wheat canopy on a sunny day. Predicted wheat grain yield outcomes over 720 seasons in dryland cropping situations across the whole of Australia with realistic weather, soil and nitrogen input using a cross-scale model.	Wu <i>et al.</i> (2023)
C <sub>4</sub> rice	Exp.	–	–	–	–	–
	Model	250%	18%	37%	Predicted high-light A <sub>leaf</sub> in rice. Predicted A <sub>canopy</sub> on a sunny day. Predicted rice biomass with unlimited water and nitrogen using a whole-rice model.	Yin and Struik (2017)
Electron transport chain	Exp.	25%	–	–	Measured high-light A <sub>leaf</sub> in Riese FeS OE <i>Arabidopsis</i> .	Simkin <i>et al.</i> (2017)
		8%	–	–	Measured high-light A <sub>leaf</sub> in Riese FeS OE <i>Setaria viridis</i> .	Ermakova <i>et al.</i> (2019)
	Model	12%	7%	–3% to 2%	Predicted ambient-C <sub>i</sub> , high-light A <sub>leaf</sub> in wheat using the biochemical model of C <sub>3</sub> photosynthesis (reflecting averaged relative changes in model parameter values inferred from changes in A–I curve observed by Simkin <i>et al.</i> (2017) and Ermakova <i>et al.</i> 2019). Predicted A <sub>sunlit</sub> of the wheat canopy on a sunny day. Predicted wheat grain yield outcomes over 720 seasons in dryland cropping situations across the whole of Australia with realistic weather, soil and nitrogen input using a cross-scale model.	Wu <i>et al.</i> (2023)
		5%	4%	–1% to 3%	Analogous to the above for C <sub>4</sub> photosynthesis, a sorghum canopy, and sorghum grain yield outcomes over 480 seasons in dryland cropping situations across the sorghum producing regions of Australia.	Wu <i>et al.</i> (2023)
	Extending photosynthetically active radiation wavelength	Exp.	–	–	–	–
Model		10% to 30%	–	–	Photosynthetic efficiency gain calculated based on (Chen and Blankenship 2011)	Long <i>et al.</i> (2015)
		1%	5%	–3% to 3%	Predicted ambient-C <sub>i</sub> , high-light A <sub>leaf</sub> in wheat using the biochemical model of C <sub>3</sub> photosynthesis (reflecting an A–C <sub>i</sub> curve with +20% PAR). Predicted A <sub>sunlit</sub> of the wheat canopy on a sunny day. Predicted wheat grain yield outcomes over 720 seasons in dryland cropping situations across the whole of Australia with realistic weather, soil and nitrogen input using a cross-scale model.	Wu <i>et al.</i> (2023)
		7%	9%	–1% to 7%	Analogous to the above for C <sub>4</sub> photosynthesis, a sorghum canopy, and sorghum grain yield outcomes over 480 seasons in dryland cropping situations across the sorghum producing regions of Australia.	Wu <i>et al.</i> (2023)

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Table 1. (Continued).

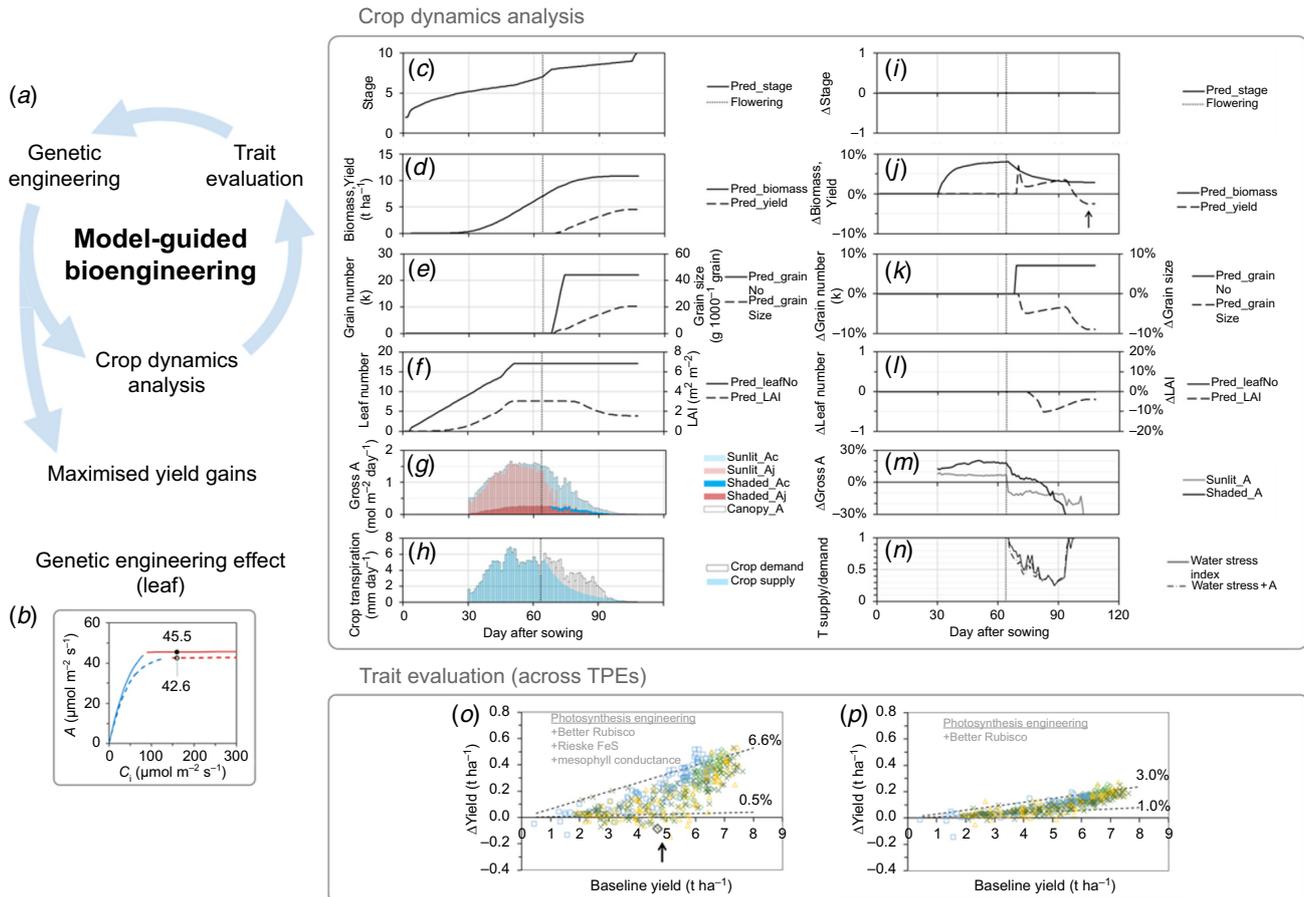
Manipulation			Leaf scale effect	Canopy scale effect	Crop biomass/ yield effect	Observed and predicted effects	References
Fluctuating photosynthesis	Accelerated recovery from photoprotection	Exp.	–	–	20% to 33% or 0%	Field soybean yield of the three top performing transgenic soybean lines from 2 years of experiment. First year results were estimated from plants grown in individual rows, second year results were from plants grown in plots with multiple rows. Results were subjected to pest and possible storm damage.	De Souza <i>et al.</i> (2022)
		Model	–	13%	–	Predicted daily $A_{\text{canopy}}$ using a ray tracing, soybean canopy architecture model with a dynamic version of the biochemical models of photosynthesis.	Wang <i>et al.</i> (2020)
Manipulation stacking		Exp.	–	–	–	–	–
		Model	–	–	14% to 19%	Predicted water non-limited storage organ biomass increase with each photosynthetic parameter increased by 20% in wheat, potato, and maize over 10 seasons (irrigated situations) across Europe.	Harbinson and Yin (2023)
			27%	15%	–2% to 7%	Predicted ambient- $C_i$ , high-light $A_{\text{leaf}}$ in wheat using the biochemical model of $C_3$ photosynthesis (reflecting an $A-C_i$ curve with combined 'better' Rubisco, higher electron transport rate, and improved gm as described above for $C_3$ photosynthesis). Predicted $A_{\text{sunlit}}$ of the wheat canopy on a sunny day. Predicted wheat grain yield outcomes over 720 seasons in dryland cropping situations across the whole of Australia with realistic weather, soil and nitrogen input using a cross-scale model.	Wu <i>et al.</i> (2023)
		7%	6%	1% to 7%	Analogous to the above for $C_4$ photosynthesis, a sorghum canopy, and sorghum grain yield outcomes over 480 seasons in dryland cropping situations across the sorghum producing regions of Australia.	Wu <i>et al.</i> (2023)	

the crop cycle, which would take the same time to reach physiological maturity (Fig. 6i). Predicted leaf number per plant and leaf size remained unchanged, so no change in the predicted canopy LAI over crop cycle (Fig. 6l). The predicted increase in leaf photosynthesis increased canopy photosynthesis before flowering: the sunlit leaf fraction by 7% (reflecting the leaf-level enhancement); and the shaded leaf fraction by up to 20% (Fig. 6m). This increased accumulated crop aboveground biomass to up to 8% more before flowering (Fig. 6j).

However, in the baseline scenario, canopy-scale photosynthesis and growth-rate advantages were diminished after flowering due to water stress, as crop water demand was not fully met from soil (Fig. 6d, g, h); water stress was made more severe with leaf photosynthetic enhancement (Fig. 6n). This was because of predicted enhanced photosynthesis, stomatal conductance, and crop water demand, which depleted soil moisture faster. Water stress caused leaf senescence and reduced canopy LAI by up to 10% during the grain-fill period (Fig. 6l). The combination of water stress on stomatal opening, and reduced leaf-area light interception and photosynthesis eliminated advantages in sunlit and shaded leaf fraction photosynthesis: the sunlit fraction was cut by about 10% across the grain-fill period (Fig. 6m). This

reduction in canopy photosynthesis reduced early advantage in the accumulated crop biomass, and finished at only around a 3% increase at physiological maturity (Fig. 6j). This biomass accumulation dynamic could not sustain the 3% yield increase achieved at around the middle of the grain-fill period, which finished with a –3% yield change at physiological maturity (Fig. 6j). The convoluted nature of the dynamic plant/crop attribute interactions makes them difficult to foresee but is made possible by using plant/crop modelling. Such *a priori* dynamic system analysis is rare in the literature, but needs to become the norm, providing the basis for deepening our understanding of plant biology beyond effects at molecular–organ scales to crops at a seasonal timescale, and supporting claims of the impacts of genetic engineering on crop-scale performance.

Such intricate photosynthesis and crop dynamics result needs to be extended to cover conditions of intended TPEs to be useful for crop improvement. Wu *et al.* (2023) has offered such simulation study. They designed a large-scale simulation, akin to conducting METs, to study the impacts of photosynthetic manipulation on wheat and sorghum grown using Australian production as a case study. Several key and environmentally contrasting locations were used,



**Fig. 6.** (a) Model-guided genetic engineering framework. (b) Modelling of  $C_4$  photosynthetic manipulation outcomes at leaf scale. The indicated  $\text{CO}_2$  assimilation rate is for an intercellular  $\text{CO}_2$  partial pressure of 160  $\mu\text{bar}$ , which is achieved with a potential stomatal conductance for the simulated assimilation rate under water non-limiting conditions. (c–h) Simulated growth and development dynamics of a sorghum crop (see text for simulation setup): phenological stages; aboveground total crop biomass and yield; components of yield: grain number and grain size; plant leaf number and canopy leaf area index; carboxylation- and electron-transport-limited  $\text{CO}_2$  assimilation rate of the sunlit and shaded leaf fractions of the canopy; crop water demand and actual supply. (i–n) Predicted changes in the corresponding growth and development attributes (note percentage change and absolute change are used in different panels). (o) Predicted variations in sorghum yield change ( $\Delta$ yield) with stacking of the indicated manipulations across 120 possible seasonal weather conditions for each of the four Australian sorghum production sites (see text for more details). The dashed lines indicate the 10th and 90th percentile regressions for  $\Delta$ yield versus baseline yield. (p) Analogous with (o) for singly enhancing Rubisco. The predicted percentage  $\Delta$ yield in Panel J (arrow) is just one outcome from the full 120 seasonal weather conditions by four sites combinations (arrow and diamond symbol in Panel o). (o) and (j) are reproduced from Wu *et al.* (2023) – an open access article.

sampled up to 120 possible seasonal weather conditions at each location. Wu *et al.* (2023) compared results for nine sorghum photosynthetic manipulation strategies; two of which are reproduced in Fig. 6o, p. The scatter of predicted yield results in these panels highlight the influence of variable location and seasonal weather conditions: the horizontal axis indicates predicted sorghum yield without manipulation; the vertical axis indicates change in yield with manipulation relative to the baseline.

The comprehensive modelling suggests that manipulation stacking strategies can result in more yield gains in more location–seasonal weather combinations, but can also result in yield losses in some seasons (Fig. 6o). The single manipulation

generated less yield gain but smaller chances of yield loss (Fig. 6p). The exact genetic engineering decision ultimately depends on the attitudes of the users (i.e. grain growers) to risk. I argue that we need to drastically increase our knowledge on crops-scale  $G \times M \times E$  and yield outcomes via this theoretical means, probing the likely benefits of molecular manipulation (or lack of it) – predicting why and how often enhanced leaf photosynthesis can boost yield or fail – to help design and focus on further manipulation strategies that are likely to have the most desirable impacts at a commercial crop production scale.

The second intriguing finding is that some modelling and experimental work suggest that enhancements at small

biological scales can be translated into yield with minimal loss or even multiplied benefits. McGrath and Long (2014) claimed that a large increase in light-saturated photosynthetic rate (simulated by a leaf-level model) could lead to significant increases in yield. The work by South *et al.* (2019) did not reconcile the fact that while canopy photosynthesis only increased by less than 10% in their photorespiration transgenics, crop biomass increased by more than 40%. These findings are not supported by many studies that predict diminishing returns (Sinclair *et al.* 2004; Wu *et al.* 2018, 2023; Hammer *et al.* 2019a). The yield-scale change predicted by Wu *et al.* (2023) is consistent with transgenic field-testing results by Simmons *et al.* (2021), which conclusively show that a single gene manipulation or several gene manipulations are unlikely to lead to significant yield advantages in crops. Given the data on photosynthetic manipulation at the leaf-scale, cross-scale modelling, and realistic expectations of gene manipulation effect, predictions of crop-yield change with photosynthetic engineering by Wu *et al.* (2019) and Wu *et al.* (2023) are likely to be more realistic. Their results suggest that many photosynthetic enhancement strategies will probably result in modest yield gains (−1% to +4%) across Australian TEPs. This points to the need to recalibrate our expectations of photosynthetic gene manipulation, and to explore and evaluate further photosynthetic engineering targets in more production environments.

To reconcile the contrasting results between model predictions, it is recommended that experimental and modelling studies adopt the informative crop growth and development analysis approach exemplified in Fig. 6 and by Wu *et al.* (2023) to support yield prediction results. This will require synergistic controlled-environment and field experiments with extensive phenotyping of transgenic plants, as well as model simulation studies to generate comprehensive information across scales of biological organisation including molecular analysis (e.g. Ermakova *et al.* 2019), leaf gas exchange, plant/canopy, soil–crop–environment measurements for validating model predictions.

### Model-guided breeding: linking complex traits with component trait and gene/QTL target

The second avenue in which plant/crop modelling can support breeding is by bridging the body of molecular and physiological knowledge with plant breeding efforts (Fig. 3). Models can tease apart the environmental and management factors (experienced across TPEs) in the performance of complex traits and dissect them into component traits, potentially providing a closer link with the underlying genetic architectures. One example is the use of a cross-scale model by Wu *et al.* (2019), which relates biomass and yield growth to underlying leaf photosynthetic CO<sub>2</sub> and light-response curves and biochemical attributes. *A priori* assessment of consequent crop dynamics and evaluation of component traits across TPEs suggests that the maximum

electron transport rate ( $J_{\max}$ ) is a major target for sorghum yield improvement (e.g. Fig. 6 and Table 1). Results from such modelling have helped fuel interest in modelling and manipulating the photosynthetic electron transport chain (Ermakova *et al.* 2019, 2022; Jaikumar *et al.* 2021; Harbinson and Yin 2023). The emergence of high-throughput phenotyping techniques across scales of biological organisation such as photosynthesis (Fu *et al.* 2020; Silva-Pérez *et al.* 2020; Zhi *et al.* 2022), root angle (Joshi *et al.* 2017), whole-plant transpiration efficiency (Geetika *et al.* 2019), and plant and panicle numbers in field crops (Zhao *et al.* 2021b) can allow for adequate phenotypic data for genome-wide association analysis. Zhi *et al.* (2022) links  $J_{\max}$  to genomic regions, effectively generating insights into the genetic architecture of a component trait that is likely to have a greater impact on crop growth. Modelling can serve as a bridge between component traits with links to molecular studies and phenotyping strategies.

The dissection of complex traits to component traits to better link with whole-genome information presents a unique opportunity for breeding. This extends the genome-to-phenome (G2P) prediction concept, which is important in plant breeding (Cooper *et al.* 2014b). Previously, whole-genome information has been used to directly predict endpoint traits such as grain yield. The extended G2P concept involves the use of whole-genome information to predict component traits of a CGM, which then simulates dynamic trait–crop–environment interactions ( $G \times M \times E$ ) and predicts emergent yield outcomes. It has been demonstrated that the incorporation of CGMs in a G2P prediction approach can enhance crop performance prediction for new genotypes and environments, especially those prone to abiotic stresses, beyond the boundaries of testing conditions in breeding programs (Cooper *et al.* 2022) and references therein. The application of the CGM–WGP approach to enhance genetic gains in leaf photosynthesis and crop growth will first require research to integrate cross-scale CGMs with whole-genome prediction methodologies.

### Implications for future roles of cross-scale plant/crop modelling

Growing knowledge in plant mechanisms and processes has prompted much interest in improving crop yield per land area via genetic/molecular manipulation approaches. But this will certainly require extensive yield assessment across TPEs, which is difficult to achieve in practice. This has motivated plant/crop modellers to critically analyse existing models (Fig. 1) and produce models that offer phenotypic prediction capabilities to close a widening phenotypic assessment gap. Yield impact information such as presented in Table 1 will continue to grow in its coverage of trait targets and simulation conditions. Confidence in models and predictions will continue to strengthen with more analysis comparing

predicted versus observed trait–crop–environment dynamics (Figs 5, 6). This area requires more attention if plant/crop modelling is to be widely applied in plant science research.

The trait dissection–integration technique has led to effective and efficient system integration (Figs 2, 4), and deepens cross-scale modelling of complex traits and establish predictive links for integration with whole-genome information via the G2P concept. Given the impact of water limitation on crop growth and yield (Leakey *et al.* 2019; Hammer *et al.* 2020; Wu *et al.* 2023), an area of modelling research is to advance plant/crop models to enable probing of traits that influence crop water productivity. Transpiration efficiency (TE) is found to offer best potential for advancing crop adaptation relevant to drought-prone and future climates (Hammer *et al.* 2020). Via the cross-scale model of Wu *et al.* (2019), TE can be related to leaf-scale photosynthesis and conductance, which can be further unravelled to their genetic underpinnings, helping with identifying molecular manipulation targets and detecting desirable breeding materials. The overall model-guided crop improvement (Fig. 3) – integrating plant/crop modelling, fundamental plant science knowledge and genetic engineering, and plant breeding – presents an innovative solution for accelerating crop yield improvement.

Optimising crop growth and development will require testing a huge number of genotypes, having unique combinations of physiological attributes, in METs and MSEs. This is technically challenging. Simulation remains the only feasible avenue for exploring the huge number of genotypic possibilities. Beyond testing individual component traits (Table 1), there is a significant role for CGMs in ‘crop design’ via integration of genotypic and agronomic combinations – the concept of  $G \times M$  for E by Hammer *et al.* (2014). Mapping the crop performance of individual  $G \times M$  combinations onto a surface can reveal a crop performance ‘landscape’ from which optimal crop designs can be identified. Hammer *et al.* (2014) used the crop design concept to explore the productivity–risk trade-offs of combinations of  $G \times M$  in different E in Australian TPEs, and reported  $G \times M$  options for advances at industry scale. Hammer *et al.* (2020) further incorporated future climatic conditions into a subsequent crop-design study and identified traits such as high-temperature tolerance to effects on seed set and TE. Such theoretical assessment is a means to generate guidance for advancing crop-scale adaptation to future TPEs. Crop design study with emerging cross-scale CGMs will enable design of components traits at smaller scales of biological organisation that may be more amenable to molecular and breeding manipulation – opening new avenues to influence important crop growth and yield traits.

Advances in plant/crop modelling are allowing the integration of plant science into interpretable and predictive frameworks that leverage knowledge across biological scales. Researchers are starting to use models for evaluating and exploring  $G \times M \times E$  interactions and crop-performance landscapes to produce guidance for plant science and decision

making for crop improvement. Cross-scale models are beginning to demonstrate reliability in simulating trait–crop–environment dynamics and phenotypic prediction skills, increasing connections with fundamental plant mechanisms and processes. The potential to add significant value to the model-guided revolution in trait dissection–integration, genetic engineering, and connection to breeding selection is a new frontier. This can only be achieved by experimental and theoretical scientists and practitioners working together to generate the model development and simulation ideas that will produce the data for model testing and accelerate crop yield advances.

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**Data availability.** The data that support the findings of this study are available from the corresponding author upon reasonable request.

**Conflicts of interest.** The author declares no conflicts of interest.

**Declaration of funding.** The author is funded by an Australian Research Council Discovery Early Career Research Award (DE210100854) during the writing of this article.

**Acknowledgements.** I thank the Australian Society of Plant Scientists for the Peter Goldacre Award and opportunity to offer this article. I thank Prof. Graeme Hammer for useful discussions.

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