Special Article

Use of computational modeling combined with advanced visualization to develop strategies for the design of crop ideotypes to address food security

A.J. Christensen*, Venkatraman Srinivasan, John C. Hart, and Amy Marshall-Colon*

Sustainable crop production is a contributing factor to current and future food security. Innovative technologies are needed to design strategies that will achieve higher crop yields on less land and with fewer resources. Computational modeling coupled with advanced scientific visualization enables researchers to explore and interact with complex agriculture, nutrition, and climate data to predict how crops will respond to untested environments. These virtual observations and predictions can direct the development of crop ideotypes designed to meet future yield and nutritional demands. This review surveys modeling strategies for the development of crop ideotypes and scientific visualization technologies that have led to discoveries in "big data" analysis. Combined modeling and visualization approaches have been used to realistically simulate crops and to guide selection that immediately enhances crop quantity and quality under challenging environmental conditions. This survey of current and developing technologies indicates that integrative modeling and advanced scientific visualization may help overcome challenges in agriculture and nutrition data as large-scale and multidimensional data become available in these fields.

INTRODUCTION

Food security is defined as adequate availability and access to sufficient, safe, and nutritious food at all times.[1] The United Nations World Food Summit in 1996 proposed guidelines for measures of food security.[2] The following components of food security were identified: availability (when states produce sufficient quantity), accessibility (when people can afford to buy the food available and the food can be transported from production to consumption sites), acceptability (when the foods available align with the cultural, social, and religious aspects of the consumer), and dietary needs (when the foods available have nutritive value and meet daily dietary demands). The International Food Policy Research Institute expands this definition by stating that the available food should also meet an individual's dietary needs and food preferences for an "active and healthy life."[3] The opposite scenario results in food insecurity, in which a household's daily per capita

Affiliation: *A.J. Christensen* is with the National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA. *V. Srinivasan* is with the Pacific Northwest National Laboratory, Richland, Washington, USA, and was with the Institute for Genomic Biology, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA. *J.C. Hart* is with the Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois, *USA. A. Marshall-Colon* is with the Department of Plant Biology, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA.

*These authors contributed equally.

Correspondence: *A. Marshall-Colon*, 1201 W Gregory Dr, 193 ERML MC-051, Urbana, IL 61801, USA. Email: amymc@illinois.edu.

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consumption is below 2100 calories.[4] The US Department of Agriculture measures food insecurity on the basis of both nutritional adequacy (calorie consumption) and household perspective of their own food security (experiential data). For example, households in sub-Saharan Africa may be food insecure because of undernourishment and limited access to food, while communities in Asian countries may perceive they have enough food yet are actually food insecure because of malnutrition from lack of diverse and nutritious food.[4] Many factors influence food security, including population size, food prices, environmental stressors, and climate change.[3] Ultimately, to overcome food insecurity, collaborative networks that integrate several components must be developed in order to enhance a community's environmental, economic and social well-being.

Crop production is one of the major components of sustainable food systems, but it is highly sensitive to changes in climate. Current climate models predict that increasing temperatures and atmospheric levels of carbon dioxide, changing global and regional precipitation patterns, and increases in the intensity and frequency of extreme weather events will significantly affect crop quantity and quality over the next 100 years.[5] Elevated atmospheric carbon dioxide has been found to increase the biomass and yield of crops that use both C_3 and C_4 photosynthetic pathways, provided water and fertilization are adequate[6]; however, recent studies have shown a decrease in the nutritional quality of grains and legumes. Crop growth under high concentrations of carbon dioxide is linked to decreased concentrations of zinc, iron, and protein in barley, rice, maize, soybean, field peas, potato, and sorghum.[5,7,8] The impact of carbon dioxide levels on seed zinc concentrations is estimated to result in approximately 138 million people at new risk of zinc deficiency by 2050.[9] High atmospheric carbon dioxide concentrations also cause declines in total nitrogen and mineral concentrations in soybean[10,11] and wheat and an increase in carbohydrate concentrations,[12] resulting in a potentially negative impact on the nutritional quality of future food supplies.

The nutritional quality of crops under projected temperatures and carbon dioxide levels is likely to shift in the future, yet four key global crops (maize, rice, wheat, and soybeans) are already showing stagnating or collapsing yields.[13,14] Maize, wheat, and rice are all expected to show reduced yields in response to the combinatorial effects of climate change in both tropical and temperate regions with poor soil nutrition and limited water resources.[15] This phenomenon is expected to have the largest impact on developing countries, where urban demand for densely nutritious food is rising, creating a need for increased production of staple crops and requiring increased use of resources.[16–18] Simply put, the existing germplasm will not be able to meet the expected demand for staple crops in 50 years.[14,19,20] The development of future crops that grow under a changing climate will require a strategy beyond traditional breeding, which is based on selection for yield or for defect elimination.[21] Cultivars for a specific purpose in a specific environment are known as ideotypes.[22,23] Ideotypes can include plants for which certain properties are enhanced, such as grain quality or nutritional balance, or plants with traits such as the ability to withstand water or nutrient deficiency. The development of ideotypes will be a key component in ensuring future food security under a changing global environment. Several modeling studies have predicted optimum phenotypic characteristics of crops under different environmental conditions.[21,24–26] More recently, efforts to couple technological advances in crop modeling with experimental canopy structural modification using Free Air Concentration Enrichment (FACE) technology under current and future carbon dioxide concentrations have been reported.[27] Unfortunately, ideotype development is slow, requiring precise genetic selection to achieve the desired expression of traits in an untested environment. This presents a considerable challenge to identify and scrutinize technologies that will accelerate the development of ideotypes for specific scenarios.

The goals of this review are to survey computational crop modeling and data visualization strategies and to explore how such strategies can accelerate ideotype breeding and engineering to increase yield and, possibly, nutrition under challenging environmental conditions. This review aims to communicate the potential of multiscale modeling and advanced visualization and reveal the current limitations in the field. At this point in history, technological advances are pushing agriculture and plant science into the realm of big data, and there is a need for strategies to comprehend and efficiently use complex data. As we approach this new frontier, technological approaches that incorporate advanced visualization are needed to facilitate user interaction with large-scale biological, agricultural, and nutritional data. Three-dimensional (3D) and immersive data visualization has the potential to improve researcher understanding of complex data by allowing observations about emergent behavior that are otherwise not readily discernible from traditional tables and graphs.[28] Here, emergent behavior refers to "unexpected properties generated by complex interconnections between subsystem components and biological (or physical) processes."[29] The recent development and accumulation of big data from the agriculture sector can improve model parameterization, while advances in high-performance computing and data visualization will enable processing and dissemination of model outputs. This review aims to summarize how computational modeling and advanced scientific visualization may help overcome challenges in agriculture and nutrition data, by (1) exploring the current use of big data in crop production and how it relates to food security, (2) surveying integrative modeling strategies aimed at ideotype development, (3) describing how advanced visualization can facilitate data discovery, and (4) examining how current visualizations of multiscale crop models are improving crop productivity. It concludes with a short perspective on the future of data exploration through modeling and visualization.

Defining and using big data in agriculture and crop science

Big data in agriculture includes large volumes of diverse data collected from individual farms. These data require aggregation and advanced analytics to enable the development value-creating tools to support decision-making.[30] Big data includes agronomic data (yield, soil properties, pesticide and fertilizer application rates, planting density, genotypes, etc), machine data (GPS and sensor-derived information, yield monitors, etc), spatial and imaging data (GIS [geographic information system], satellite, and remote sensing imagery, near-infrared reflectance, etc), and meteorological data (precipitation, temperature, atmospheric gas levels, etc) (Table 1).[30–49] Although agronomic and meteorological data have been recorded for decades via historic monitoring of farms, it is the digitization of this information, along with the terabytes of data collected from remote sensing and other technologies, that has moved agriculture into the era of big data. Likewise, with the advent of high-throughput technologies, crop science research is now producing vast amounts of "-omic" scale data from the genome, transcriptome, metabolome, and proteome.

As the volume and diversity of data rapidly increase, agricultural technology providers are developing data services to store, compile, and analyze this data, resulting in advice on precision agriculture practices. These services are generally supplied by agricultural input providers, such as John Deere, Monsanto, and DuPont Pioneer, who then use the data to prescribe their products (ie, genetics, fertilizers, pesticides) for field-specific treatments.[30,45] For example, Monsanto's FieldScripts is a paid-subscription program, facilitated by certified dealers, that uses farmer-collected field data to generate planting prescriptions for use with Monstanto's DEKALB seed types and also offers monitoring and real-time advice throughout the growing season.[30] Likewise, John Deere outfits their equipment with sensors that stream data about soil and crop conditions through the Internet of Things. The resulting analysis can inform farmers with paid subscriptions about best management practices.[45] In general, the precise data collected by for-profit farm management services are not publically available and are only accessible through paid subscriptions.

Nonprofit and government organizations provide open-access, integrated data reports and/or tools to process agricultural data. The National Agricultural Statistics Service and the World Agricultural Outlook Board prepare monthly forecasts for crop supply and demand, using data collected from farm surveys, field observations (ie, weather), stocks, and trade data. These services provide estimates for the United States and the world that serve as benchmarks in world commodity markets.[46] These estimates include acres to be harvested and yield per acre on regional, national, and global scales, but they do not offer specific advice on crop and soil management. Another limitation of these services is that National Agricultural Statistics Service does not use long-range weather forecasts and thus can only provide yield predictions on a monthly basis. Furthermore, results from these reports must be interpreted by commodity statisticians and are usually not easily understandable by farmers and other stakeholders. Results from these reports are visualized through dense tables and so-called snapshot maps that do not take into consideration predictions over time.

Other organizations have improved the dissemination of data and predictions to the public through the development of simulation tools that display model outputs as interactive visualizations, which couple agricultural data with geospatial information (eg, geographic information systems). The Food and Agriculture Organization of the United Nations (FAO) developed the Global Information and Early Warning System on Food and Agriculture (GIEWS), which monitors major food crops around the world. The GIEWS uses precipitation and remote sensing data to calculate an Agricultural Stress Index that serves as an indicator for early identification of areas that will be affected by water deficiency.[47] This information is publically accessible via interactive geospatial maps that provide near real-time indices of vegetation health and water availability within a 10-day period. Likewise, the Famine Early Warning Systems Network (FEWS NET), created by the US Agency for International Development (USAID), provides evidence-based, unbiased analysis on global food security using big data from physical science (eg, US Geographical Survey), remote sensing of agroclimatic factors (eg, National Oceanic and Atmospheric Administration and National Aeronautics and Space Administration), economics, and politics. This information is cataloged and made available through the FEWS NET data center, which also

Table 1 **Resources to access and process big data in agriculture and biology**

Type of resource	Description	Reference(s)
Modeling software		
FieldScripts by Monsanto	Analysis of field data trends to provide planting advice	Sykuta (2016)[30]
Food Insecurity and Climate Change, web tool by the World Food Programme	Geographic data used to predict food insecurity	Met Office (2015)[31]
Functional–structural plant models such as ADEL-Maize and ADEL-Wheat, MLCan, BioCro, and the Chinese Academy of Science's 3D rice model	Computational models of plant canopies to understand yield under different growing conditions	Fournier et al. (1999)[32]; Fournier et al. (2003)[33]; Drewry et al. (2010)[34]; Drewry et al. (2010)[35]; Miguez et al. (2009)[36]; Wang et al. (2015)[37]; Song et al. (2013)[38]
L-system-based functional–structural plant models such the barley model by Wageningen University & Research and by Brandenburg University of Technology Cottbus; the wheat and pea model by LUNAM University and by INRA; and the beetroot hairy root culture by the Technical University of Dresden	Procedural computational models of plant canopies to understand yield under different growing conditions	Buck-Sorlin (2007)[39]; Barillot et al. (2014)[40]; Lenk et al. (2014)[41]
SimRoot by Penn State University	Geometric computational model of plant root growth to understand how root physiology affects yield	Lynch et al. (1997)[42]
L-PEACH by the University of California, Davis and by Irrigation Technology, Institut de Recerca i Tecnologia Agroalimentàries	Geometric computational model of peach tree growth to understand yield	Allen et al. (2005)[43], Lopez et al. (2008)[44]
Databases and analytical resources		
John Deere Internet of Things	Sensor data for planting advice	Bronson & Knezevic (2016)[45]
National Agricultural Statistics Service and the World Agricultural Outlook Board	Survey, observation, and trading data for commodity market advice	National Agricultural Statistic Service (2012)[46]
Global Information and Early Warning System on Food and Agriculture by the FAO	Precipitation and satellite data for early drought detection	GIEWS (2016)[47]
FEWS NET by USAID	Physical science, satellite, economic, and political data to predict food insecurity	Famine Early Warning Systems Network (2017)[48]
Volumetric model of F4 tornado-forming thunderstorm by Robert Wilhelmson	Computational model of atmospheric effects in a constrained volume to analyze and understand the dynamic processes that lead to formation of tornados	Public Broadcasting Service (2004)[49]

Abbreviations: FAO, Food and Agriculture Organization of the United Nations; GIEWS, Global Information and Early Warning System on Food and Agriculture; INRA, Institut National de la Recherche Agronomique (French National Institute for Agricultural Research); USAID, US Agency for International Development.

provides visualizations of aggregate data. This collective information is used to identify areas of current and future vulnerability to food insecurity. For example, FEWS NET monitoring identified countries at new risk of food insecurity in response to the 2008 global financial crisis. They also predicted the current drought in the Horn of Africa and have predicted that this food security emergency will continue into early 2018.[48] The integration and visualization of large-scale agriculture, climate, and economic data by FEWS NET provides objective analyses to decision-makers and aid organizations to assist in the development of response plans. Real-time observations are mapped and used to develop scenarios to forecast future events. However, these projections are limited to 8-month stretches of time, although they are updated every 4 months. This invaluable service has directly prevented massive famine-related humanitarian crises for the past 25 years by integrating big data from agriculture and other sectors and using effective visualizations to pinpoint areas at risk. However, with the rapid rate of global climate change, there is a need to use big data for long-term, decadal predictions of crop production and food security.

The World Food Programme has developed a web-based tool called Food Insecurity and Climate Change, which allows users to explore multiple scenarios of carbon dioxide levels and crop adaptation to identify areas vulnerable to food insecurity over the next 60 years. Vulnerability is determined on the basis of a country's exposure (average length of flood and drought events over areas with > 1% of the area in crop production) and sensitivity (amount of forest cover, rainfed land, and cereal crop yields per country) to climate-related hazards and its adaptive capacity (socioeconomic indicators such as access to water, population growth rate, poverty, employment, etc).[31] Future predictions represent the average vulnerability index based on calculations using 12 existing CMIP5 (Coupled Modeled Intercomparison Project Phase 5) climate models.[50] The range of results across scenarios shows the best and worst cases for each country. The value of this tool lies in its empowerment of the user to test different scenarios and identify specific areas in which to focus adaptation and mitigation strategies and initiate change. These simulations can assist vulnerable nations and aid organizations in developing contingency plans for worst-case scenarios.

Each of the above-mentioned tools relies on models that integrate various types of big data to make predictions on a local or global scale. Yield forecasts are based on both high-tech and low-tech observations, such as satellite imagery and grower surveys, respectively. However, most open-source projections do not take into consideration crop genetics or genotype-by-environment interactions, which are widely considered critical for determining quantitative traits such as yield and yield stability across environments.[51] Precision data owned by for-profit companies, including crop variety and nutrient inputs, has the potential to better parameterize models designed to predict crop performance under different environmental conditions; however, this information is not freely available. There is a need today for the scientific community to develop predictive models that take into consideration factors that influence the whole crop system, including large-scale genetic, genomic, and biochemical data, to more accurately forecast how specific crop varieties will perform under future conditions. Ideally, these simulations will also have the power to assist the design of ideotypes that express desired traits and can be prescribed for specific locations.

Data integration, modeling, and visualization for ideotype development

Technology is in place for the development of robust crop models that integrate information from the environment to the ecosystem to the organ and to the cell. In particular, the integration of climate models with crop models holds great potential for the development of ideotype simulation tools. Such an approach was used to design a tomato cultivar adapted to water-deficient conditions; process-based model simulations identified 8 genotypic parameters that directly influence fruit size under water deficiency.[52] Likewise, biophysical models were used to design a drought-resistant maize ideotype that could outperform existing hybrids under a variety of climates, water availabilities, and nutrient regimens.[53]

Simulations of virtual crops under different climate scenarios have helped researchers perform ex ante evaluations of ideotypes and design fertilizer, water, and management strategies for predicted future environmental conditions.[53,54] However, the majority of crop models include phenotypic properties only and neglect or poorly connect to the underlying genetic properties driving the observed traits.[23,55]

Recent studies have expanded crop simulations to include genetic information such as quantitative trait loci, a section of DNA (the locus) that correlates with variation in a phenotype. Genetic mapping (identifying the locus of a gene and the distances between genes) has been combined with biological process-based models (reviewed by Buck-Sorlin[56]) to predict genotype-by-environment interactions that influence leaf elongation in maize[57] as well as with an ecophysiological model of spring barley genotypes to predict flowering traits under various environments.[58] Further inclusion of genetic and molecular data, such as gene expression and metabolic fluxes, into existing crop models could significantly enhance model simulations and better direct crop breeding and engineering efforts to improve nutrition, yield, and resource use efficiency[55] under specific environments, which is at the core of ideotype design. One recent success story comes from the integrated process-based e-photosynthesis model[37,59] that was used to simulate the relaxation of nonphotochemical quenching of chlorophyll fluorescence.[60] Motivated by model simulations, which predicted that increasing the relaxation rate of nonphotochemical quenching could improve photosynthetic efficiency and yield,[61] targeted experimental genetic engineering of plants with faster nonphotochemical quenching response resulted in a 15% increase in crop productivity under field conditions.[60] This example shows one of the strengths of integrative and multiscale modeling that takes whole-system response into consideration[55,62] for the engineering of crop ideotypes.

The remaining challenge is to build virtual crops by combining existing molecular and climate models with architectural models. The inclusion of plant architecture at the level of individual leaves and roots, as well as crop canopies, is needed to begin to predict emergent, whole plant response to environmental perturbations.[23,38] It is doubtless that plant architecture influences plant–environment interactions. Defining plant architecture within a 3D space allows the virtual plant to explore that space for resources.[63] The bidirectional flow of information between integrated model components results in "movement" and spatial simulation of architecture, which allow the researcher to observe emergent behavior and complex patterns that would remain hidden otherwise. The model-linked connection between phenotype and genotype would allow researchers to discover the molecular underpinnings driving crop response to specific environmental conditions. The genes underlying this response could then be targeted for molecular and/or traditional breeding of crop ideotypes.

Functional–structural plant models of crop architecture, such as the ADEL-maize and -wheat models,[32] MLCan,[34,35] BioCro,[36,37] and a 3D rice model by Song et al.,[38] are routinely employed in crop science. The explicit coupling of spatial structure with physiological function creates modular functional–structural plant models, facilitating communication between different components of the model.[64,65] Functional–structural plant models begin to address visualization of agricultural data beyond tables, graphs, and simple 2D images of crop architecture. However, an essential next step is to expand these models to include cellular-level biological processes and ecosystem-scale interactions in order to observe and interpret emergent behaviors of crop response to various environmental scenarios or predict how the nutritional quality of crops will change. These multiscale models will require innovative strategies to visualize and interpret the integrated model outputs to then be used for ideotype design.

Advanced scientific visualization for discovery

According to Donalek et al., "Data visualization is the bridge between the quantitative content of the data and human intuition."[66] Visualization, in simplest terms, is creating imagery to help describe information or data. The field of visualization is a vital tool for scientific research. With the beginning of computer-aided research, the field of visualization has also experienced a renaissance.[67] Since the 1980s, computer visualization of data has been aiding digitally enabled research and leading to new discoveries. In the human brain, the visual cortex, associated with visual perception, processes information more quickly than the cerebral cortex, which performs general cognition.[68] Visualization takes advantage of this, balancing the cognitive load and making complex multivariate data easier to understand, both for education and for expert analysis. Scientific visualization has become increasingly important in understanding large, multivariate datasets that are becoming more accessible as high-performance computing resources and data-sharing capabilities increase. Visualizations are most effective when they create a mapping between data attributes collected by scientists and the dimensions of an image, such as position, color, opacity, depth, motion, blurriness, etc. While charts and graphs do this in a very simple way, subject-matter experts can easily be taught to function at a higher level of visual literacy,[69] which demands more complex image-based solutions.

Approaches for advanced visualization of complex, large-scale data have been developed in the fields of atmospheric science, physics, and astronomy, in which terabytes of spatial and temporal data have been translated from numbers into 3D moving images. For example, visualization of multivariate data recorded from inside an F4 tornado that touched down in South Dakota in 2003 revealed a counter-rotating anticyclone that had not been observed by researchers and was not obvious from the raw numbers.[49] The dataset used for visualization covered 100 square kilometers of terrain by 25 vertical kilometers at 100-meter resolution and was housed in 3D grids containing dozens of attributes such as humidity, temperature, pressure, and the 3 components of wind velocity. From this data, several visual assets, called glyphs or visaphors, were derived: (1) isosurfaces, which are geometric meshes generated at points where adjacent grid cells have humidity values on opposite sides of a given threshold value to create a descriptive shell of the storm cloud, (2) advected particles, which are massless points pushed from grid cell to grid cell on the basis of the grids' evolving wind velocity values to show areas of high vorticity, (3) streamtubes, which are geometric trails showing the history of a subset of particles to preserve temporal characteristics as shapes, and (4) ground vectors, which are cones designed to point in the direction of wind vectors along the ground plane. Because the data grids were overlapping, the visualization team could then communicate attributes like humidity and temperature with, respectively, opacity and color, as seen on the spheres at the center of the vortex (see Movie 1 in the Supporting Information online). Color was also used to communicate vertical velocity, as seen on the blue-to-orange gradient on the streamtubes, which atmospheric scientists had identified as a key attribute in their work. The researchers who generated this data knew anticyclones were a potential weather phenomenon, but the visualization of this data revealed an emergent phenomenon that was not visible through the thick clouds to storm chasers on the ground, and the numerical data would have required extensive analysis. This visual recreation of natural phenomena through numbers can be applied to any multivariate data but is especially intuitive for data with spatial and/or temporal dimensions.

As data from agricultural and biological fields begin to approach the level of big data, researchers in these domains can utilize and learn from visualization approaches developed for traditional big data from astronomy and atmospheric science. Large-scale data from agriculture, crop science, nutrition, and food security often have inherently spatial characteristics that can be presented directly on top of geographic maps or as stand-alone 3D models. Even when these data seem natively constrained to a 2D context, it is often helpful to explore them in 3D, either with an aerial perspective viewpoint or by expanding the data into 3D by mapping some data attributes to height in the virtual environment[70] (Figure 1). For example, FEWS NET calculates various measures of food security, such as rainfall and dryness, which are related to drought, or relative vegetation and food prices, which are related to food distribution, and fits the values by geographic region on interactive maps of Africa and Central Asia. These regions are then colored by transferring those calculated values to colors, where green indicates relative food security and red indicates relative food insecurity.[71]

As another example, 1D canopy light absorption data from a field of soybean plants over the course of a day was visualized in 3D (see Movie 2 in the Supporting Information online). The input data for the ray-tracing model included an evolving time series of triangulated meshes in which each vertex stored the light-absorption parameter. The format of the output data from the simulation included geometric positions of leaves and a magnitude of absorbed light. The visualization mapped the geometry to triangular meshes in the 3D environment and mapped the magnitude of absorbed light to a color transfer function that displayed low values as dark blue and high values as bright red. This data was combined with a simple data source, the daily path of the sun represented as an animated virtual light source, to render moving shadows that help clarify which time step in the model is being shown. In the final visualization, it is clear to the viewer that leaves closer to the ground are heavily shaded by the higher leaves, and that more sunlight is absorbed near midday than near dawn or dusk. With the visualization pipeline built to render this data format, researchers can easily compare new visualizations of plants modeled under different environmental conditions. Such precise measurement of light absorption by every leaf of every plant in a field would be experimentally impossible, while output of these model simulations as tables would be time consuming and difficult to use for identifying patterns. It is the 3D rendering of model outputs as realistic plants that makes the data intuitive to researchers. The realistic rendering of model-simulated plants is an important step toward the in silico "testing" of ideotype designs under different environmental conditions, enabling researchers to make dozens of observations about ideotype performance under varying scenarios. In silico exploration can help researchers target components of the underlying genetics to enhance crop yield and nutritional quality.

An advanced visualization tool that is becoming increasingly useful is immersive visualization, in which a user feels they are part of a simulated environment. Immersive environments have been proven to increase spatial comprehension,[72] and a community has formed to establish standards for immersive theaters and to ensure comprehension of visual material.[73] Scientific data exploration through immersive visualization enables a researcher to interact with and probe complex spatial and temporal data. This can be accomplished using virtual reality platforms, either in specialized spaces such as CAVE Automatic Virtual Environments and similar rooms consisting of display walls,[74] or, more recently, via portable hardware such as the Oculus Rift head-mounted display or the Microsoft Kinect sensor for manual input. Virtual reality has improved data exploration in the medical,[75–78] chemical,[79] and physical[80] science fields. Both 2D and 3D virtual graphical environments can be placed into interactive virtual reality headsets and immersive displays, where scientists can intuitively explore a multidimensional representation of their numerical models and quickly and iteratively discover emergent phenomena in their data.[81]

Immersive visualization can promote more efficient data mining by helping researchers observe meaningful patterns in multidimensional data, identify and remove bad data, and choose the best algorithms to fit the data on the basis of observed structures.[66] Studies have shown better retention of the perceived relationships in the data using immersive data exploration.[66] Immersive visualization techniques are also effective for the exploration of nonspatial data, which would normally be represented using 2D tables and graphs. Kwon et al.[82] found that 3D stereoscopic representations are useful for visualization of even simple network graphs. They reported that graph exploration using immersive visualization with depth routing increased the rate of task completion and correctness while reducing the number of user interactions necessary to complete the assigned task. Study participants performed tasks better using virtual reality than using traditional 2D graph visualization.[82] This sort of immersive data exploration using virtual reality holds great potential for exploring outputs from multidimensional models that integrate data across temporal and spatial scales, including economic and nutrition data as well as climate-, ecosystem-, and (crop) organism-level data. Researchers in China have

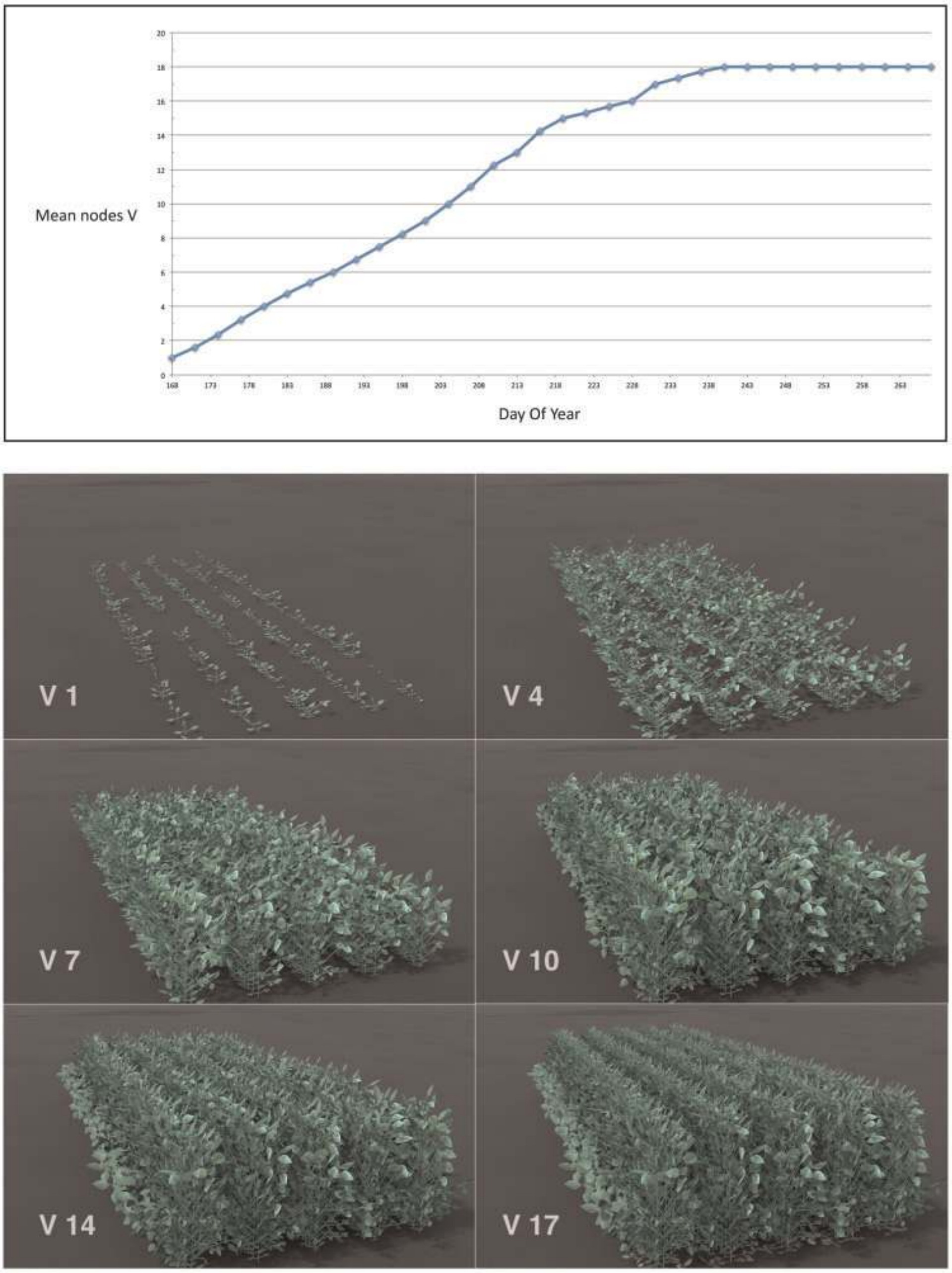

Figure 1 **Comparison of data visualized in 1D vs 3D representations.** (**A**) Average number of internodes per soy plant grown in ambient carbon dioxide levels over a growing season. (**B**) 3D representation of the same data in (**A**), except that spatial information is taken into account. The 3D representation of the data allows many more properties of the plants to be observed and explored. For example, it can be observed that, over time, plants grow taller and fuller, and the effectiveness of the use of space between plants can be analyzed. Both images (**A** and **B**) show when plants reach their maximum height, but the 3D representation also shows time of flowering and fruit set, time required for development of flowering and fruit set, and time required for leaves to senesce.

used virtual reality visualizations of farmland as an educational tool to help students understand pollution and crop land preservation.[83] However, immersive visualization has not been widely used to analyze data from agriculture or crop sciences. An exception is the KeyGene company, which is currently using virtual reality to manage large datasets obtained from plant phenotyping.[84]

The agriculture and nutrition fields have lagged behind in advanced scientific visualization of data, but as the datasets within these fields grow in size and complexity, creative visualization strategies, such as those described above, are becoming necessary. In particular, the plant sciences community is beginning to embrace computational simulations to integrate massive datasets with spatial coordinates to generate virtual fields of crops with quantifiable traits that can be measured in silico and under conditions difficult to obtain in a laboratory or field. These datasets naturally call for 3D scientific visualization. The computational science of crop simulation works across a wide range of scales: molecular, genetic, cellular, organ, plant, and stand. Each of these scales depends on scientific visualization to provide insight and foster discovery at the current scale, but also uses the visualization to communicate these insights and discoveries across the scales, eg, to facilitate communication between the molecular biologists, geneticists, plant biologists, and crop scientists collaborating on a project.

At the finest scale of crop simulation, molecular visualization techniques reveal how atoms form molecules and molecules form proteins. Such techniques expand efforts to understand how proteins function by visualizing how the molecules fold into the protein structure and how the resulting protein behaves at an atomic level. Protein structures can be visualized experimentally using X-ray crystallography, but even today, this procedure is technically challenging and yields low throughput. Owing to experimental limitations, few plant-specific proteins have been obtained, and the geometry of their structures has been inferred from homologous proteins in other organisms. Such visualizations, such as those surveyed by Dunker et al.,[85] for example, commonly utilize the concrete geometry of a ribbon to visually communicate the arrangement of molecules into the α-helices and β-sheets of the protein structure as well as their relationships to each other. In one example of investigator-led visualization, a ribbon was used to track the interface between two helices wrapping around each other. Untwisting of the ribbon (and the helices) better revealed the interactions along the interface.[86]

Visualization has also been instrumental in understanding plant development through computational simulation. Developmental models of botanical structures have been modeled using a formalism known as Lindenmayer systems (L-systems).[43,87–89] This algorithmic description of plant growth is more computationally efficient than explicit modeling and provides a basis for experimentation through computational simulation of a large quantity of detailed plants at varying levels of resolution (Figure 2 [43,88,89]). Photorealistic rendering of a simulated plant provides a basis for visual comparison and verification of the simulation with real-world photographs and other measurements of the growing plant, leading to an L-system model that reveals new insights into the underlying processes of plant development. A recent model of inflorescence and phyllotaxis, shown in Figure 2C,[89] provided a means to experimentally verify, through simulation and visualization, hypotheses of flower morphogenesis that are exceedingly difficult to observe physically at such small spatial scales and such long time scales.

The L-system formalism has also been used to model crop canopy architecture, in particular to predict the effects of light partitioning and shading on many individual crops, including barley,[39] faba bean,[90] wheat,[91] and maize,[32] and on crop mixtures such as wheat–pea[40] and chickpea and the weed sowthistle.[92] These models are able to link L-system architecture models, which simulate the recursive behavior of plant growth, with physiological models and ray-tracing algorithms. The exchange of information between these modules results in accurate simulations of canopy response to environmental inputs, both abiotic (temperature, carbon dioxide, humidity) and biotic (disease or competition with weeds). For example, a functional–structural model of barley was built on the basis of L-system formalism to generate a semiquantitative phytochrome-based shade detection model.[39] The ray tracer was designed to model the local ratios of red to far-red and was shown to be capable of reliably reproducing a range of radiation values encountered in nature. Importantly, model simulations were able to relate tiller number to level of radiation, where there is reduced tillering at low phytochrome ratio values.[39] The importance of this model is that it opens the door for integration of signaling pathways controlled by photoreceptors, which would represent a significant advance toward a functional multiscale model that takes into account how both physiological and biochemical processes influence crop response to environmental signals. This linkage across biological scale would also expand the usefulness of the model to other scientific domains such as nutritional science. The ability to relay information from the physiological scale to the biochemical scale could provide valuable insights about the modification of pathways and lead to predictions about differential accumulation or depletion of metabolite pools or other biochemical products important for nutrition.

Likewise, architectural models have been used to understand growth dynamics and physiological properties in multispecific stands. L-system-based functional–structural models of wheat and pea were interfaced with a radiative transfer model (or light model) to generate contrasting architectures of crop canopies and to explore how those architectures influence light partitioning.[40] This study found that the key determinants for how light is partitioned in a mixed stand of wheat and pea include leaf area index and plant height. In particular, pea internode length was found to have the strongest effect on both pea and wheat dominance in terms of light interception; that is, longer pea internodes resulted in pea dominance, and shorter pea internodes resulted in wheat dominance, more so than an increase in wheat internode length of the same proportion.[40] The results of these model simulations could be used to

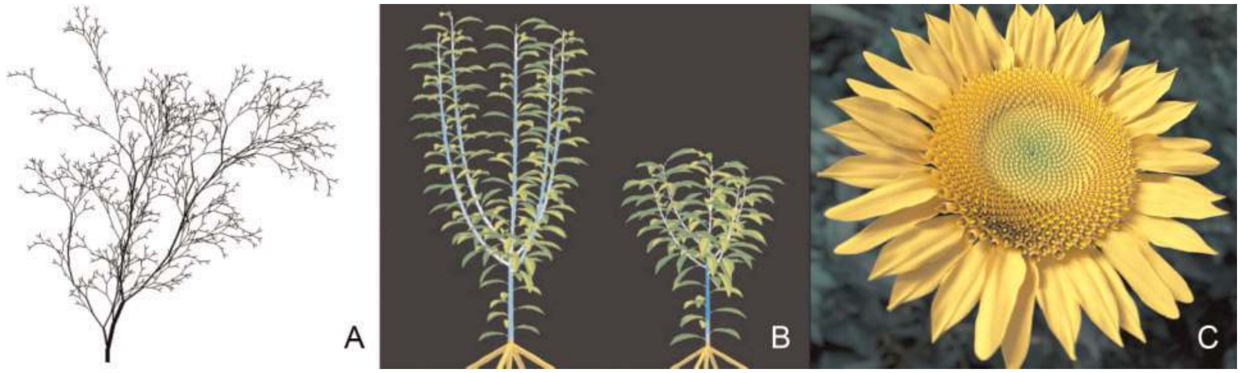

Figure 2 **Examples of L-systems to model plant architecture.** (**A**) A fractal tree generated from Horton-Strahler branching patterns.[88] (**B**) Peach trees modeled under different water stress using L-PEACH[43] and (**C**) a photorealistic sunflower model.[89] L-systems can be used to address a breadth of biological questions related to the evolution of plant morphology over development and in response to environmental perturbations.

identify wheat and pea cultivars with ideal canopy morphologies to increase productivity of grass–legume intercropping systems. Alternatively, canopy architecture models can be used to study competition between crops and weeds. Cici et al.[92] developed the first model of crop–weed competition and also used L-system-based architectural models to test the ability of different chickpea cultivars to outcompete sowthistle via light interception. Their model was heavily parameterized on the basis of data collected from four chickpea cultivars. Afterward, simulations were run to quantify sowthistle growth under the different canopy architectures. They identified the morphological characteristics that allowed certain varieties to outcompete sowthistle, such as short phyllochron and large leaflet size.[92] Identification of important traits via simulations can provide plant breeders with useful information to make informed decisions during selection for breeding.

Recently, L-system formalisms have been modified and expanded to perform 3D modeling in an agent-based, structured growth model of beetroot hairy root cultures.[41] In this work, the Virtual Experimentator for Root Networks was developed to simulate the development of hairy root culture morphology to generate data that would help optimize media recipes and improve the design of bioreactor environments. The rationale for this study was to identify optimal bioreactor conditions for the production of secondary metabolites, such as betalains, in hairy root cultures. The results of this study would have implications for the industrialization of plant products. The agent-based model produces emergent behavior through the interaction of simple units that describe processes of nutrient uptake and transport. This study found that simulated results closely matched experimental results for the traits of total number of root segments and total root length, with only a 4% to 6% deviation.[41] Model outputs included changes to plant properties and to the nutrient matrix and oxygen concentration within the simulated petri dish environment. The depletion of nutrients within the media over time was visualized using changes in color of both the media and the plant. The 3D visualization was zoomable and rotatable to allow visual inspection of the hairy root in real time. Uniquely, this model can be used to predict secondary metabolite accumulation and observe morphological response to changes in the nutrient environment. This is an important example because it is a rare instance of a model that links biochemistry and physiology. A similar linkage applied to functional–structural root models would be a step forward in achieving predictions about how fluctuating nutrient environments result in different nutritional composition and quality of crops.

In each of the above examples, 3D visualization of plant structure was instrumental for the realistic simulation of crop response to abiotic and biotic interactions. Although these models are built using intense parameteriztion based on empirical data, visualization via L-systems results in the generation of data that reveal emergent properties upon system perturbation. The qualitative and semiquantitative model outputs can inform researchers and breeders about important plant properties and traits that can improve crop production. The major limitation of these examples has been the lack of molecular and genetic information, which makes it difficult to associate plant traits with the underlying genetics. Such integration should be considered a priority in future crop and/or nutritional modeling efforts.

Future directions for advanced visualization of agriculture and nutrition data

Scientific visualization, including 3D, immersive, and photorealistic rendering, can improve researcher comprehension and promote discovery in large-scale agriculture, plant science, and nutrition data as it becomes available. One of the best examples of scientific discovery through visualization of agronomic data comes from outputs of the SimRoot software. SimRoot[42] is a functional–structural plant root model that can simulate several root-related parameters and render model outputs as 3D images. SimRoot was used to simulate the utility of root cortical aerenchyma in 3 maize genotypes growing in different soil environments[93] (Figure 3[93–95]). Model simulations predicted growth and yield benefits in plants that form root cortical aerenchyma in lateral roots. Simulations suggest that increased formation of root cortical aerenchyma improves crop performance on low-fertility soils, resulting in 70% and 55% greater yield under phosphorus and nitrogen deficiency, respectively, compared with low aerenchyma root types. This finding would affect grower use of inorganic fertilizers, in that substantially less would be needed to achieve sufficient yield. Field studies were then conducted under different environments using maize root phenes selected on the basis of model predictions. Field trials in Pennsylvania using high root cortical aerenchyma lines resulted in a 58% increase in maize yield under low-nitrogen conditions[94] (Figure 3B[94]). Likewise, maize genotypes with high root cortical aerenchyma had 78% to 143% greater yield than those with low root cortical aerenchyma grown under water stress in Malawi[95] (Figure 3C[95]). In this example, observations, along with quantitative data obtained from the model, allowed the researchers to choose existing crop varieties for field trials by comparing root architecture phenotypes between model simulations and available cultivars. Here, advanced visualization of model simulations, using measured agronomic data, resulted in an immediate and positive impact on grain yield under challenging environmental conditions through selection of existing ideotypes.

Functional–structural models that take into account empirical data about biological processes are particularly useful in predicting emergent plant architecture for horticultural trees. The IMapple model is able to simulate the growth of a whole apple orchard in 10 minutes on a desktop computer; such growth would take at least 10 years in real time.[96] IMapple's realistic tree model can immediately help growers make decisions about pruning strategies to optimize future fruit weight and/or nutritional quality, on the basis of visual outputs of model simulations. Likewise, the L-PEACH model[43,44] was developed to help peach growers in their decision-making for orchard management (Figure 2B).[43] The L-PEACH model includes algorithms for water potential and carbon allocation driven by source–sink interactions between tree organs.[43,97] L-PEACH simulations have been used to calculate rates of seasonal water uptake, which allowed researchers to estimate developmental and yield responses to various irrigation schemes.[97] Annual sink and source behavior for carbohydrate storage was simulated over 6 years and in response to field treatments such as severe pruning, defruiting, or remaining unthinned. The L-PEACH outputs revealed patterns of whole-plant carbohydrate storage and mobilization and uncovered the emergent property that replenishment of carbohydrates back into storage sinks is a slower process than mobilization out of storage.[97] Importantly, the model exposed gaps in field data that informed researchers how to proceed with future sampling and field observations.

Functional–structural and algorithmic models demonstrate the power of 3D rendering of model-simulated data to observe emergent crop architecture in response to interaction between plants and their environment. Although the models themselves are very large, requiring intensive parameterization, they are not designed to process large, "-omic" scale data and therefore do not account for the complex biochemical and signaling pathways that occur at the cellular level. In today's era of big data, a key challenge faced by the plant sciences community is effective integration and visualization of large experimental or simulated datasets in order to reveal hidden insights. However, several modeling platforms have recently been launched to address these issues, including the Agricultural Model Intercomparison and Improvement Project,[98] the Decision Support System for Agrotechnology Transfer,[99] and the Crops *in silico* project.[55]

In particular, the Crops *in silico* initiative aims to create a graphical user interface to access model integration tools that will enable multiscale modeling across molecular, cellular, tissue, organ, and ecosystem levels. The Crops *in silico* user interface will allow model outputs to be visualized as easy-to-interpret graphs, tables, animated simulations of plant growth, and ecosystem interactions. Interactive visualizations of early outputs from this integrated architecture will help plant scientists to test and validate the results of their computational simulations against experimentally measured data. It is anticipated that interactive visualizations of output from the integrated models will intuitively convey simulation dynamics and reveal emergent behaviors that will help researchers identify new biological questions for investigation. For example, an integrated model of soybean growth and dynamics has been generated using the Crops *in silico* framework, and 3D rendering has been applied to integrated model simulations (see Movie 3 in the Supporting Information online). The model incorporates a leaf submodel

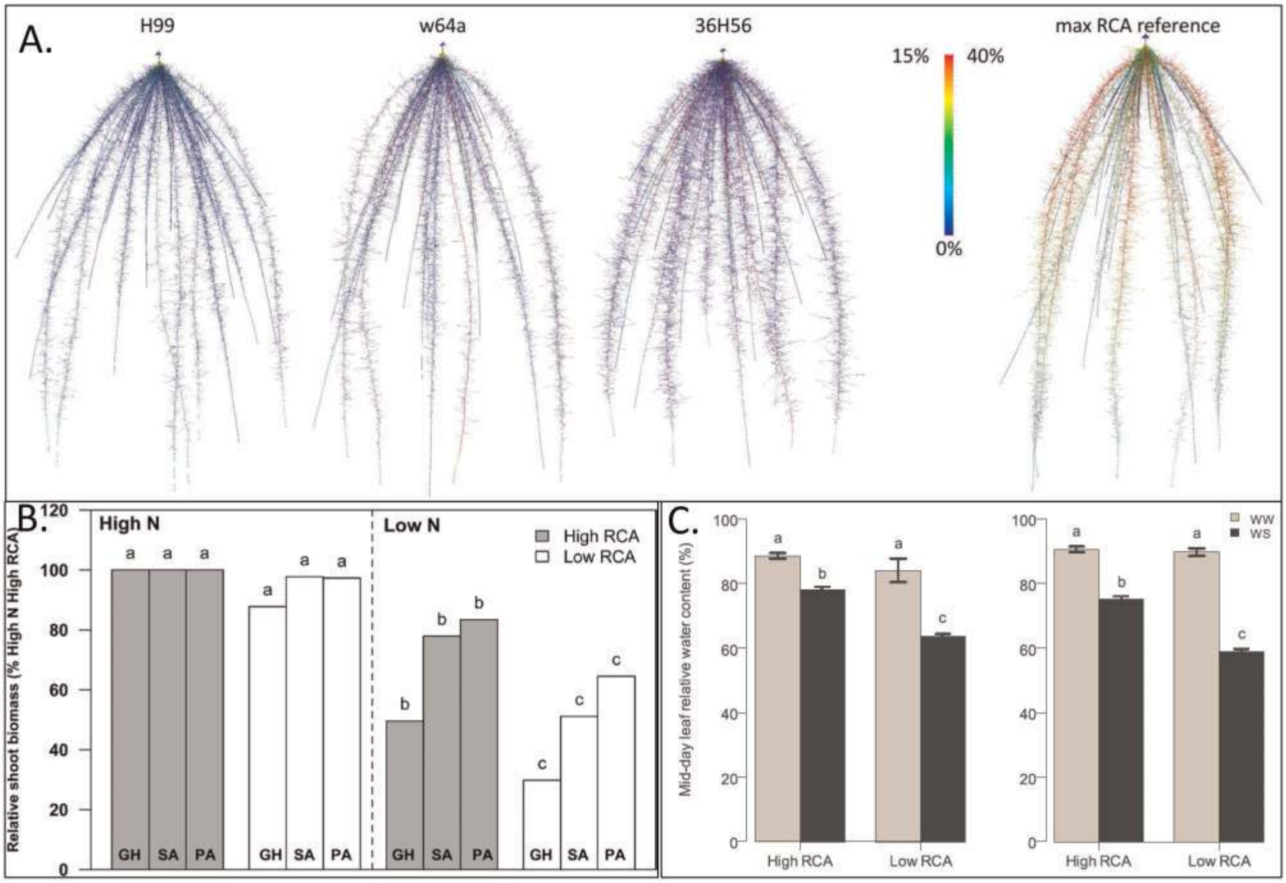

Figure 3 **Example of SimRoot model predictions to enhance crop production under challenging environments.** (**A**) Spatial map of RCA formation in simulated root systems at 40 days after germination. Color scale/shading indicates RCA formation as a percentage of root cross-sectional area.[93] (**B**) Relative shoot biomass under high nitrogen (high N) and low nitrogen (low N) conditions at 35 DAP in soil mesocosms (GH) in 2010 and at flowering (63 DAP) in fields in South Africa and Pennsylvania.[94] (**C**) Leaf relative water content for 10 high-RCA and 10 low-RCA maize genotypes under water stress and well-watered conditions at 70 DAP in 2 field environments in Bunda, Malawi (left), and Chitala, Malawi (right)[95] *Abbreviations:* DAP, days after planting; GH, greenhouse; PA, Pennsylvania; RCA, root cortical aerenchyma; SA, South Africa; WS, water stress; WW, well-watered.

coupled with interactions between photosynthesis, energy balance, stomatal conductance, and leaf boundary layer conductance.[35] It employs an explicit 3D soybean architecture with a ray-tracing algorithm to obtain light absorbed at different parts of the canopy.[38] It then partitions the photosynthetic carbon uptake to different plant parts, using a thermal time-based carbon allocation model[100] that predicts the growth and maturity of soybean plants.

The long-term goal of Crops *in silico* is to push the limits of general visualization tools to motivate development of novel approaches that are specialized to reveal insight into the dynamics of crop simulation. Explicit 3D geometric models can be explored and analyzed to function as interactive tools that will inform the modification of input variables used in the simulations. In particular, the 3D rendering of the soybean crop canopy, mentioned above, is able to provide more-accurate canopy architecture such as leaf area and leaf angle measurements as inputs for the raytracing module,[38] resulting in improved simulation of light interception and photosynthesis by the crop canopy (see Movie 2 in the Supporting Information online). Another goal of integrative, multiscale modeling and visualization is to enable researchers to make real-time observations of crop response to the environment, including untested environmental conditions such as elevated levels of atmospheric carbon dioxide (see Movie 4 in the Supporting Information online). Ideally, developing a visually appealing and accessible platform to perform model integration and simulations will facilitate the use of Crops *in silico* as a modeling tool for plant biologists and as a teaching and training tool for students. High-quality visualizations of the results from integrated and multiscale modeling will be valuable not only to domain experts but also to producers, farmers, breeders, and the broad public. This transition from investigator-based interactive visualization to end-user and public-based presentation visualization can increase the transparency of scientific research and make it understandable to a broad audience.

A future direction for integrative modeling and visualization would be the expansion of multiscale crop models to include large-scale data from nutrition and health studies, which would facilitate forecasting of how future climate scenarios will affect global human nutrition and well-being. Such integration could potentially improve overall modeling of food insecurity, provide better estimation of uncertainty, and guide strategies for assessment and management of risk. For example, integration of crop system and climate models with the Global Expanded Nutrient Supply (GENuS) nutrition model[101] could refine model predictions of nutrient deficiency by country on the basis of simulated changes in access to food or in the nutrient composition of crops. The GENuS model uses FAO food balance sheets in combination with data on individual crop production, trade, and utilization to estimate the role of individual foods in the nutritional status of a given population.[101] As stated earlier, the outcomes of global change, such as elevated levels of atmospheric carbon dioxide, have a known impact on the nutritional quality of crops.[5] A model that integrates biological, economic, and nutrition information would be a valuable tool to provide predictive and assessment capabilities to decision makers in public and private sectors.[102]

CONCLUSION

Historically, the availability of numerical models and established visual metaphors in agriculture and nutrition has been limited. Researchers have had to rely either on simple graphics tools available through their word processing software or on commissioned artistic illustrations to communicate important phenomena and information. For example, infographics have recently become a popular visualization tool to convey health information to consumers and policymakers by communicating complex data in a digestible format that can quickly be consumed.[103–105] Health educators are taking advantage of social media to share infographics about nutrition guidelines containing constructs of health behavior theory to change consumer behavior related to dietary practices and exercise.[103] However, research exploring the effectiveness of nutrition infographics found that action-oriented titles, more so than illustrations, are the most important design component to make infographics memorable and compelling.[104] The Scientific Animations Without Borders program, established at the University of Illinois, Urbana-Champaign, Illinois, and now at Michigan State University, East Lansing, Michigan, has linked agricultural researchers with professional animators to create and distribute short educational films to low-literate farmers in developing nations.[106] Its ability to redistribute these visual elements across the world in regions of low literacy, repackaged with culturally appropriate language recordings,[107] suggests that visual presentation of information is universal and effective. Although these simple visualizations are useful for communicating research outcomes to the public, there is a need for advanced visualization to enable researchers to glean more from their data, especially as the volume, diversity, and complexity of data increase.

Advanced scientific visualization is now being adopted as a tool to reveal emergent trends in computational data in diverse fields. However, the use of modern visualization in agriculture and nutrition presents many challenges. Researchers will need to find ways to integrate and understand the intersectionality of models at molecular, cellular, organism, ecosystem, and consumer scales. The datasets from diverse fields vary from spatial to relational, from computational to observational, and from intuitive to counterintuitive data. Scientists can leverage decades of visualization research to reconcile differences and develop a visual language to communicate with each other, with the public, and with policymakers.

This review surveys the use of computational biology in integrative, multiscale modeling and advanced scientific visualization as one approach to the design of ideotypes aimed at improving food security over the next 75 years. Climate change is having an increasingly profound and complex effect on global food security and nutrition. Therefore, a realistic, visual representation of crops can enable a more accurate prediction of crop response to environmental conditions and can aid in targeted crop breeding and engineering. Likewise, the acceptance and use of advanced scientific visualization technology can enhance the exploration and comprehension of multivariate agriculture and nutrition data, which can inform crop models and, in turn, lead to the design and generation of crop ideotypes that will be better suited than the existing germplasm to meet future yield and nutritional demands. Scientific visualization can also affect future food security by shaping popular opinion and influencing public policy through its ability to reveal, educate, convince, and inspire.

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Declaration of interest. The authors have no relevant interests to declare.

Supporting Information

The following Supporting Information is available through the online version of this article at the publisher's website.

Movie 1 **Visualization of an F3 tornado**

Movie 2 **Soybean growth in ambient carbon dioxide**

Movie 3 **Sunlight absorbed by soybean plants over the course of a day**

Movie 4 **Comparative growth of soybean plants in ambient and elevated carbon dioxide**

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