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Enhancing sorghum yield and risk management via optimizing crop design

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Abstract. Globally, the need to intensify food production and accelerate crop yield gains requires new strategies for crop improvement. Agricultural production outcomes, such as grain yield and crop failure risk, are complex and emerge from interactions that occur between genotype (G), crop management (M), and the environment (E) during crop growth and development. With no feasible means to assess all possibilities, these G × M × E interactions complicate crop improvement decision-making and limit our ability to enhance production over diverse environments and conditions. Further complicating this problem are productivity-risk trade-offs, which make simultaneous improvements in multiple production criteria difficult. This study introduces the CropGen platform, which offers a simulation-based approach to explore crop-adaptation landscapes to identify optimal G × M strategies, called crop designs, for target E. By connecting the Agricultural Production Systems Simulator sorghum model with an evolutionary optimization algorithm, the CropGen platform enables the exploration of crop-adaptation landscapes and the generation of optimized crop designs allowing for the trade-offs among production criteria. This study details the testing and development of the CropGen platform, including its application to a sorghum crop improvement case study in situations varying in yield potential. Findings indicate the CropGen platform is capable of generating physiologically sensible sets of Pareto-optimal solutions that represent a range of trade-offs between yield and crop failure risk. The potential for CropGen to help guide and focus research and breeding efforts for the adaptation of crop production and the advancement of crop improvement is highlighted.

Keywords: crop modelling; G × M × E; APSIM; simulation; crop improvement

1. INTRODUCTION

New strategies for accelerating crop improvement are required to help meet increasing future demands on food production and to cope with changing environmental conditions (Ray et al. 2013, Fischer et al. 2014). Capturing effective interactions between genotype (G), crop management (M), and environment (E) in crop growth and development is imperative for enhancing the improvement of complex traits and agricultural production outcomes, including grain yield and crop failure risk. However, these G × M × E interactions complicate current breeding and agronomic approaches to crop improvement and limit our ability to devise strategies that perform over diverse environments and conditions. With myriad possible G × M strategies for target E, the complex and high-dimensional nature of the G × M × E factorial means there is no feasible, cost-effective means to test all possibilities (Hammer et al. 2014, Cooper et al. 2021). To further complicate this issue, seasonal climatic variability and climate change act to shift the Es being targeted, inhibiting our ability to predict to what extent current crop improvement strategies will be relevant in future conditions (Ray et al. 2019, Hammer et al. 2020).

Crop growth models (CGMs) have emerged as powerful tools to interpret and predict how crops grow and develop in response to genetics, management practices, and environmental conditions (Sinclair and Seligman 1996, Hoogenboom et al. 1997, Hammer et al. 2010). Suitably structured CGMs are designed to capture the dynamics involved in crop growth and development, making them capable of predicting the emergent outcomes of complex crop traits, such as grain yield, with consideration of the influence of genetic, management, and environmental factors through the crop life cycle (Hammer et al. 2019, Peng et al. 2020). In this way, CGMs can be used to assess the potential value of genetic and management interventions for crop improvement and provide a basis to explore the performance of multiple G × M combinations under different Es (Jones 1993, Boote et al. 2001, Peng et al. 2020).

How best to gauge crop performance is, however, a complicated task, as crop production is a multifaceted endeavour that can be evaluated using a combination of metrics, including not only grain yield but other factors like crop failure risk, profitability, water use, and input requirements (Dobermann and Nelson 2013). Many of these factors are known to trade-off with each other, requiring a decision-maker to balance possible improvements in productivity with commensurate increases in the risk of yield penalty under adverse conditions (Clarke et al. 2019, Hammer et al. 2020). With each individual's unique circumstances, there exist many different attitudes to risk, which dictate their prioritization of these factors and their trade-offs. Hence, capturing a way to represent this is crucial for informed decision-making. Currently, explicit assessment and consideration of these trade-offs that exist in crop production is emerging as a topic of focus in crop improvement discourse (Hammer et al. 2014, Rotili et al. 2020, Wu et al. 2023). Strategies to quantify and balance these trade-offs will be necessary to develop sustainable cropping strategies and robust improvements in production into the future (Klapwijk et al. 2014).

With crop improvement encompassing efforts related to both cultivar improvement and improvement in crop management, the concept of crop-adaptation landscapes has been used to help unify these domains and to aid in understanding the search space in which both breeding and agronomic research programmes operate. Adaptation landscapes describe the performance of chosen criteria (e.g. grain yield) across all possible combinations of G and M factors in the target population of Es (Fig. 1; Kauffman 1993, Cooper and Hammer 1996, Hammer et al. 2002, Messina et al. 2011). Given that we know there are many metrics with which to measure this performance, there exist many adaptation landscapes that must be simultaneously navigated to manage the trade-offs that occur between them in order to find the optimally performing G × M combinations. As such, this complex problem of crop improvement can be thought of as a search strategy that acts on and between these vast crop-adaptation landscapes, aimed at finding improved adaptive positions (Messina et al. 2009, Hammer et al. 2016, 2002, Hsiao et al. 2024). Currently, despite the potential of these crop-adaptation landscapes to contribute to crop improvement, we remain constrained in our ability to predict their structure and indeed to produce strategies for navigating to desirable or specific regions on the landscapes (Hammer et al. 2016). Due to their ability to deal with the complex G × M × E factorial, sophisticated CGMs are emerging as powerful tools to generate these crop-adaptation landscapes (Messina et al. 2009).

To help translate the information from these landscapes into strategies for crop improvement, the concept of crop design can be implemented. Crop design is the optimal pairing of G and M combinations for specific Es, in essence, the identification of optimal G × M strategies for E (Hammer et al. 2014, Hsiao et al. 2024). This can be applied for broad or specific adaptation, depending on the goals of the specific crop improvement programme. Furthermore, the concept of crop design can be undertaken with respect to a range of criteria, addressing the multi-objective nature of crop production.

In order to execute this crop design concept, there is a need for the development of tools that can work across adaptation landscapes associated with the different objective criteria (e.g. yield, evapotranspiration, and crop failure risk) to identify common superior adaptive positions, or indeed positions with

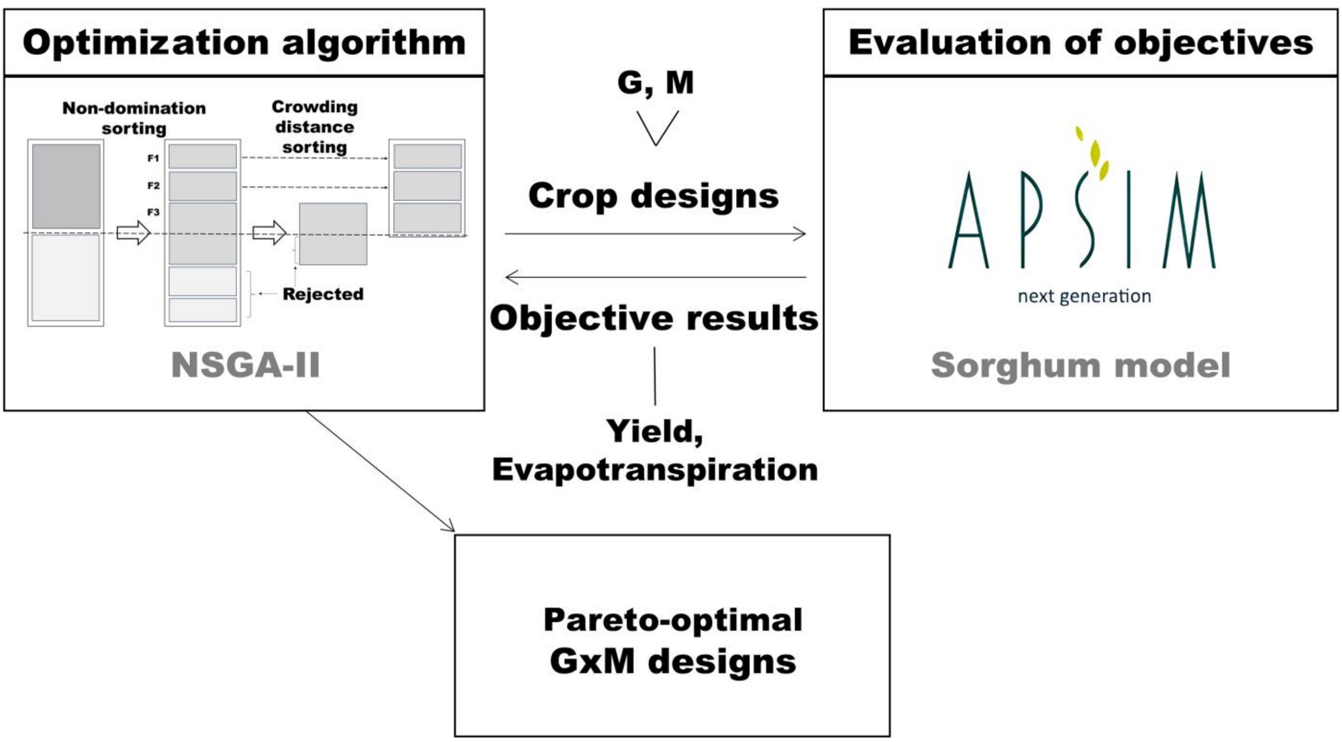

Figure 1. Schematic of the CropGen optimization platform, based on the connection of the crop growth model, Agricultural Production Systems Simulator (APSIM) sorghum, to the evolutionary optimization algorithm, nondominated sorting genetic algorithm II (NSGA-II). Schematic of the NSGA-II algorithm after Deb et al. (2002).

acceptable trade-offs between them. As such, this problem can be framed as a multi-objective optimization problem, where the best result is represented by a set of Pareto-optimal solutions, in which each strategy involves a different level of trade-off between the objectives (Coello Coello 1999). Having been successfully demonstrated in similar problems, evolutionary optimization algorithms are indicated to be effective techniques for solving multi-objective optimization problems such as this (Devoil et al. 2006, Quilot-Turion et al. 2012, Xiao et al. 2024). However, due to the high level of complexity involved, this problem of exploring crop design and optimizing trade-offs in crop-adaptation landscapes is not simple, and there exists no available tool directly suitable for this purpose (Hsiao et al. 2024).

This work aims to address this deficiency via the development of a crop design optimization tool, the CropGen platform. As identified previously, the importance of the use of a mechanistic and biologically robust CGM for this purpose cannot be understated. As such, although the platform design is model agnostic, due to the significant research effort regarding both its development and validation, the core of the platform was chosen to be the Agricultural Production Systems Simulator (APSIM) sorghum model (Hammer et al. 2010, 2023, Holzworth et al. 2014). This model has been well tested in Australia, where sorghum production typically occurs in highly variable, dryland production systems where water availability is typically the major production constraint (Passioura 2002). In these systems, confounding G × M × E interactions are common, and high year-to-year variability can cause significant production risk for growers (GRDC 2017). With trade-offs between productivity and risk particularly significant in this system, this case of sorghum production in Australia is the application evaluated.

This work aims to advance current crop design exploration capabilities by increasing the efficiency of evaluating large numbers of G × M combinations using a Pareto (multi-objective)-optimization approach. Specific crop design strategies for sorghum crop improvement in Australia are assessed, particularly with respect to water limitation. Due to their significant impacts on crop performance and adaptation, maturity, tillering, and planting density have been chosen as the G and M factors of focus (Saeed and Francis 1986, Jordan et al. 2012). There are three objectives for realizing this aim:

1. Develop a new crop design optimization platform that combines the APSIM sorghum model with a multi-objective optimization approach—CropGen.
2. Use a Pareto-optimal approach to explore maturity, tillering, and planting density combinations for specific water use conditions and understand consequential G × M × E interactions.
3. Evaluate CropGen in a case study of sorghum crop design optimization that quantifies trade-offs between maximizing grain yield and minimizing production risk in contrasting yield potential scenarios.

2. MATERIALS AND METHODS

2.1 CropGen platform overview

The CropGen optimization platform was developed to generate and navigate crop-adaptation landscapes for crop design through the connection of the APSIM sorghum CGM (Hammer et al. 2010, Holzworth et al. 2018) with the evolutionary optimization algorithm, nondominated sorting genetic algorithm II (NSGA-II, Fig. 1, Deb et al. 2002). This specific algorithm was chosen for the optimization component due to its suitability in solving biological problems such as this and its successful demonstration with similar problems (Quilot-Turion et al. 2012, Xiao et al. 2024). CropGen was implemented in Python, with pymoo (Blank and Deb 2020), a multi-objective optimization framework, used as the basis for the platform.

2.1.1 Design and objective spaces. To understand the operations of the CropGen optimization platform, it is useful to think in terms of a 'design space' and an 'objective space'. When setting up the optimization problem to be run by CropGen, all design variables to be optimized are specified, alongside their respective bounding minimum and maximum values. In this work, these design variables are APSIM parameters in the sorghum model and can include both physiological traits and management factors. Given that it is the space in which the optimization is working, this is called the design space, with unique combinations of the specified variables referred to as crop designs (Fig. 2). Another factor specified during the optimization set-up is the objective space, which includes the different criteria of interest that are used to measure performance, such as grain yield, evapotranspiration, or crop failure risk. When the different crop designs forming part of the design space are evaluated by APSIM, they are mapped into this objective space, with these objective criteria results guiding the exploration of the design space as the optimization progresses.

2.1.2 CropGen platform set-up. Alongside the definition of the design and objective spaces, the set-up of the CropGen platform involves the specification of the simulation (.apsimx) file to be run by APSIM, which includes all other simulation details and parameters, such as weather data, soil information, sorghum cultivar coefficients, and additional agronomic specifications. These factors do not directly form part of the optimization in this study. The final stage of the CropGen set-up is the initialization of the NSGA-II algorithm, which involves the specification of the optimization parameters and the different variation operators. In CropGen, the optimization parameters to be specified are the size of the working population used in each iteration of the algorithm, called population size, and the number of iterations of the algorithm before termination, referred to as the generation number. The population size and generation number are typically chosen on a case-by-case basis depending on the specific optimization undertaken.

The elements of the NSGA-II algorithm that introduce variation in the populations and hence allow exploration of the design space, called variation operators, must also be specified. For all CropGen optimizations, the sampling of the initial population is undertaken using Latin Hypercube sampling, which is a random sampling method highly suited for use in multi-dimensional problems. To introduce variation from one generation to the next, and to ensure effective exploration of the design space, both crossover and mutation operators are used. For crossover, the specific method adopted is simulated

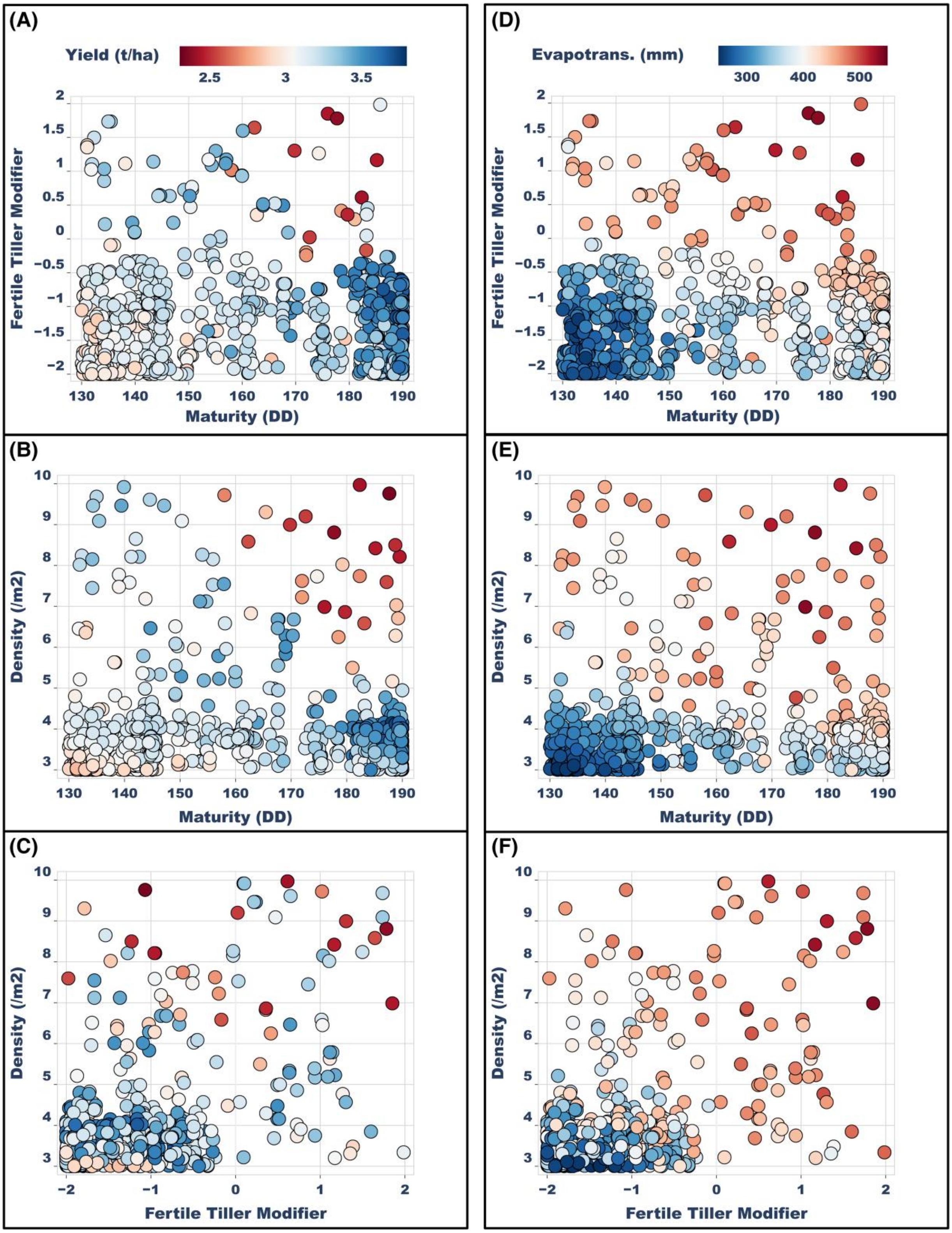

Figure 2. Pairwise representations of the crop-adaptation landscapes for the yield and evapotranspiration of different sorghum maturity, tillering, and planting density combinations in the single-season scenario. The results are from the single-season sorghum simulation, with the yield ($t\ ha^{-1}$) crop-adaptation landscape representations shown on the left (A, B, C) and the evapotranspiration (mm) landscape representations shown on the right (D, E, F). The colour of each point indicates the yield or evapotranspiration level as per the colour scales at the top of each set of landscape representations. Each point represents a different maturity, tillering, and planting density combination evaluated.

binary crossover, which is a real-parameter recombination operator, with the probability of occurrence set to 0.8 and the spread for the distribution of the offspring solution with respect to the parent solutions set to 15. After crossover, the real polynomial mutation operator is used to perturb the created offspring solution, with the value for the distribution spread set to 20 (Deb et al. 2007). For further details on these variation operators and their parameters, see Blank and Deb (2020) and the associated pymoo package website.

2.1.3 CropGen running and operations. Once CropGen has been set up, the platform can be used to initiate a run. When running the optimization through the pymoo framework, APSIM is called from Python to evaluate the objectives specified in the objective space, such as yield and evapotranspiration, for the different crop designs being evaluated. Specifically, this call happens over the APSIM server, which holds the simulation file open in memory during the optimization and evaluates the objective results for the modified crop designs when called.

CropGen is first initialized with a randomly sampled population of crop designs that are used to start the optimization. This initial population is sent to APSIM for evaluation of the objective results, which are then returned and used to perform multicriteria sorting of the crop designs to establish a ranking. To form an offspring population, parents are chosen from this initial population using tournament selection, with each offspring then perturbed by subsequent application of the crossover and mutation operators to introduce variation (Blank and Deb 2020). By using the highest ranking individuals and variation operators to help produce the offspring population, high-performing solutions are maintained in the population, and the design space is adequately searched so as to not remain in locally optimal regions. This offspring population of equal size to the parent population is then sent to APSIM for evaluation of its objective results. With both the parent and offspring populations evaluated for their performance, ranking of all individuals is performed using both nondomination and crowding distance. Finally, the generation that will form the parent population in the next iteration of CropGen is chosen, using firstly the nondomination ranking, and also the crowding distance measure if competing solutions are of equal rank. This process of population generation, objective evaluation through APSIM, and nondomination ranking will continue for the number of generations specified in the set-up, at which point CropGen will output the Pareto-optimal $G \times M$ designs.

By searching the design space to identify the best-adapted regions with respect to a range of objective criteria, the CropGen platform is designed to facilitate the navigation of multiple crop-adaptation landscapes and the identification of Pareto-optimized crop designs.

2.2 CropGen component detail

2.2.1 APSIM sorghum model. The APSIM sorghum model in APSIM Next Generation was chosen as the CGM component of the CropGen platform due to its thorough validation for use in the north-east Australia region (Hammer et al. 2010), its use globally (Kholová et al. 2014, Tirfessa et al. 2023), and its robust framework of ecophysiological determinants of crop growth and development, which allow the prediction of complex agronomic trait outcomes as emergent consequences of model dynamics.

In brief, the APSIM sorghum model is based on a framework of the physiological determinants of crop growth and development and is focused at organ scale. It generates the phenotype of a crop as a consequence of underlying physiological processes by using the concept of supply and demand balances for light, carbon, water, and nitrogen. Phenology is simulated through a number of development stages by using a thermal time approach. This also determines leaf number, and with a leaf size distribution function and tiller number, canopy size development can be simulated. The thermal time approach is used to determine time to flowering and grain filling duration. Above-ground biomass accumulation is simulated as the minimum of light-limited or water-limited growth through the use of radiation use efficiency and transpiration efficiency coefficients which interplay with the supply and demand of light, water, and nitrogen. Daily above-ground biomass accumulation is partitioned to plant parts in ratios that depend on the growth stage of the crop. Grain yield is simulated as the product of grain number and grain size, with number determined by components of biomass growth around flowering. During grain filling, crop biomass growth is allocated to the growing grains. Full details of the implementation and testing of the APSIM sorghum model can be found in Hammer et al. (2010, 2019).

2.2.2 NSGA-II optimization algorithm. NSGA-II was chosen as the multi-objective optimization algorithm for the CropGen platform due to its suitability to this style of biological problem as a result of its use of the principles of natural selection and biological evolution (Sarker et al. 2003). The algorithm works with populations of candidate solutions over generations and is driven by the repeated application of variation and selection operators, resulting in increasing fitness in consecutive generations. Through its use of the Pareto concept, NSGA-II is able to incorporate multiple objectives and generate a set of optimal solutions with respect to trade-offs of the different objectives, as is required here for this application to crop design. For full details of the NSGA-II algorithm, refer to Deb et al. (2002), and for the implementation of this algorithm in the pymoo optimization framework, see Blank and Deb (2020).

2.2.3 Software specifications. The CropGen software is written in Python and has a minimum memory requirement of 8 GB. The minimum free hard drive space is 15 GB, and it requires a minimum of 8 CPUs. Refer to https://github.com/APSIMInitiative/CropGen for documentation and availability.

2.3 Crop design optimization set-up

All scenarios evaluated are based in Dalby, a prominent rainfed Australian sorghum production region, using a local soil parametrization and historical daily weather data. The Dalby region has a subtropical/temperate climate with hot summers, mild winters, and summer dominant rainfall. Year-to-year rainfall variability is high and is a key risk factor in crop production. The sorghum season (between September and March) has an average daily maximum temperature of 29°C (but can reach above 35°C during December to January) and an average daily minimum temperature of 16°C. The timing of the sorghum season aligns with the wetter period in the region, during which the average total sorghum season rainfall is typically close to 400 mm.

The soil used in all simulations was a 180 cm deep Vertosol with 324 mm plant-available water capacity. For the cultivar coefficients, the 'Buster' sorghum hybrid (a representative commercial variety) was used as a reference (Hammer et al. 2010), with the standard tiller number calculated using known effects of location (latitude), planting density, row configuration, and time of sowing, as per Hammer et al. (2014). In all simulations, sowing was on 1 m rows with a solid row configuration and a sowing depth of 25 mm.

All optimizations were undertaken with the same design space variables, evaluating combinations of maturity (thermal time from end juvenile stage to floral initiation, APSIM parameter 'TTEndJuvToInit'), tillering, and planting density. To assess genetic differences in tillering, tillers were either added onto or taken away from the E- and M-determined standard tiller number outlined above using a fertile tiller modifier (FTM), meaning the tiller number was increased or decreased by the value of the FTM, with a lower limit of zero tillers. This use of the FTM to modulate tillering is used to represent variability in the genetic tillering propensity that is observed in different sorghum genotypes (Hammer et al. 2023). The parameter range set to evaluate for maturity was between 130 and 190 degree days, which results in total leaf number ranging between 15 and 18 leaves (Ravi Kumar et al. 2009). The FTM was allowed to vary between –2 and 2 tillers, and planting density was set to between 3 and 10 plants m^{-2}, representing the wide range of planting density used across diverse sorghum production conditions in Australia. It is important to note that each of the variables was treated independently in the analysis, meaning changes to each factor occurred separately and were not influenced by the other variables. In all runs, the size of the working population used (i.e. number of crop designs assessed) in each generation of the optimization was 50, and the number of generations (i.e. iterations) was set to 25.

2.3.1 CropGen testing using a single year of seasonal weather data. A single-year simulation was first undertaken to test the CropGen platform. The Dalby 2017 season was used, with the simulation initiated with 100 mm of plant-available water filled from the top and sowing on 15th November. The objective criteria used for the optimization were the yield ($t\ ha^{-1}$) and the simulated crop evapotranspiration (referred to as evapotranspiration, mm) during the crop life cycle of the different maturity, planting density, and tillering combinations evaluated, with the optimization seeking Pareto-optimal combinations to maximize yield and minimize evapotranspiration.

2.3.2 Sorghum crop design optimization case study. A case study with multi-year simulations was also undertaken for optimizing crop design with the CropGen platform. Two scenarios were evaluated, low-yield potential and high-yield potential. The low-yield potential scenario evaluated had 100 mm available stored soil water and 15th November sowing, reflecting the single-year case described previously, but expanded to incorporate results from over 122 seasons. For contrast, the high-yield potential scenario was initialized with 300 mm of available stored soil water and sown on 15th September. In both cases, the soil water, nutrients, and surface organic matter were reset to the initial conditions at the time of planting each season. For the optimizations, the objective criteria used were the overall average yield over the 122 seasons ($t\ ha^{-1}$) and the average yield in the worst-performing 20% of years, as a proxy for production risk. In this case, the optimization of maturity, tillering, and planting density is seeking Pareto-optimal combinations to maximize average yield and minimize production risk (i.e. maximize performance in the worst-performing 20% of years).

3. RESULTS AND DISCUSSION

3.1 Crop design using a Pareto-optimization approach

An initial evaluation of the CropGen platform was undertaken using a single-year simulation. To understand the adaptation landscapes that the optimization must traverse, it is advantageous to visualize relationships in the design space and to assess the performance of different combinations of the design variables. In this scenario, performance is measured by both grain yield and evapotranspiration, and as such, there exists a unique adaptation landscape for both criteria. The design space evaluated includes three variables, maturity, tillering, and planting density, meaning that assessment of the performance of different combinations in this space is highly dimensional and difficult to visualize. As such, three pairwise relationships are presented (Fig. 2).

The CropGen platform has sampled the design space thoroughly and focused on particular regions, evidenced by the higher proportion of points in specific areas (Fig. 2). This behaviour is a feature of the optimization process, whereby sampling is random at the start of the optimization and subsequently focuses on the better performing regions as it progresses. By removing the need to evaluate the design space using a gridded approach, optimization in this way allows for the identification of the best regions to occur in a faster and more efficient way, unlocking the potential to explore more complex and higher dimensional problems (Hammer et al. 2014, 2020, Hsiao et al. 2024).

Another feature highlighted in Fig. 2 is the contrasting nature of the performance of the two objective criteria evaluated. In the optimization, the objective is to determine the best combinations of maturity, tillering, and planting density to maximize grain yield and minimize evapotranspiration for the evaluated season. This multi-objective optimization is not trivial, as the objectives are somewhat in opposition, meaning that combinations of the design variables that maximize the yield do not minimize evapotranspiration, and vice versa. This is evidenced in the adaptation landscape representations in Fig. 2, where the points with desired levels of each of the objectives are shown in blue. Results show that combinations maximizing yield do not typically overlap with those that minimize evapotranspiration (Fig. 2A and D). This behaviour is due to trade-offs that exist between the two criteria, meaning that there is a cost associated with the improvement of each variable on the other. In circumstances where we place equal weight on both performance criteria, there is no clear way to ascertain the best possible crop designs with respect to both of the objectives.

To resolve this type of multi-objective optimization problem, there is a need to navigate between the adaptation landscapes, to quantify the trade-offs between them and to identify optimal regions with respect to the performance of all the evaluated criteria. To help facilitate this assessment of performance with multiple criteria, the concept of Pareto-optimal has been adopted, allowing both the different maturity, tillering, and planting density combinations to be ranked with respect to both yield and evapotranspiration, and representation of the levels of trade-offs between the specified criteria for the set of Pareto-optimal solutions.

To assess the ability of the CropGen platform to generate physiologically appropriate and Pareto-optimal solutions, results from the single-season simulation and optimization were further plotted (Fig. 3). The objective space plot (Fig. 3A) shows the performance of all crop designs evaluated as part of this optimization and the trade-offs that they generate between the two criteria. There is an initial positive relationship between the objective criteria, whereby increased evapotranspiration is associated with increased yield. However, this trend peaks at the highest yielding points, after which further increases in evapotranspiration are accompanied by diminished yields. As such, the optimal region of this plot is only in the increasing portion, with the Pareto-optimal set representing the section with trade-offs in line with the criteria, i.e. maximizing yield and minimizing evapotranspiration. The Pareto-optimal solutions represent the maturity, tillering, and density combinations that give the greatest yield at a given level of evapotranspiration or the least evapotranspiration for a given level of yield. Those combinations away from the Pareto front are 'dominated' as a superior combination exists. The different outcomes in the Pareto-optimal set of solutions represent different cropping strategies, whereby those that completely maximize yield and accept the associated high evapotranspiration might be considered as 'aggressive' strategies (Fig. 3, blue outlined points), while those that minimize evapotranspiration as much as possible at the expense of yield might be considered 'defensive' strategies (Fig. 3, green outlined points).

The design space plot (Fig. 3B) shows the maturity, tillering, and planting density combinations associated with this Pareto-optimal set. As can be seen in the plot, all the Pareto-optimal crop designs are very low/no tillering and have low planting density. In this case, maturity drives the variability of the designs in the Pareto-optimal set of solutions, with the more defensive positions having shorter maturity, and the aggressive strategies having longer maturity.

3.2 Understanding consequential G × M × E interactions in evaluated crop designs

To understand why crop designs with the attributes outlined above optimize performance in this scenario, it is necessary to explore the seasonal dynamics of crop traits that are associated with crop growth and water use. Assessment of these factors will allow evaluation of the consequential G × M × E interactions that are occurring through the season and provide an understanding of the factors driving performance in this scenario.

To facilitate this analysis, three crop designs have been selected (Fig. 3): the most defensive Pareto-optimal strategy, the most aggressive Pareto-optimal strategy, and the non-Pareto-optimal design with the highest evapotranspiration. The exact design variable values and performance outcomes for each of these strategies are shown in Table 1.

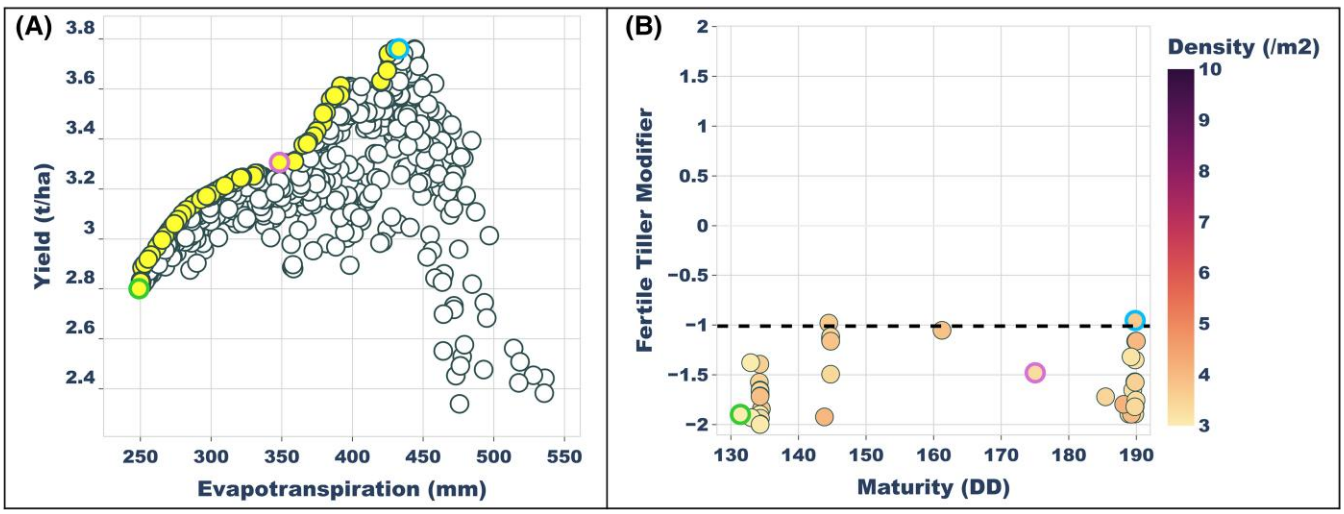

Figure 3. Objective and design space outcomes of the CropGen optimization maximizing yield and minimizing evapotranspiration in a single-season scenario. In the objective space plot on the left (A), each point is a different maturity, tillering, and planting density combination evaluated, with the Pareto-optimal set shown in yellow. On the right is the design space plot (B) showing the maturity, tillering, and planting density combinations of the individuals in the Pareto-optimal set, with the colour of the points indicating the planting density. The black dashed line in the design space plot indicates the level at which no fertile tillers occur, meaning FTMs below this value have the same effect of causing no fertile tillers in the evaluated season. The points outlined in green, purple, and blue are highlighted to facilitate connection between the two plots, with the outcome of the design shown on the left-hand side (A) and the crop design generating that outcome on the right-hand side (B).

For each design, the seasonal trajectories of traits associated with crop growth and water use have been evaluated and compared. Specifically, the extractable soil water (ESW), crop evapotranspiration, rain, and water supply/demand ratio have been assessed on a daily timescale, alongside crop leaf area index (LAI), biomass, and grain yield (Fig. 4). The water supply/demand ratio evaluated is an integrated measure of soil water availability and crop water demand, indicating the level of water sufficiency for the crop, with 1 representing no water limitation and lower ratios indicating higher levels of limitation (Hammer et al. 2014).

The trajectories of these crop attributes throughout the season are shown in Fig. 4, with the water-related factors in the left-hand panels and the growth-related attributes in the right-hand panels. Note that all simulations had identical starting conditions and were sown on the same day, with differences in the timings of anthesis and harvesting driven by differences in maturity and differences in canopy size driven by the FTM and planting density. The Pareto-optimal defensive strategy had the shortest crop duration, followed by the Pareto-optimal aggressive strategy, and finally the non-Pareto-optimal strategy with high evapotranspiration, which had the longest crop duration (Fig. 4).

When evaluating differences in the growth trajectories between the different designs, a stark contrast is visible between the Pareto-optimal and non-Pareto-optimal designs. Specifically, the non-Pareto-optimal strategy had high LAI early in the season, indicating a larger initial canopy size due to the high tillering and high planting density of this design (Fig. 4F). As a result of this, the water demands of this crop design are very high at the start of the season, causing swift drawdown of the ESW and early preflowering severe water limitation (Fig. 4E), which greatly diminished the LAI by the time of anthesis and caused reduced seed set and lower yield despite some recovery due to late rainfall events.

The behaviour of this non-Pareto-optimal crop design is in contrast to the Pareto-optimal strategies which were able to maintain their modest initial LAI through anthesis (Fig. 4B and D), indicating canopy growth that matched the prevailing seasonal conditions. The primary distinction between the two Pareto-optimal designs was their maturity (Fig. 4A and C), with the long maturity of the aggressive strategy allowing late-season rain in this specific scenario to be captured and better exploited during the key period around anthesis and grain filling (Fig. 4A). Whilst this extended maturity resulted in increased levels of water use when compared with the defensive position, it was not to the level of the non-Pareto-optimal strategy.

To further evaluate the differences in the trajectories of water use over the season among the different strategies, a rolling average of the daily evapotranspiration is instructive (Fig. 5). It is evident from the figure that the Pareto-optimal strategies have more balanced evapotranspiration through the season, whereas the non-Pareto-optimal strategy has evapotranspiration heavily skewed to the start of the season, as a consequence of the large initial canopy size as noted above. Evidently, the low/no tillering and lower density nature of the Pareto-optimal designs allow them to best ration evapotranspiration across the crop lifecycle, resulting in superior performance in the evaluated season.

When interpreting these results, it is essential to acknowledge that this analysis has occurred with consideration of only a single season. The implication of this season-specific optimization is that all results and performance outcomes are tightly linked to the specific conditions experienced, in particular the amount and timing of rainfall. Specifically, given the focus on combinations of maturity, tillering, and planting density, this work has optimized the crop canopy development to the dynamics of water available through the season in the particular year evaluated. As such, the Pareto-optimal crop designs identified are advantageous in this scenario due to the fortuitous timing of late rainfall in the evaluated season. In a more water-scarce season, some of the identified designs would be too aggressive, and in a more water-abundant year, many designs identified as Pareto-optimal would not effectively exploit the conditions. Clearly, the utility of optimization in single-year scenarios is limited, and while it enables understanding of the G × M × E interactions and testing of the CropGen platform, there is a need to evaluate scenarios over multiple years of production to obtain more widely applicable findings.

3.3 CropGen application for crop design—a case study for guiding sorghum improvement in north-east Australia

To expand the focus from the initial CropGen testing in the single-year simulation, this analysis includes two long-term scenarios with contrasting production conditions. The starting conditions from the single-year run were applied in a multi-year simulation to represent a low-yield potential scenario, while a high-yield potential scenario with different seasonal initialization was also assessed.

3.3.1 Crop design optimization in a low-yield potential multi-season scenario. The results of the CropGen optimization in the low-yield potential multi-season scenario are shown in Fig. 6. The objective space plot shows a strong trade-off between overall average yield and production risk (i.e. average yield in the worst-performing 20% of years) in these conditions, with

Table 1. Attributes of the crop designs chosen for seasonal evaluation from the CropGen optimization.

Design strategy	Maturity—end juvenile to floral initiation (degree-days)	Fertile tiller modifier	Density (plants m^{-2})	Yield (t ha^{-1})	Evapotranspiration (mm)
Pareto-optimal—defensive	131.41	−1.90	3.00	2.80	249.02
Pareto-optimal—aggressive	189.82	−0.96	3.71	3.76	432.74
Non-Pareto-optimal	176.00	1.85	6.98	2.44	536.16

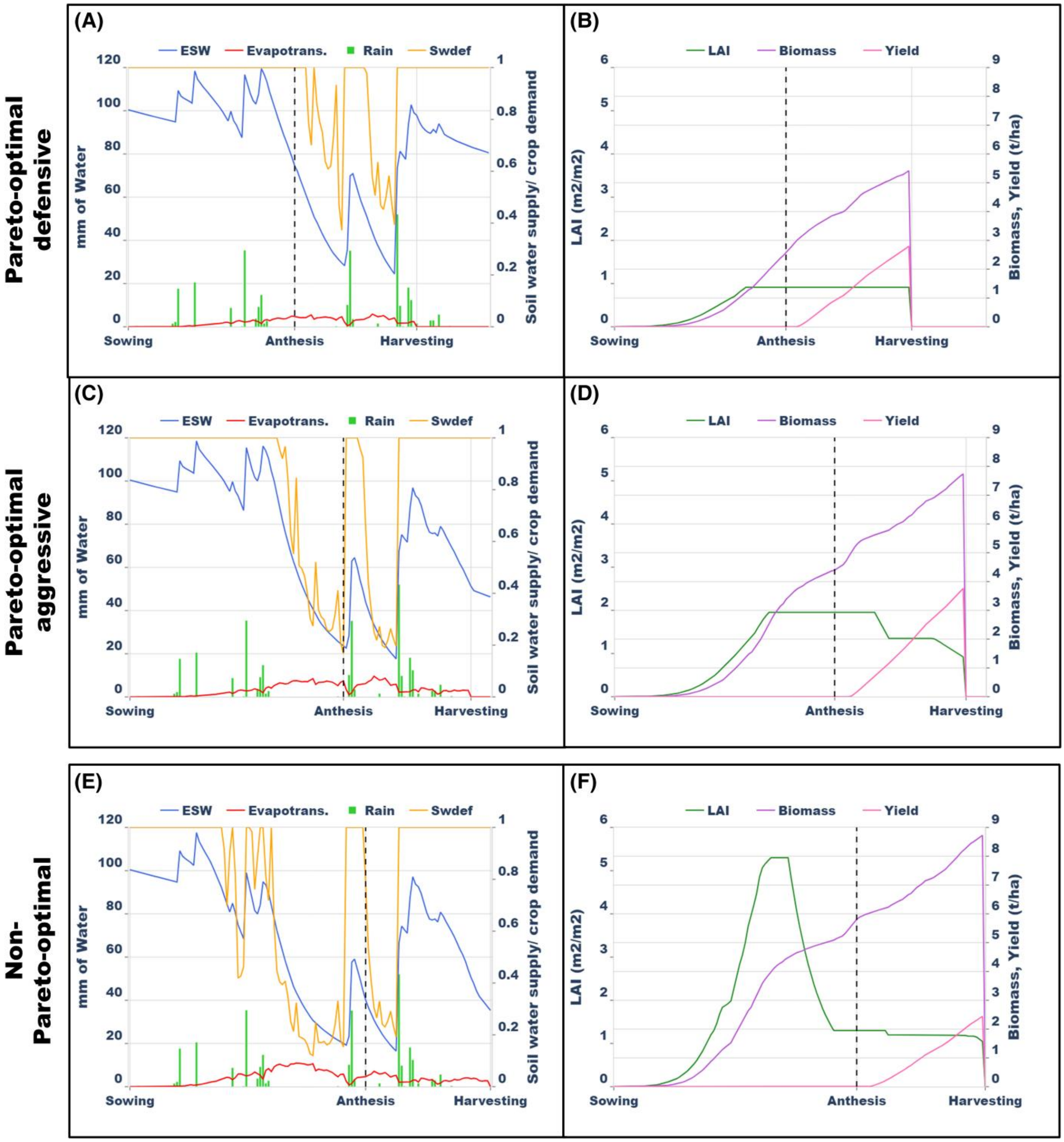

Figure 4. Seasonal crop attribute dynamics of Pareto-optimal and non-Pareto-optimal crop designs. The top two rows of panels show the seasonal results for the Pareto-optimal designs, with the defensive crop design strategy on the top (A, B) and the aggressive crop design strategy below (C, D). The lower row (E, F) shows the results for the non-Pareto-optimal strategy evaluated. The plots on the left of the figure (A, C, E) show the seasonal trajectories of the extractable soil water (ESW), crop evapotranspiration, and rainfall, alongside the water supply/demand ratio (Swdef). On the right side of the figure (B, D, F), the plots show crop leaf area index (LAI), biomass, and yield across the season.

improvements in risk accompanied by significant declines in overall average yield (Fig. 6A). In this scenario, the aggressive position sees the maximization of average yield at the expense of performance in poorer seasonal conditions, whereas the defensive scenario prioritises downside risk and accepts accompanying low average yields. The Pareto front in this scenario spans the outside edge of the points evaluated, excluding the section where the criteria do not trade-off with each other.

In this low-yield potential scenario, the optimal performance outcomes are associated with crop designs with low density (Fig. 6B). Designs that are more defensive also show short maturity and low/no tillering (Fig. 6B; lower left corner of the

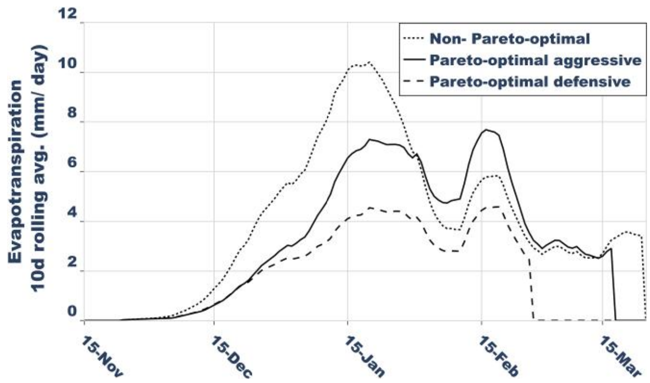

Figure 5. Comparison of crop evapotranspiration through the growing season for Pareto-optimal and non-Pareto-optimal crop designs. The 10-day rolling average of evapotranspiration (mm day^{-1}) over the crop season is shown for each design of interest: a non-Pareto-optimal design (dotted line), the most aggressive Pareto-optimal design (solid line), and the most defensive Pareto-optimal design (dashed line).

design space), whereas aggressive designs have progressively higher tillering and longer maturity (Fig. 6B; top half of the design space). The optimization identifies the addition of tillers before extending maturity as the avenue to enhance average yield while maintaining the lowest risk possible (i.e. best production in poor seasons), albeit at risk levels greater than that of the defensive strategy. Designs with low tillering and long maturity are non-Pareto-optimal with lower average yields for the same risk levels (data not shown).

There are some similarities between the results of this low-yield potential scenario optimization and those of the single-season optimization undertaken previously with the same starting conditions (Fig. 3). In particular, the defensive strategies (outlined in green) are fundamentally the same, with short maturity, no tillering, and very low planting density. This suggests that designs minimizing evapotranspiration on a single-year basis for a low-yield potential season will also likely minimize downside risk over the long term. The fact that the other Pareto-optimal designs are different between the two optimizations is driven by the sampling of many seasonal conditions with variable dynamics of water availability in this multi-season optimization.

Overall, given that this is the low-yield potential scenario, the results are physiologically sensible and appropriate for the conditions. The low density of all Pareto-optimal points and the maximization of yield with designs that are high tillering and longer maturing are sensible and in line with known responses of these factors (Hammer et al. 2014, 2020).

3.3.2 Crop design optimization in a high-yield potential multi-season scenario. Optimization in a high-yield potential multi-season scenario (Fig. 7) was also evaluated to assess the ability of the CropGen platform to generate different Pareto-optimal solutions to suit different growing conditions. As highlighted previously, beyond the seasonal starting water and sowing date, all other simulation and optimization parameters were kept consistent between the two scenarios.

Under these high-yield potential conditions, there is less trade-off between the overall average yield and production risk. As such, the Pareto-optimal designs have more similar outcomes and are condensed in the design space (Fig. 7B). Interestingly, the non-Pareto-optimal designs in the objective space have a recursive trend, with designs generating very different average yields with the same risk level (Fig. 7A). On inspection, the higher average-yielding designs are typically long maturity, high tillering, and high planting density, whereas the lower average-yielding designs are short maturity, low tillering, and low planting density. This behaviour stems from these sets of designs having different yield distributions over the multi-season analysis, with the higher average-yielding designs having much more variable yields due to their more aggressive strategies, and the lower yielding points having reduced, more stable yields.

When assessing the Pareto-optimal combinations in the design space, it can be seen that they all have high tillering and moderate/high planting density (Fig. 7B). For the more defensive designs, maturity is short, whereas in the aggressive designs, maturity is more moderate. When comparing these findings with those from the low-yield potential scenario, it is interesting to note that whilst high tillering and high planting density are identified in this optimization, maturity is not extended significantly, remaining relatively short in the Pareto-optimal designs.

This preference for increasing tillering and planting density over maturity in this high-yield potential scenario is driven by the relative advantage of larger canopies under favourable starting conditions. With ample water available initially, bigger canopy growth can be supported and maintained through to anthesis in this scenario, conferring yield advantages. Despite this, whilst this scenario is initialized with favourable conditions, there are still limitations and significant seasonal variability present. This is particularly the case when considering water availability later in the season, such as during grain filling. As such, extending maturity alongside the increased tillering and planting density pushes performance back along the top edge of the objective space plot (Fig. 7A), leading to non-Pareto-optimal outcomes with increased risk.

4. SYNTHESIS

The CropGen platform can identify situation-specific and physiologically sensible crop designs that manage trade-offs between relevant production criteria. Previous research efforts in this capacity have been limited in their ability to comprehensively assess all relevant factors of the G × M × E factorial in a time and resource-efficient manner. Past studies have adopted a gridded approach, whereby all combinations of the factors of interest were assessed, often resulting in a very large set of simulations to be completed (Hammer et al. 2014, 2020). Furthermore, without an explicit Pareto-optimization approach, capturing trade-offs and assessing optimal solutions with respect to several criteria has been challenging (Hsiao et al. 2024).

By addressing the problem of crop design exploration as a multi-objective optimization problem and connecting the APSIM sorghum model with the evolutionary optimization algorithm, the CropGen platform introduces an efficient

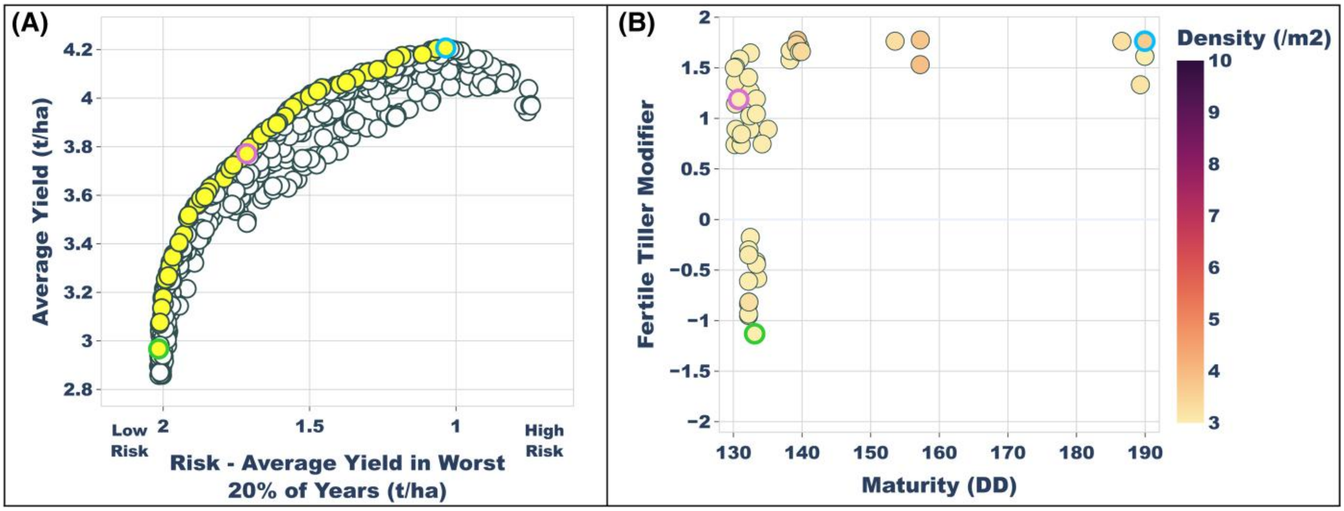

Figure 6. Objective and design space outcomes for the CropGen optimization maximizing the overall average yield and minimizing production risk (through greater average yield in the worst-performing 20% of years) in a low-yield potential scenario. In the objective space plot on the left (A), each point represents a different maturity, tillering, and planting density combination evaluated during the optimization. The points in the Pareto-optimal set, which quantifies the trade-off between yield and risk, are shown in yellow. On the right (B) is the design space plot showing the maturity, tillering, and planting density combinations of the individuals in the Pareto-optimal set, with the colour of the points indicating the planting density. The points outlined in green (defensive strategy), purple, and blue (aggressive strategy) are highlighted to facilitate connection between the two plots, with the outcome of the design shown on the left-hand side (A) and the crop design generating that outcome on the right-hand side (B). All results are generated from a simulation spanning 122 years of production in a prominent sorghum-growing location in Australia with mid-season planting and low initial stored soil water.

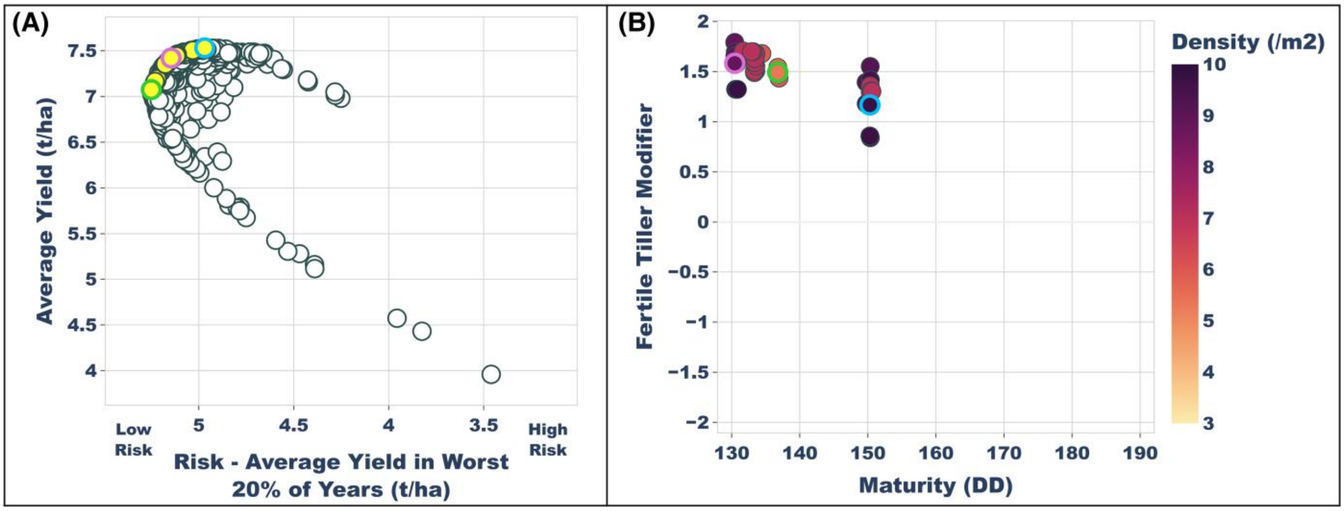

Figure 7. Objective and design space outcomes for the CropGen optimization maximizing the overall average yield and minimizing production risk (through greater average yield in the worst-performing 20% of years) in a high-yield potential scenario. In the objective space plot on the left (A), each point represents a different maturity, tillering, and planting density combination evaluated during the optimization. The points in the Pareto-optimal set, which quantifies the trade-off between yield and risk, are shown in yellow. On the right (B) is the design space plot showing the maturity, tillering, and planting density combinations of the individuals in the Pareto-optimal set, with the colour of the points indicating the planting density. The points outlined in green (defensive strategy), purple, and blue (aggressive strategy) are highlighted to facilitate connection between the two plots, with the outcome of the design shown on the left-hand side (A) and the crop design generating that outcome on the right-hand side (B). All results are generated from a simulation spanning 122 years of production in a prominent sorghum-growing location in Australia with early planting and high initial stored soil water.

and targeted way to explore these problems. By focusing the analysis into areas with better performance, CropGen reduces the amount of simulation required, lowering both time and computational demands, and unlocking the potential to assess more complex and higher dimensional scenarios.

However, one factor of the multi-objective optimization approach that must be addressed is its reliance on the use of a

CGM fit for this purpose. For this style of work, model perspicacity is essential, with the types of possible analyses dictated by the scope and structure of available models (Martre et al. 2015, Hammer et al. 2019). For a specific trait to be suitable for this type of optimization, the cost of variation in that trait on other factors must be captured by the model. As such, traits and practices that are modelled without such internal linkages may not be amenable to optimization, a fact that underscores the importance of understanding the scope and implementation of the CGMs being used in this way. The popular modelling adage of obtaining 'the right answer for the right reason' rings true here and should be front of mind when evaluating the application of CGMs for such optimization purposes (Keating 2020).

A further consideration with the optimization approach of the CropGen platform is its generation of a set of Pareto-optimal solutions as opposed to a single best strategy. Whilst this behaviour is a feature of the optimization, which allows for all criteria to be prioritized equally and a full range of trade-offs to be generated, it means subsequent application of the results will require end-user input and decision-making (Hsiao et al. 2024). Despite this, the generation of a set of Pareto-optimal solutions allows for many positions and preferences to be represented in the optimization results, making findings relevant for a wide range of circumstances, and allowing users to integrate personal and commercial factors to determine the best strategy for their situation. Ultimately, to fully exploit the potential of this approach, it is likely that field validation of findings and recommendations will be needed to build adequate trust and confidence. Considering the exploratory nature and large scale of this work, evaluating the outcome of specific strategies identified as part of the optimization against observed data would likely be the most appropriate course of action, although this lies beyond the scope of this study.

Lastly, application of the CropGen platform could extend beyond optimization at the crop-level. It could be configured to explore questions at the cropping system level, including evaluating and optimizing crop rotations (Devoil et al. 2006), optimizing nitrogen fertilizer rates or timing (Pardon et al. 2017), and assessing irrigation practices (e.g. area vs. amount) for a set water budget. It could also be possible to assess different strategies across numerous fields, such as exploring risk reduction by optimizing a sowing rule to spread sowing across different dates or to use varieties with differing maturity (crop duration). Furthermore, this style of crop design exploration and optimization could also be extended to include finer traits, such as those underpinning photosynthesis (Wu et al. 2023). The CropGen platform offers the ability to explore genetic and M intervention strategies *in silico* before the investment of significant time and effort.

5. CONCLUSION

Optimizing crop design is a complex concept that requires the consideration and balance of many factors. The nature of crop production is such that performance is nonlinear and driven by many complex and interacting factors. Different measures of crop performance will trade-off with each other, with improvements in one factor of interest often accompanied by commensurate deteriorations in another. The need to explore and address this problem *in silico* for accelerated crop improvement cannot be understated, with the novel approach adopted in this work offering the potential to explore a much wider crop design space and to optimize multiple production objectives.

The CropGen platform is a powerful tool to support crop improvement decision-making by enabling crop design assessment and unlocking information present in crop-adaptation landscapes. By facilitating the comprehensive assessment of G × M strategies for target Es, CropGen can help to prioritize research efforts and identify avenues for further investigation, including the likely value of traits for detailed pursuit in genetics and plant breeding programmes (Cooper et al. 2021, 2022) combined with M options for agronomic research programmes (Tirfessa et al. 2023).

Ultimately, the questions addressable by CropGen are limited only by what can be implemented in an APSIM crop or farm simulation. Future work will see the CropGen platform and this multi-objective optimization approach applied to a broader range of traits and M practices, with the potential to even evaluate optimal cropping strategies for future climates and conditions. To unlock the full potential of this crop design optimization concept, a sustained investment into the development of biologically realistic and mechanistic CGMs will be required (Martre et al. 2015, Wu et al. 2019, Hammer et al. 2023, Wu 2023).

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DATA AVAILABILITY

All software developed as part of this work can be found in the following GitHub repository: https://github.com/APSIMInitiative/CropGen. The data underlying this article will be shared on reasonable request to the corresponding author.

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