CH02 - Advances in root architectural modeling during the last decade

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Abstract

Root architectural models (RSA) have become important tools in root research and plant phenotyping for studying root traits, processes, and interactions with the environment. The models have been used to simulate how various root traits and processes influence water and nutrient uptake. At a more technical level, they have been used to develop phenotyping technology, particularly for testing algorithms for segmenting roots. To compute these quantitative estimates regarding plant nutrition and root functioning, much development occurred in the last decade increasing the complexity of the models. In this chapter, we describe first the application of the models to questions in plant biology, breeding, and agronomy, and second the development of the models. We end with a small outlook suggesting that models need benchmarking and validation and that new developments are likely to include better descriptions of root plasticity responses and focus on biological interactions among (soil) organisms, including mycorrhizal fungi.

Keywords: FSPM, Simulation, root system architecture, plant nutrition, ideotype development, plant-soil interactions

Introduction

Mathematical models of plant roots are formulations that quantitatively describe the morphology, size, growth, or physiology of plant roots. These models have a long history of development, and different root models have been presented in the literature. Among the different models, root system architectural models (RSA models) are distinguished from other model types by their specific concern for which roots of what types are where in space, and they give arguably the most explicit and detailed representations of the root system. The first root architectural models were developed at the end of the 1980s (Fitter, 1987; Diggle, 1988; Pagès et al., 1989). At the time the simulated root systems were relatively small and the simulations were mainly concerned with representing the geometric aspects of root architecture. Since those early beginnings, these models have been developed further and the range of applications has expanded. The models have added physiological aspects of root growth and functioning and thereby in effect have become what we now call functional structural plant models (Vos et al., 2010), albeit with the focus belowground, not aboveground. The functionality and application of RSA models were reviewed by Dunbabin et al. (2013). Since then new model codes have been released and many model studies published. The RSA models have been coupled to soil and shoot models, and have acquired more detail and functionality. Significant effort went into improving the code, and the model development typically expanded from single researchers to development teams. In this chapter, we aim to describe the advances of these models during the last decade (2010-2020) and how the simulation exercises contributed to our scientific understanding of root and plant functioning.

Advances in the application of RSA models

During the last decade, RSA models have been applied to study an increasing number of plant species, root traits, and plant physiological processes. The models have been coupled to increasingly more complex simulations of the (soil) environment (see chapter 3) and many papers focus on the interaction between environment and phenotype. This has led to applications in the area of breeding, agronomy, and ecology, although these fields are strictly speaking at a higher scale than single plant models. Currently, our understanding of the function of phenotypic root traits is still fairly limited, but the RSA model studies that we highlight here have demonstrated the complexity of, and provided insights into, phenotype by environment interactions.

Root traits studied

RSA models contrast with root length density models by explicitly simulating the placement of each root whereas root length density models typically assume homogeneous distribution of roots within a given soil layer (Postma et al., 2008). Simulating competition for nitrate among different species (maize, bean, squash), Postma and Lynch (2012) showed that a homogeneous root distribution gave much greater nitrate uptake than a root distribution determined by root architecture. We can conclude from this that root architecture restricts the foraging capacity of the root. This immediately raises the question as to what the optimal architecture is for the acquisition of various nutrients. Several studies were published in which the sensitivity of nutrient uptake for root architectural parameters was tested. These parameters are usually directly translated to root architectural traits. In many cases, the sensitivity depended on the simulation environment and nutrient simulated, giving some insight into the complex interactions between the environment and root architecture. Additionally, the studies suggested some tradeoffs exist for optimizing root architecture towards the acquisition of different nutrients.

A relatively simple to understand trait is root growth angle of branch- or adventitious roots (Figure 1). Although various angles might be measured during phenotyping, including insertion angles, set-point angles, and the rate of the gravitropic response (Freschet et al., 2020), the overall angle causes the root system to be either shallower or steeper. Dathe et al. (2016) simulated steeper and shallower root growth angles in maize and showed that the optimum for nitrate uptake depended on the rate of nitrate leaching, with fanned phenotypes (larger variation in root growth angle) achieved relatively good performance in many environments. Already in 2001, Rubio et al. (2001) showed that shallow root growth angles may be advantageous for P uptake by basal roots in bean, and this work was recently followed up by a much larger set of simulations including mechanistic simulation of P-uptake and simulating phenotypes that varied both in root growth angle and the number of basal roots (Rangarajan et al., 2018). The study gives support for the existence of phenotypic variation in both traits, as the optimum is strongly dependent on the environment simulated. Nevertheless, the overall picture is that plants are faced with a tradeoff between shallow and deep placement of roots through a change in root growth branching angle and that the tradeoff determines the relative uptake of shallow (P) and deep (nitrate) resources. Experimental papers confirming the relation between P and nitrate uptake and root growth angle include greater P uptake by bean phenotypes with shallow basal root growth angles (Miguel et al., 2015) and greater N uptake by deep rooting maize (Trachsel et al., 2013).

Phenotypic variation in the number of root axes was studied in several papers. We already mentioned the simulation study of Rangarajan et al. (2018) (Figure 2), in which 2 or 3 whorls of basal roots were both the most frequently observed phenotype and the optimal number in many simulation scenarios. Lateral root branching density, which is the inverse of the interbranching distance, has been studied experimentally in many species (Pagès, 2019; Freschet et al., 2020). Postma et al. (2014a) simulated observed phenotypic variation for this trait and predicted a tradeoff between phenotypes with many short and few long lateral roots. The many short phenotype would be advantageous for P uptake whereas the few long phenotype would benefit nitrate uptake. Experimental confirmation of the results came from two papers studying the same set of genotypes under P deficiency (Jia et al., 2018) and N deficiency (Zhan and Lynch, 2015). With a semi RSA model, Heppell et al.

(2015) concluded that higher branching in the topsoil and lower in the subsoil could increase P uptake by 42%. In another simulation study, dense root systems were beneficial to quickly capture in-season rainfall but not for exploiting water stored before the growing season (Tron et al., 2015). Recently, Muller et al. (2019) took the concept of branching a step further and distinguished randomness in branching from structured variation. RSA models will be well suited to simulate these various kinds of variation in branching and might estimate the utility of the different phenotypes in various soil environments. The lateral root branching density not only interacts with the environment but also with other traits. For example, Postma and Lynch (2011a) simulated a positive interaction between the number of branches and the amount of root cortical aerenchyma (discussed further below).

RSA models have also been used to investigate anatomical traits. So far the function of these has been difficult to study, so RSA models have been used to pose and simulate hypotheses on how anatomical traits influence nutrient uptake and plant physiology. Root cortical aerenchyma, the formation of air spaces in the root in this case through programmed cell death, is an interesting example. Aerenchyma formation is negatively correlated to both root respiration and root nutrient content (mol cm^{-3}) and was hypothesized to reduce the metabolic cost of roots, allowing new root growth and thereby greater nutrient uptake (Fan et al., 2003; Postma and Lynch, 2011a; Postma and Lynch, 2011b). The simulation studies suggest large benefits from a metabolically more efficient root system, especially in maize where aerenchyma formation covers a relatively large percentage of the cortex as opposed to bean where aerenchyma formation is much less prevalent and is in part replaced by the loss of the whole cortex (cortical senescence) due to secondary growth. Variation in secondary growth itself, however, may be a form of metabolic efficiency that can be achieved when stressed plants with smaller shoots have reduced water requirements (Strock et al., 2017). Loss of the whole cortex also occurs in barley and several other Poaceae, due to programmed cell death rather than secondary growth (Schneider et al., 2018). Cortical senescence is not only associated with reduced respiration and nutrient content but also reduced water and nutrient uptake (Schneider et al., 2017b). Simulating these processes showed that cortical senescence is beneficial when it occurs in the major root axes, but not in the lateral roots (Schneider et al., 2017a). Indeed, cortical senescence in lateral roots was not observed.

One of the most studied anatomical traits in plant nutrition is the formation of root hairs. Different approaches to simulating the function of root hairs have been published. Zygalakis et al. (2011) presented a dual-porosity model for root hairs in which they take account of the interaction between root hair geometry and soil particle geometry. The model simulated greater uptake from P in micropores and showed that uptake was less sensitive to soil moisture content than previously simulated. Leitner et al. (2010) took a different approach and used homogenization, a mathematical procedure, to derive an analytical solution for the uptake of nutrients by root hairs. Such analytical solutions can compute much faster and thereby be useful when simulating 100,000+ root segments.

Thus far we have treated the architectural traits as static traits, but in reality, many of these traits are influenced by the environment. Simulation models currently include some of this root growth plasticity, even though much about the mechanisms and regulation of root growth plasticity is still unknown. The models often include empirically derived relations between environmental conditions, plant status and root growth responses (Dunbabin et al., 2011; Tournier et al., 2015; Postma et al., 2017). Root responses are typically defined in terms of tropisms (change in the growth direction), branching (change in the rate of primordia formation) or elongation rate. These empirical relations may be sufficient to study root growth plasticity as a functional trait. Henke et al. (2014) concluded that root growth plasticity in a heterogeneous soil would enhance N uptake. Similarly, Chen et al. (2013) produced a simulation study with root proliferation in response to P banding which suggested large benefits from the proliferation response.

Root processes studied

Functional structural plant models (FSPM) not only simulate structure, but also the relevant processes associated with that structure. In this respect, root architectural models advanced strongly as they were coupled to models of plant metabolism, nutrient and water uptake. Besides the interactions between structure and environment, the mechanics of the structure and soil were explored.

To simulate plant metabolism, RSA models were coupled to shoot models, albeit not often geometric shoot models (see section 3). This coupling allowed simulation of nutrient and carbon balances and source-sink relations, which play an important role in many simulations. The models typically restricted total carbon consumption to the carbon available from photosynthesis and carbon storage. Carbon consumption is restricted by reducing the growth rate of the root system. Several conclusions resulted from these simulations: 1) plants might cycle dynamically through periods of source and sink limitations, 2) large uncertainty exists with regard to what causes plant growth to be source or sink limited, and 3) oscillatory behaviour in source-sink ratios arises when the functional equilibrium responds to current plant status through allocation which is inherently slow and not corrected for future uptake efficiencies (Postma et al., 2014b). Source-sink models treat a trait like branching density as an increase in the sink term. Assuming no change in the source term, roots will have to stay shorter (Postma et al., 2014a). Although much uncertainty exists around source and sink limitations, especially of nutrient-deficient plants, it is currently one of the easiest ways to understand tradeoffs among RSA traits and foraging limitations. Similar to carbon-based source-sink relations, nutrient use efficiency concepts (defined as the amount of nutrients needed to construct the root system) have been implemented. Greater nutrient use efficiency (NUE, here the amount of nutrients invested for the amount of nutrients acquired) for N and P, for example, was achieved by simulating root cortical senescence and aerenchyma formation (see the section above). Interestingly, the model was more sensitive to the NUE effects than to the carbon saving effects, which may suggest that the cost of the root system might be computed in terms of nutrient "investment costs" (Schneider et al., 2017a; Postma and Lynch, 2011a,b).

There has been much interest in nutrient and water uptake by root systems. Current models for nutrient uptake typically rely on a reaction-diffusion-advection equation for nutrient transport in the soil and a Michaelis-Menten based nutrient uptake term. It is often said that the models are relatively insensitive to the Michaelis-Menten kinetic parameters, as in many scenarios the soil becomes the limiting factor. York et al. (2016) showed that under competitive conditions the maximum uptake rate, Imax, can give a (small) competitive advantage, and that sensitivity to Imax depends on other RSA traits and soil conditions (Figure 3). This is an important realization, especially when scaling up from single plants to competitive stands, and to understand interactions among plant species.

The RSA modeling community has been especially active in the area of simulating plant water uptake and transport. A short history of the simulation of water flow from the soil through the root system to the plant starts with representing flow using electrical analogies (e.g. Honert 1948). Based on these analogies, Alm et al. (1992) developed a numerical model of water transport for an unbranched root. This was extended to branched root systems by Doussan et al. (1998). Javaux et al. (2008) coupled the Doussan model to the well known SWMS (forerunner of Hydrus) soil water model and thereby enabled further studies of compensatory water uptake and hydraulic lift. Lobet et al. (2014) expanded this work to include water transport through a geometrically explicit shoot. Doussan’s equations were originally based on root water potentials which are 'corrected' for gravity, such that gravity does not appear in his equations. Schnepf et al. (2018b) present a version that introduces gravity into the equation. Meunier et al. (2017b) and Meunier et al. (2017a) present a hybrid analytical-numerical solution for a branched root system.

Thus far, model studies suggested there is no optimal root architecture for water uptake, as it all depends on the environment (Tron et al., 2015). This is by itself not surprising, as water and roots need to coincide in time and space. This means that deep rooting is only beneficial in environments with deep water available, and with deep water recharge during rainy seasons. However, the model studies gave more precise insights into these interactions between environment and root phenotype. A long-standing issue in plant hydrology has been whether root to shoot signaling occurs via hormonal transport from root to shoot. Huber et al. (2014) concluded that shoot responses to soil drying might be explained just as well or better by a hydraulic signal (a change in xylem water potentials as the soil is drying) than by hormonal transport.

Trait synergies and integrated phenotypes

One of the great challenges in understanding the utility of a trait is that interactions among traits can result in both synergistic and antagonistic effects on root functioning. For example, Miguel et al. (2015) demonstrated experimentally that bean phenotypes with either long root hairs or shallow basal root angles had greater growth on low P soils. However, phenotypes that had both long root hairs and shallow root angles had far greater growth than phenotypes with only one of these traits. Such interactions were easily explored with RSA models. Examples are found for tiller number interacting synergistically with root cortical senescence (Schneider et al., 2017a) and lateral root branching density positively interacting with aerenchyma (Postma and Lynch, 2011a). Integrated phenotypes that combine variations in multiple traits and may represent real-world phenotypes, can be explored further. Such integrated phenotypes were simulated by Rangarajan et al. (2018) and York et al. (2016) (Figures 2 and 3). Phenotypic variation is not a continuum but tends to group in what might be termed root system types. Bodner et al. (2013) worked out such types based on statistics and these types were simulated to study water uptake in different scenarios (Leitner et al., 2014b; Tron et al., 2015).

Simulating the soil environment

Plants in the natural environment grow their roots in a complex, dynamic, heterogeneous soil matrix. At the beginning of the decade, most RSA models largely ignored this environmental complexity to focus on simulating growth under uniform and nonrestrictive conditions. These simplifying assumptions were made partly to simplify initial model development, but also because model representations of many soil processes (even uncoupled from RSA models) were still under development (Vereecken et al., 2016). Further, most RSA models were initially parameterized using data from experiments conducted under glasshouse or laboratory conditions at the mesocosm scale or smaller, meaning many of the parameters available for calibration were, in fact, observed under uniform and nonrestrictive conditions. Therefore, credit for progress in modeling the soil environment must go as much to the researchers developing improved methods for field measurements that can be used for model validation as to those writing down the model code.

Whether root growth responses to soil hardness should be thought of as primarily driven by average responses or by local heterogeneity (i.e. roots grow through cracks and biopores) is an unresolved research question. It is therefore not surprising that modeling of the interactions between soil hardness and root growth has taken two differing directions: one investigating how root architecture responds to hard soil at the macroscopic scale, and another trying to represent soil heterogeneity at the scale of the root tip. De Moraes et al. (2018) used RootBox to simulate the effect of soil strength and water status on soybean root extension rates. They calculated soil strength using a soil-specific exponential function of bulk density and water content, and additionally assumed that root growth was affected directly by soil matric potential (independently of the effect of water status on soil strength) according to the classic Feddes et al. (2001) root water uptake function. One intriguing feature of the de Moraes model is that by adjusting its empirical parameters it can account for the macroscopic changes in root architecture attributable to soil biopores without requiring highly detailed simulations of individual pores. Similarly, SPACSYS (Wu et al., 2007) has included a term for the effect of soil impedance on root growth since the initial description of the model. This term can only be varied at the root class level and requires user calibration, but when sufficiently detailed soil profile data are available it has been used to reproduce the observed root distribution of field-grown wheat (Bingham and Wu, 2011). By contrast representation of biopores in R-SWMS takes an explicitly detailed approach. The magnitude and direction of each root tip's growth vector is scaled by the frictional forces from the immediately surrounding soil, represented as a tensor (array of force vectors) computed from the conductance (inverse of penetration resistance) of the eight nearest soil grid nodes (Landl et al., 2016). This approach allows simulation of, in 3D space directed, root responses to individual pores down to the scale of the simulated soil mesh. Using this approach, Landl et al. (2019) showed that root penetration of strong soil layers via large-diameter biopores is likely a substantial benefit to net plant water uptake, even when accounting for a loss of water uptake caused by incomplete contact between the root and the pore wall.

Simulating rhizosphere processes and soil biota

Rhizosphere models are typically at a scale below RSA models, simulating single root tips or segments and the rhizosphere around. These models have been reviewed by Darrah et al. (2006). RSA models, however, have been used to up-scale the rhizosphere models to whole-plant level. Although some difficulty exists with respect to overlap between rhizospheres of different roots, this problem is typically mitigated by setting the outer boundary to the mean mid-distance between roots and by the assumption that overlap is relatively small (Postma and Lynch, 2011a; Postma and Lynch, 2012). Alternatively, the rhizosphere models are scaled up to 2 or 3-dimensional models including several root segments. This approach was taken by de Parseval et al. (2017) who specifically simulated facilitation as it may occur between roots differing in the amount of organic acid exudation. Nevertheless, reduced dimensionality of the models allows the rhizosphere to be simulated with greater detail around the root. The utility of organic exudates was thus simulated by Schnepf et al. (2012) who coupled a citrate exudation model to a P uptake model. The more computational intensive 3D approach was used by Fang et al. (2019) who coupled the RSA model RootBox to the eSTOMP chemistry model. The coupled model thereby simulated the chemical interaction between different solutes and the uptake of multiple nutrients. The detail around the root, including the importance of root diameter and root hair geometry, however, is typically lost in the 3D approaches which treat single root segments as sinks with a given surface area.

Rhizosphere processes not only include chemistry, but also microbial activity. Thus far little has been achieved in modeling these systems, in part because they are not well understood. In studies simulating the mycorrhizal system, Schnepf et al. (2016) and Schnepf et al. (2011) simulated the hyphal network of mycorrhizal fungi around a root to estimate the uptake of P by the hyphal network. Additionally, the SPACSYS model has been used to produce field-scale representations of microbially-mediated processes including N_2O emissions (Wu et al., 2015) and N fixation (Liu et al., 2013), but to our knowledge these were only validated with a 1D root profile and have not been extended to the full 3D RSA model.

Application of RSA models in breeding

RSA models have application in breeding. Thus far, the application has been mostly limited to ideotype development by simulating trait-environment interactions and integrated phenotypes (see above). This is possible for an increasing number of crop species including lupin, maize, bean, squash, rice, wheat, barley, and the model species Brachypodium (Liu et al., 2012; Postma and Lynch, 2012; see for example Dunbabin et al., 2013). Beyond the species level, parameterization at the genotype level has allowed understanding functional aspects associated with specific genotypes (Postma and Lynch, 2011a; York et al., 2015; see for example Fang et al., 2019). York et al. (2015) used the RSA model SimRoot to show that changes in root phenotype that were introduced during a 100-year timeline for breeding were associated with greater N capture. So far, however, the direct application of models in breeding has been limited, possibly because of a perception that RSA models have not yet been sufficiently validated (Koevoets et al., 2016; Ndour et al., 2017). However, an encouraging counterpoint to this perception comes from Zhao et al. (2017), who noted that observations of pea seedling root phenotypes had little predictive power when correlated directly to mature root traits, but that using these same seedling traits to parameterize RootBox simulations resulted in predicted root lengths that corresponded well with observations of the mature plants. This suggests immediate applications of models to aid phenotyping, and we expect a greater role for these models in breeding in the future, as outlined by Lynch (2007), Tracy et al. (2020) and in detail by Ndour et al. (2017) for breeding for drought tolerance.

Application of RSA models in agronomy and ecology

Although agronomy and ecology are strictly speaking at a higher scale than these plant models, they have been used to understand plant-plant interactions and in the ecological realm, species diversity. By simulating stands of multiple plants, RSA models are useful to understand how plant traits affect root competition (Figure 4). Multiple plant stands are featured in CRootBox (Schnepf et al., 2018b) and OpenSimRoot (Postma et al., 2017). Using the later, Rangarajan et al. (2018) showed that the optimal number of basal roots in bean was lower when the planting density was higher. Such interactions between plant density and root architecture are currently poorly understood (Hecht et al., 2019) but of importance when breeding for high production at high plant densities and also for the translation of single plant phenotypes to an agricultural context (Hecht et al., 2020).

Future sustainable agriculture should be biodiverse. Intercropping studies are of renewed interest as robotics might solve long-standing issues in the mechanization of such cropping systems. Postma and Lynch (2012) simulated the competition between maize bean and squash root systems for nitrate and phosphorus and concluded that the architectures and acquisition strategies of these plants are complementary. The maize-bean-squash intercropping system is an ancient one, and the simulation study merely provides some mechanistic insights into the functioning of the intercrop as observed experimentally (Zhang et al., 2014). However, Evers et al. (2019) proposed that functional structural plant models can be used to explore many more intercropping schemes and combinations, in order to reduce the number of systems tested experimentally. Such studies not only have utility in agriculture but will also contribute to our ecological understanding of biodiversity. Pagès et al. achieved much progress in this area by developing a relatively simple RSA model such that they were able to parameterize it for a wide range of species (Pagès et al., 2014; for example see Pagès and Picon-Cochard, 2014). This work in the future might be linked to databases of functional trait variation in ecology in order to explain the variation in functional root traits.

Application of RSA Models for refining experimental measurements

Once an RSA model has been validated to produce a realistic 3D root system, it immediately becomes useful not just for asking questions about root architecture, but also as a tool for producing known root architectures that can be used to calibrate measurement techniques. For example Lobet et al. (2017) used ArchiSimple to create a ground-truth library of images of root systems with known dimensions and then used these images for training of an image analysis tool. Similarly, Leitner et al. (2014a) used RootBox models to improve segmentation of neutron radiography images of living root systems by adding weight to detected paths that lie within the growth trajectory expected by RootBox and downweighting as probable errors the paths that do not. Schulz et al. (2013) tested the presented segmentation algorithm for roots in MRI images and used artificial generated images with varying resolution and noise levels to ground-truth the algorithm and find acceptable values. The images were generated with SimRoot. Rao et al. (2019) used modeled electrical conductivity of root-soil systems in order to interpret measurements.

Similarly, simulated root systems provide a ready method for testing field sampling methods. While this is not new (c.f. Pagès and Bengough, 1997), it continues to be a fruitful way of interpreting the reliability and bias of core, trench, and minirhizotron samples (Miguel et al., 2015; Wu et al., 2018; Morandage et al., 2019). Pagès et al. (2012) took a different approach and compared the output of an RSA model against a collection of possible root length density models fitted to the same data used to parameterize the RSA model, and showed that the results were largely congruent. This was reassuring and, given the differing goals and parameterizations of RSA and RLD models, not a foregone conclusion.

Advances in model development

Model development in the last decade has been dominated by a desire for implementing an ever-increasing number of processes, more precise presentation of morphology, and inclusion of the environment. This required greater flexibility in the code, but also lead to more complex and extensive models. Communicating what the model do has become ever more difficult. Nearly all codes were developed modularand adopted forms of object-oriented programming in order to accommodate team development and included more flexible implementation of new algorithms. This has led to model names such as CRootBox and OpenSimRoot which, in practice, are rather names for code bases with which different models can be constructed, depending on modules and parameters used. Modularity, in this case, leads to the encapsulation of different parts of the model, not necessarily transparency about what the model does. Few models have trackable public histories or backward compatibility and it is even a question as to what extent published results can be repeated, assuming licenses do not restrict access to the code. Because of this, there is a need for more transparency, simplification and better, more formal ways for parameterization of the models.

Continued model coupling

Multiscale-multiphysics is a current buzz-word that carries over into systems biology and visions have been expounded to simulate from gene regulatory networks up to the crop (Marshall-Colon et al., 2017). Root architectural models are supposed to play an important scale and discipline bridging role in this vision (Zhu et al., 2016). At the lower end of the scale, it has been explored how multi-cell models of roots and root tips, and the cellular networks that they simulate, can be scaled up to the whole-plant level (Baldazzi et al., 2012; Band et al., 2012). At even greater scales, Warren et al. (2015) explored how root models can be coupled to terrestrial biosphere models.

Modeling across scales and coupling processes that function at different scales is, however, a difficult task. This challenge was well summarized by Koevoets et al. (2016) in a discussion about using RSA models to advance crop breeding:

> "Current models, however, are often not easy to integrate [into breeding programs]. When developing a model, the general challenge is to make it comprehensive, widely applicable and simple. [....] As soon as models tend to be more widely applicable or incorporate more conditions, they tend to become more complex and the number of parameters increases. This decreases the ease of interpretation and especially the ease of integration into a larger model (including soil and plant performance models)."

One of the challenges currently being explored is the coupling of roots to soil models. In this coupling, the geometries of both models do not necessarily match and matching them would, because of the deforming nature of root growth, require a computationally intensive solution (Postma et al., 2008). Adaptive meshing was tried in the RSWMS model (Schröder et al., 2009) but abandoned as it did not seem to provide more speed or accuracy than a static mesh. A challenge is posed not only by the geometry but also the required resolution of the mesh around the roots. To circumvent these issues, Mai et al. (2018) coupled a high-resolution rhizosphere model around the roots to a much coarser 3D soil domain model. The work demonstrated that in doing so, the sink term at the higher scale might be improved, as well as the outer boundary condition at the lower scale, but that conflicting assumptions at both scales remain.

A more straight forward development of model coupling is the coupling of RSA models to FSPM of the shoot. An early approach was presented by Lobet et al. (2014) who used a coupled model to simulate water transport from roots to leaves, and more recently Fang et al. (2019) have taken a similar approach using different component models and adding nutrient ion flux as well as water flow. The advances in FSPM-shoot models were recently reviewed by Evers et al. (2018). Coupling of shoot and root seems a logical step forward and will enable a much better understanding of shoot-root interactions than thus far possible.

Modeling platforms to aid in defining new models

To facilitate the development of coupled models, different software platforms have been developed which are able to couple various submodels. From an IT perspective, this is best achieved through what is called loose coupling (Figure 5). Loose coupling is achieved when different components of software (in this case different models) are coupled over a standardized programming interface, without the components having any specific information about the implementation of the other component. This means that the data exchange between models is abstracted, such that one model can have implementation changes without the need to reprogram other models. This enables independent development, and crucially independent testing, of the different coupled components. It also facilitates the extension of the software by introducing new models and coupling them over the standardized programming interface. Software platforms for simulation typically implement some form of this modularity concept and various platforms have been developed. Various FSPM and RSA models have been constructed using such software platforms for simulation (SPFS).

CrossTalk (Draye and Pagès, 2006) is such an SPFS and was used to construct a coupled model of root and shoot architecture (Lobet et al., 2014). The coupling interface in CrossTalk defines the simulation theme as it requires a model for the root, the shoot, and the environmental components. OpenAlea (Pradal et al., 2008) is a general-purpose platform for constructing FSPMs and has a large code base containing many models. It has been used in various publications in diverse ways, but development activity on its Git repository seems to have stalled in recent years. AMAPstudio (Griffon and de Coligny, 2014) with AMAPsim (Barczi et al., 2008) describes a scene, but the implementation is more abstract and extensible. The software includes a root architectural component, called DigR (Barczi et al., 2018). The approach taken in AMAPsim may be similar to approaches found in the gaming industry where the scene is made up of different geometric models, all expressed in data structures that are defined in the programming interface. This approach allows interactive editing of the scene, and to incorporate geometric models extracted from 3D measurements, including laser derived point clouds. The designers of AMAPsim see this as a clear advantage over OpenAlea's more developer and process focused approach (Griffon and de Coligny, 2014).

L-systems have long been used to construct FSPMs (Prusinkiewicz and Lindenmayer, 1990). Although useful as a formalism to construct plant geometries, L-systems do not define the functional aspects of these models. As an alternative, 'Growth Grammar' was developed to have a complete formalism to describe FSPMs (Kurth and Lanwert, 2011). To our knowledge, GroImp (Kniemeyer, 2008) is the only SPFS that implements 'Growth

Grammar'. It is mostly used to simulate shoot architectures, however an RSA model was implemented by Henke et al. (2014).

The majority of the SPFSs discussed above are either limited to integrating models written in a single language or rely on generic cross-language bindings. By contrast Yggdrasil (Lang, 2019) provides interprocess communication through message-passing, thus allowing models written in different languages to synchronize information at each timestep even when running in parallel with each other. This tool is part of the larger 'Crops in Silico' project (Marshall-Colon et al., 2017), an ambitious SFPS that aims to support coupling plant models across all scales from molecular to ecosystem. As part of this ambition, Yggdrasil's developers claim it will be extended to support automatic runtime coupling of ODE models, effectively allowing models written separately to be solved as a single model. Although this automatic coupling facility remains to be seen, if successful it should provide a major step forward in model coupling and co-simulation.

Many of the models that are coupled to construct an FSPM can and, in our opinion, should be mathematically defined as conditional algebraic equations, or as often will be the case, ordinary and partial differential equations (ODE, PDE). Too often they are only defined as programmed algorithms with discontinuities and time-step dependencies hidden. The models can be regarded as a system of coupled differential equations. In numerical mathematics, it is well known that the stability of such systems is strongly problem-dependent. Finding the right solution can be challenging, and loose coupling further complicates this as it introduces the numerical challenges associated with co-simulation. Most SPFS ignore this and often rely on a single step, first order, explicit coupling method. OpenSimRoot was specifically developed as an SPFS for coupling ODEs using predictor corrected methods. This, in theory, should provide more robustness and reduce numerical errors, but is no guarantee that the right solution will be found. Thus far users have little way to know how accurate the solution is other than checking mass balances and sensitivity for time and space discretization. These issues are not specific to RSA models, and present a challenge to nearly all dynamic models in biology. Numerical accuracy has been much more of a concern in areas of physics and soil science, possibly in part because plant biology is plagued by other formidable sources of uncertainty.

In addition to large multi-model platforms, recent advances in web technology have allowed the development of a variety of new interfaces for individual models, in some cases even allowing users to run the entire model inside their browser with no further computing resources required. For example CRootBox itself is a compiled C++ application, but its developers also maintain shinyRootBox (Schnepf et al., 2018a), a live interactive modeling environment that allows users to explore predefined parameter sets and experiment with new parameter values by adjusting sliders in a web browser while the simulation updates in real time (Figure 6).

Simplification of models

The ever-increasing complexity of RSA models has led to important work towards their simplification. Specifically, Archisimple (Pagès et al., 2014) is an RSA model implemented in the scripting language R and has a reduced parameter set. This was achieved by assuming correlations among certain parameters. Archisimple takes advantage of experimentally observed correlations for branching patterns (Pagès, 2014), lateral root traits (Wu et al., 2016) and axial root traits (Wu et al., 2014). Sensitivity analysis is more easily achieved with a model that has a reduced parameter set (Pagès, 2011) and the relation between root length density profiles and RSA models could be determined (Pagès et al., 2012), as well as studies of the stochasticity of root systems (Pagès et al., 2013).

Although RSA models constructed with, for example, Crootbox and OpenSimRoot are often complex, their modularity allows simple models to be built. This raises a relevant question concerning what complexity can be left out. In general, this is answered through sensitivity analysis (e.g. Schnepf et al., 2018a; Morandage et al., 2019). However, complete sensitivity analyses of complex parameter sets are prohibitively large, so too often the analysis is performed on a subset of parameters already suspected to be sensitive. This leads to the conclusion that the processes included significantly influence results and therefore should not be ignored. For example, Thomas and Pollen-Bankhead (2010) concluded that root failure calculations cannot ignore soil type when parameterizing root friction angle. This demonstrates that there is still significant uncertainty in how to define RSA models and that different concepts varying in complexity are likely to be developed.

One way to reduce the RSA model is to see if the modeled root distributions can be represented by simpler continuous models containing fewer parameters. Different approaches are found in Zhang et al. (2014) and Bonneu et al. (2012). But since these models are not FSPM, they fall outside the scope of this review.

Better handling of input and output

In addition to uncertainty about which model parameters to include, RSA model operators suffer from uncertainty in deciding which values to assign to the parameters. This task is easier when parameters correspond to directly measurable root traits (e.g. root diameter in mm rather than a scaling factor in arbitrary units), but is still challenging. The de facto standard for most models has been to begin from an existing parameterization for the species of interest, then to measure plants or perform a meta-analysis (e.g. Pagès et al., 2012). Further, models differ in which parameters they need and in the units, names, and interpretations of the parameters they share, which means parameters developed for one model are of limited value for simulating the same plant using a different model.

Several researchers have proposed systems for converting image data (scanned root systems, rhizoboxes, minirhizotrons, MRI scans) into model parameters. One pipeline relies on the partially automated extraction of images into a machine-readable format, e.g. RSML (Lobet et al., 2015), then computing relevant parameters from the RSML input using the R package archiDART (Delory et al., 2016). Several RSA models can also now read and write RSML directly (Postma et al., 2017; Schnepf et al., 2018b), in some cases allowing simulations to begin from a digitized real architecture and continue growing as if this architecture had been generated by the model. An alternate pipeline for image data is to estimate the parameters through a reverse-modeling approach, as Garré et al. (2012) did for a minirhizotron dataset that was too sparse to fully constrain the model, and as somewhat more elaborately done by Ziegler et al. (2019) using an approximate Bayesian computation that increased the reliability of the procedure on noisy datasets.

In any case, the rise of more detailed inputs leads to the need to rethink what constitutes a valid output. Comparisons between observed and predicted traits require that the model be parameterized for the same scale and using the same experimental treatments as the observations, whether that is whole-field biomass, root length density (e.g. Bingham and Wu, 2011), root length of individual plants (Postma and Lynch, 2011b), or detailed time series of root placement and water flow (Koch et al., 2019).

This handling of input and output is one area where modeling platforms (discussed above) have potential to help. An example from the field of ecological modeling, and of which we are not aware of a root-modeling equivalent, is PEcAn ("**P**redictive **Ec**osystem **An**alyzer"; LeBauer et al., 2013), a meta-analytic data-assimilation pipeline built for ecosystem forecasting models that is intended to make it easy to assimilate all available data about an experimental site, species, or climate dataset, update it when new observations become available, and feed it to many models at once. If a similar platform existed for parameterizing and comparing RSA models, it would greatly reduce the effort needed to run existing models with new data and to evaluate the same scenario using multiple RSA models. Such multi-model comparisons could greatly aid benchmarking efforts (Schnepf et al., 2019) by showing divergence or convergence between predictions from models expected to be equivalent, and could also be used for scaling results up or down (to the extent that is valid for the available inputs) by running detailed and generalized models alongside each other.

Current challenges and future directions

Future RSA model development will likely be focused on the inclusion of more mechanisms and concepts. These will be multi-scale (from cell to crop), but also at the plant scale will include, among others, root-shoot coupling, rhizosphere processes, plasticity responses, and root sensing and signaling. A curiously ignored subject in this area is plant protection. This is probably because model development typically ignored interactions among organisms possibly because such interactions are still not understood very well. Despite this, there is a need for new concepts and their implementation. Although model complexity will continue increasing by introduction of new processes, the time and mental capacity of model developers will not, and the quality of the code bases must be tested and maintained. Fortunately the software industry has also developed and many tools are now available to ease the quality-assurance process. For example, every code change in

OpenSimRoot is tested using CI (continuous integration) functionality built into its GitLab repository. The number of tests, however, is limited and needs extending. Benchmarking is one way of testing that the code basis can achieve sufficient accuracy but this has so far not been widely attempted, The first benchmarks for RSA models have been described (Schnepf et al., 2019) but benchmarking requires that models are to some extent made comparable. Currently, the variation in algorithms used and the assumptions made are large and documentation and unification will be themes in the years to come. Besides benchmarking, validation of the predictions is necessary. Although good agreement has been achieved between the utility of traits simulated and experimental genotypic contrast studies, more detailed validation is lacking.

Lack of validation raises questions about the usability of the models for non-specialists, but the number of researchers that would like to test a hypothesis in silico is increasing. Nevertheless, the current software has steep learning curves. GUI development, better documentation, and adopting modern development practices may help.

Conclusions

In the last decade, RSA models moved from close-sourced, single-user or lab developments to open-source community-driven development. This was necessary as the models have incorporated much more complex processes. RSA models have proven to be of relevance to many functional questions in plant nutrition and plant phenotyping. They have become useful tools for testing the functional benefits of RSA traits for nutrient and water acquisition. However, many challenges remain. Conceptually, the models do not represent the rhizosphere very well and the biological interactions with soil microbes are poorly represented if at all. Furthermore, validation of the models is still scattered, and benchmarking of model components, to arrive at an agreed level of quality is needed.

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Tables and Figures

Tables

Table 1: List of cited models.

Model software	Citation
ArchiSimple	Pagès et al. (2014)
CRootBox	Schnepf et al. (2018b)
DigR	Barczi et al. (2018)
GroImp	Henke et al. (2014)
OpenSimRoot	Postma et al. (2017)
RSWMS	Javaux et al. (2008)
RootBox	Leitner et al. (2010)
SimRoot	Postma and Lynch (2011b)
SPACSYS	Wu et al. (2007)

Figure legends

Figure 1: Rendering of a simulated bean and maize root system with indication of various root traits. Simulations were run with OpenSimRoot and rendering was done with Paraview. Figure was reproduced with permission from Postma et al. (2017).

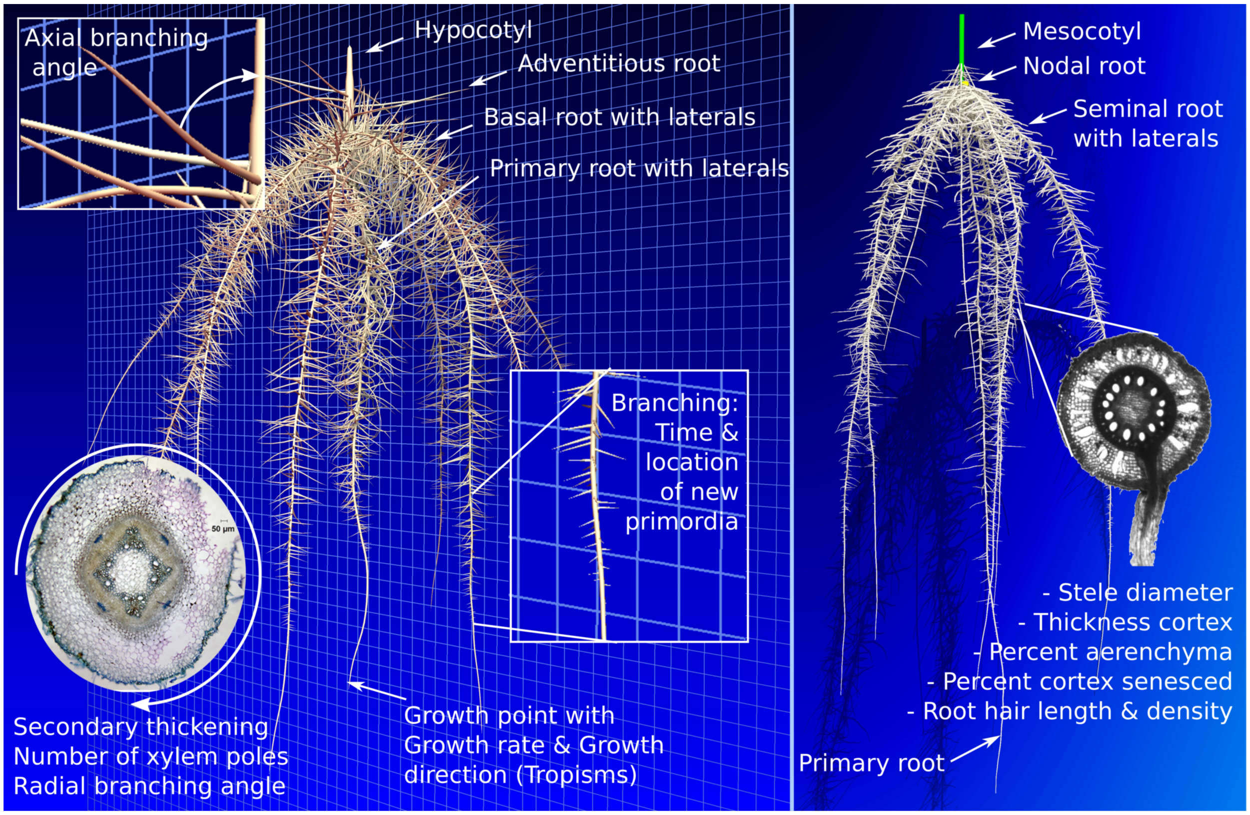
Figure 2: Simulated shoot biomass of 40 day old bean plants as a function of basal root whorl number (BRWN), number of hypocotyl born roots (HBR), basal root angles type (deep, fanned, shallow) and nutrient availability (low P, low N, low N+P, high N+P). Figure reproduced with permission from Rangarajan, Postma, and Lynch (2018).

Figure 3: Simulated shoot biomass of maize as a function of Imax (x-axis), nodal root number (NRN), and two soil types (sand and clay). Image printed with permission from L.York. For full study see York, Silberbush, and Lynch (2016).

Figure 4: Simulation of barley growing at a high planting density. Roots were simulated with OpenSimRoot and rendered with Paraview. A Roots with pseudo colors indicating different root types in order of diameter laterals (blue), seminals (yellow), nodals (green), mesocotyl (red). B Simulation of nitrate depletion by a high planting density of barley. For pseudo colors see legend.

Figure 5: Conceptual diagrams illustrating "loose" vs "tight" coupling between model components. Shown are two possible implementations of a hypothetical model calculating the elongation of a single root based on assimilate supply, genetic potential, and carbon partitioning factors. Each box represents a group of related calculations or values (which would likely be implemented as a class), and arrows indicate information lookup (e.g. read x -> y as "x uses y"). Top panel: Tightly coupled design. Each calculation requires detailed knowledge of the internal details of other modules. Bottom panel: Loosely coupled design. Modules share information through standardized interfaces "Potential Growth", "Stress Response", and "Carbon Available", thus isolating the growth rate calculation from the details of e.g. where and how parameters are stored or whether the potential growth rate of the current root is limited more by developmental factors or by root type parameters. Note that both implementations ultimately perform the same set of calculations; thoughtful code design can improve maintainability and interoperability even within a set mathematical framework.

Figure 6: Screenshot of Shiny web app for generating root system architectures with CRootBox (https://plantmodelling.shinyapps.io/shinyRootBox/).



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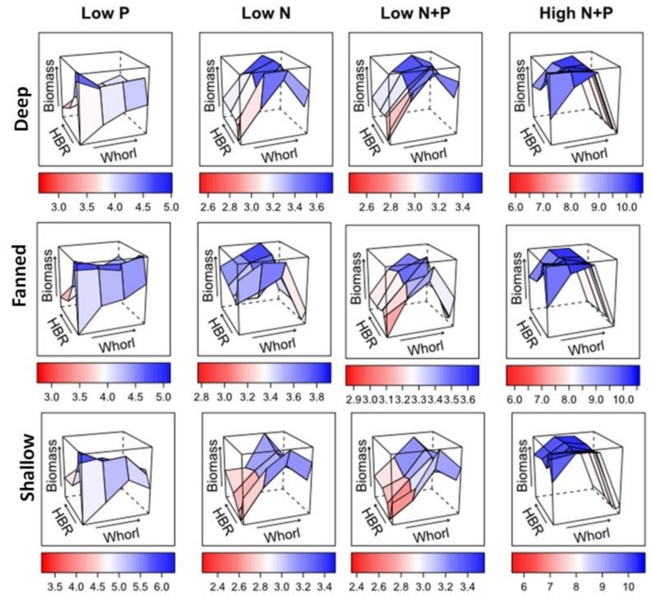

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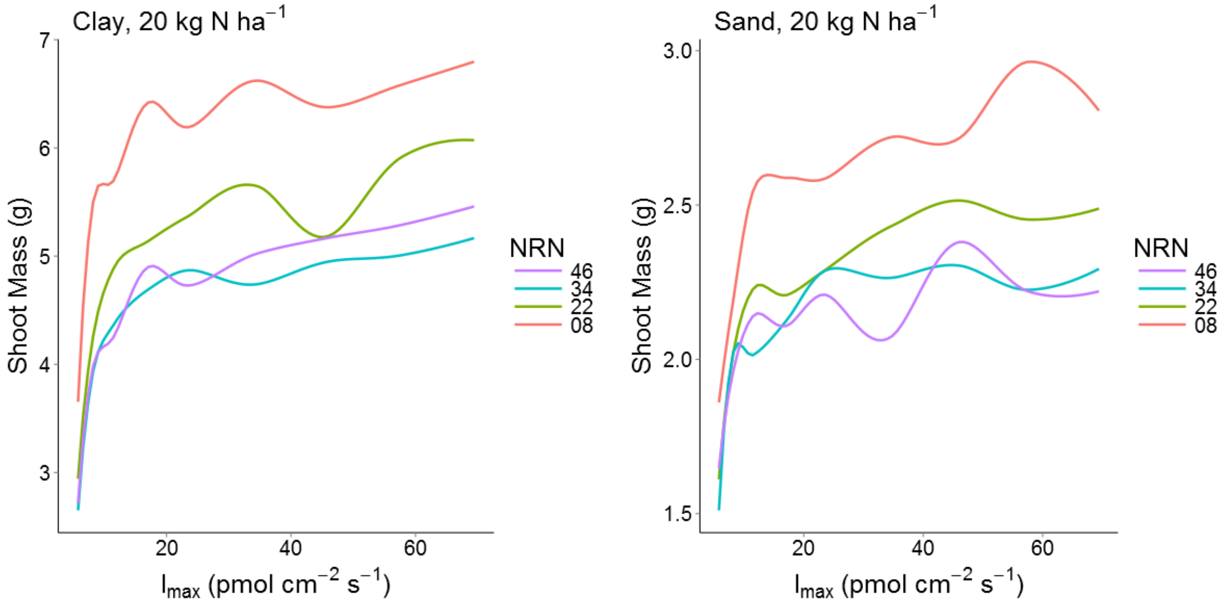

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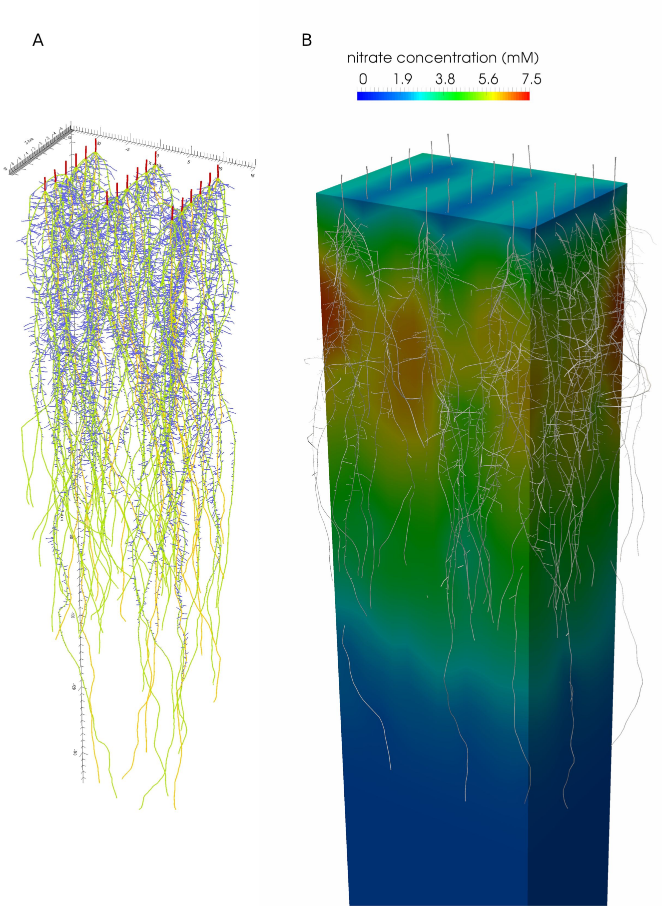

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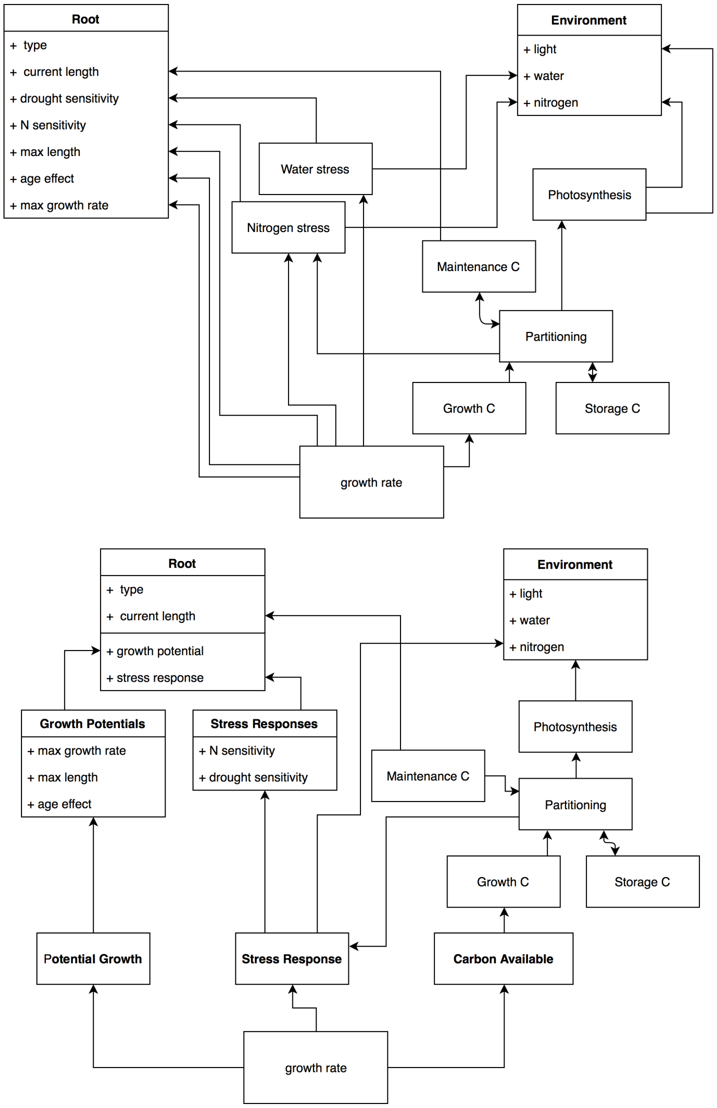

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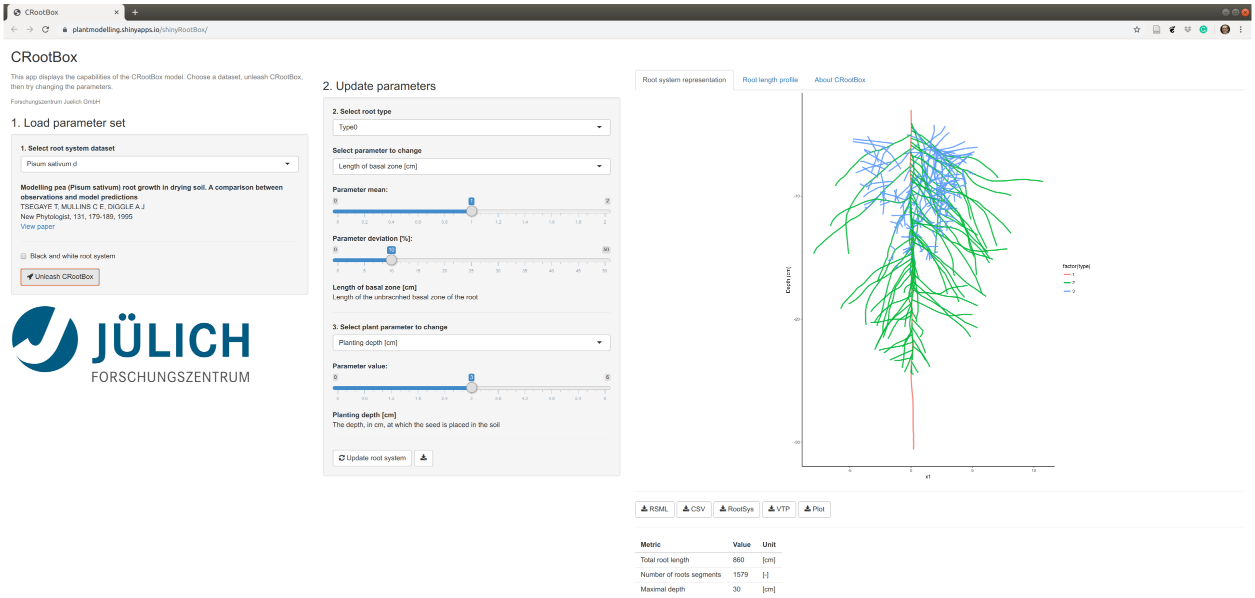

CRootBox

This app displays the capabilities of the CRootBox model. Choose a dataset, unleash CRootBox, then try changing the parameters.

Forschungszentrum Juelich GmbH

1. Load parameter set

1. Select root system dataset

Pisum sativum d

Modelling pea (Pisum sativum) root growth in drying soil. A comparison between observations and model predictions
TSEGAYE T, MULLINS C E, DIGGLE A J
New Phytologist, 131, 179-189, 1995
View paper

☐ Black and white root system

Unleash CRootBox

2. Update parameters

2. Select root type

Type0

Select parameter to change

Length of basal zone [cm]

Parameter mean: 1 (0–2)

Parameter deviation [%]: 10 (0–50)

Length of basal zone [cm]
Length of the unbracnhed basal zone of the root

3. Select plant parameter to change

Planting depth [cm]

Parameter value: 3 (0–6)

Planting depth [cm]
The depth, in cm, at which the seed is placed in the soil

Update root system

Metric	Value	Unit
Total root length	860	[cm]
Number of roots segments	1579	[-]
Maximal depth	30	[cm]

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