



Root2Res

Root phenotyping and genetic improvement for rotational crops resilient to environmental change

D6.2: updated version of OpenSimRoot

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OpenSimRoot is a root architectural model used for root trait utility exploration and ideotype development. A new version was released as part of the Root2Res modelling toolbox.

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1. Introduction

OpenSimRoot is a code for simulating functional structural root and plant models. It simulates plant structure (root architecture) in a given environment. The acquisition of necessary resources, C, N, P, K, H₂O and their utilization are simulated. The root and shoot growth respond to the availability of all these resources aiming at achieving a functional balance, optimal for growth.

Through templates, described in .xml, different models can be constructed. Thus, the user sets what processes are simulated with what module. This enables both backward compatibilities as well as flexibility for simulating different plant species and scenarios.

Input files describe parameterization using .xml formatting and including meta data like names and units, which are thoroughly checked, to avoid errors. Default parameterizations are available for different plant species and genotypes.

OpenSimRoot is an open-source version of SimRoot, originally developed in the Lynch Lab at Pennsylvania State University during the early 1990's and first published in 1997 as a purely structural model (Lynch et al. 1997). A major update was released in 2011, which included the carbon and nutrient models (Postma and Lynch 2011a,b). The code base was much improved and extended in a 2017 release (Postma et al. 2017). Now, in 2025, in the context of the Root2Res project (<https://root2res.eu/>), there is a new release, with many further improvements.

These improvements notably supported the development of models for **new crop species**, root **plasticity** responses to soil conditions such as local soil drying, proliferation in nutrient patches, and soil compaction. The new code represents the **rhizosphere processes** better, couples those to the larger scale water flows thus enabling interactive effects of water and phosphorus. We enabled the possibility to add Python-based plugins that allow the exploration of metabolic flux balance models coupled to OpenSimRoot.

We extensively tested the code, comparing runs to the previous release and benchmarking against known scenarios (Schnepf et al. 2023).

2. Summary of publications

OpenSimRoot is modular and open-source, which enables it to be used in many different projects. This has led to numerous publications in international journals, and simulation results were part of at least three PhD theses.

Publications involved **parameterization of new crop species** such as rice (Gonzalez, Postma, and Wissuwa 2021; Ajmera et al. 2022), cassava (Punyasu et al. 2025), pearl millet (Ndoye et al. 2024), and barley (Schneider et al. 2017; Schäfer et al. 2022).

Parameterization for wheat, sweet potato, faba bean, and *Arabidopsis thaliana* are under construction and are expected to be published shortly.

Root architecture is plastic, and the benefits and drawbacks of observed changes in root architecture related to nutrients, water, and soil compaction were explored (Strock et al. 2022; Griffiths et al. 2022; Schäfer et al. 2022; Schneider et al. 2022). Multiple quantitative traits may have synergistic functions, such that the benefit of one quantitative trait depends on the value of another. This was illustrated in the exploration of integrated phenotypes and multiple trait sensitivity analysis.

Domestication and, in recent times, modern breeding have significantly modified the crop phenotype, with selection primarily focusing on aboveground traits. Retrospective studies of older cultivars show changes in root architecture, and OpenSimRoot was used to understand some of these changes and how they might relate to the agronomic growth environment (Lopez-Valdivia et al. 2025; Rangarajan and Lynch 2024; Perkins and Lynch 2021).

Several papers were published on **the endo-rhizosphere, the root cortex**. Using cost-benefit analysis, several root anatomical traits were explored, including cell number, size, and senescence (Lopez-Valdivia, Yang, and Lynch 2023; Sidhu et al. 2024; Sidhu et al. 2023; Strock, Morrow de la Riva, and Lynch 2018; Schneider et al. 2017). These papers share a strong focus on metabolic costs and the importance of these metabolic costs during drought stress, when stomata close, was simulated using a new photosynthesis module based on the Farquhar-von Caemmerer-Berry models (Schäfer et al. 2022).

Phenotyping roots in the field is still challenging. OpenSimRoot was used to develop methods for field phenotyping. Using virtual coring, a 'best-practice' coring scheme for maize plantings was worked out (Burridge et al. 2020). Using the 3D root architecture renderings, new image segmentation methods were developed for images of cassava root crowns (Wilhelm et al. 2022). Last, pipelines were developed to model root architectures imaged by MRI and CT (Griffiths et al. 2022).

OpenSimRoot is an advanced simulation platform with a very flexible input file format, which allows the user to define many different models. This flexibility comes with a price of complexity and a steep learning curve. We keep a wiki with instructions, and a more detailed and systematic manual was published (Schäfer et al. 2022).

3. Code management

We maintain OpenSimRoot on a GitLab repository, making use of the issue board, version control, and continuous integration, which runs several tests automatically.

In agreement with the data management plant of Root2Res, the repository is open-access with open-source licensed code (GPLv3). It contains the required metadata, input files, and environmental data to run the model. Users typically fork the main repository

for their purposes and file merge-requests so that these changes can, after review, flow back into the main repository. Since not all changes passed review or were requested to be merged, some publications are based on code not found in the main repository. There are currently 26 direct forks listed.

4. Major changes in OpenSimRoot since last release in 2017

4.1. Code changes

Number of lines increased from 42 to 52 K lines (not counting the 38 K line math parser).

Many minor bugs fixed, small code improvements and improvements in the numerical solving to simulate more challenging scenarios with improved mass balances and accuracy. Many messages have been added to inform users about events in the current simulation.

4.2. Build system

- Compilation simplified with a single make file for linux, windows, and mac.
- New make file with different build options included, with or without Python support, with or without writing of dependency graphs.
- Updated to the 2023 C++ standard.

4.3. Command line interface

- Option to write warnings directly to screen, and not just at the end of the simulation.
- Build and git version info in output.

4.4. Reading of input files

- Option to define mathematical equations in input files, so that not all modules need to be written as C++ class.
- Option to use a python script as a module.

4.5. Writing of output

- Writing of dependency graphs. The model will write a graph illustrating the simulated dependencies among state variables.
- Writing of RSML output format. RSML is a new standard for writing root architectural data.
- Writing of tables with statistics on root data.

4.6. Engine

The time step logic was updated with more controls, and stricter global rules and less reliance on interpolation.

4.7. Modules

4.7.1. water

- Stomatal Conductance module added.
- Benchmarking of infiltration, root water uptake, and evaporation
- Standardization of water retention curve
- Stability of the solution so we can simulate much drier scenarios.
- Drought response functions developed

4.7.2. nutrients

- Phosphorus model coupled to water code
- New numeric implementation
- Provisions for repeated fertilizer applications

4.7.3. carbon

- Seedsize bug fixed. The ambiguous use of Seedsize is removed in favor of Seedmass, and the use of Seedmass is made consistent across modules.
- StemRespiration bug fixed. StemRespiration had a reference to leaf rather than stem mass.
- Added optional extra carbon sink/source which is the starch in a storage organ. Code was necessary for cassava and sweet potato simulations.
- Unified use of light in photosynthesis and transpiration modules with auto conversion between molar and energy units.
- Farquhar photosynthesis model was implemented as alternative photosynthesis model.
- Gas exchange model for CO₂ and O₂ added.
- Metabolic-flux balance model of photosynthesis coupled over python interface.
- Alternative handling of carbon allocation, using stress factors.

4.7.4. root architecture

- OSR scales the root diameter relative to the variation in longitudinal growth rates, but this failed due to a wrong reference. This bug fix has some effects on the overall results when distributions are log-normal, causing the average root diameter to be slightly smaller.
- Root plasticity responses were generalized.
- A root growth Impedance model was added simulating root plasticity to, water dependent, soil strength.

4.7.5. shoot

- Crop height added.
- Simulation of leaf temperature added.

4.8. Backward compatibility

Old input files run, with minor changes which are signaled by the code and are on purpose not backward compatible as they involve ambiguous interpretation (e.g. seedsize which now needs to be declared as seed mass). There are a couple of bug fixes that change the results somewhat. Backporting these bugfixes resulted in the same results between the backport and the current version. To our knowledge, the bugfixes had no significant influence on the interpretation of the published studies.

5. Conclusions

Changes made to OpenSimRoot have resulted in gained functionality, precision, and scope. It proved useful in many root studies and is ideally positioned to explore root ideotypes. Code can be downloaded here:

<https://gitlab.com/rootmodels/OpenSimRoot>

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