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An algorithm for the simulation of the growth of root systems on deformable domains

Lionel Xavier Dupuy [a,*], Matthieu Vignes [b]

[a] The James Hutton Institute, Invergowrie, Dundee DD2 5DA, Scotland
[b] UR875 UBIA, INRA, 31326 Castanet-Tolosan Cedex, France

HIGHLIGHTS

- ► We model the growth of root systems using density functions on deformable domains.
- ► Growth is modelled using PDE and root trajectories are used to deform the domain.
- ► We showed root domains can be predicted using developmentally meaningful parameters.
- ► Deformable domains are computationally efficient and can be used in population models.

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ABSTRACT

Models of root systems are essential tools to understand how crops access and use soil resources during their development. However, scaling up such models to field scale remains a great challenge.

In this paper, we detail a new approach to compute the growth of root systems based on density distribution functions. Growth was modelled as the dynamics of root apical meristems, using Partial Differential Equations. Trajectories of root apical meristems were used to deform root domains, the bounded support of root density functions, and update density distributions at each time increment of the simulation.

Our results demonstrate that it is possible to predict the growth of root domains, by including developmentally meaningful parameters such as root elongation rate, gravitropic rate and branching rate. Models of this type are computationally more efficient than state-of-the-art finite volume methods. At a given prediction accuracy, computational time is over 10 times quicker; it allowed deformable models to be used to simulate ensembles of interacting plants. Application to root competition in crop–weed systems is demonstrated.

The models presented in this study indicate that similar approaches could be developed to model shoot or whole plant processes with potential applications in crop and ecological modelling.

1. Introduction

Plant architectures are involved in key biological and environmental processes (Fourcaud et al., 2008). Root architectures in particular are optimised to capture and assimilate large amounts of water and mineral elements from the soil, thereby contributing to crop yield and effective food production (Lynch, 2007). Root architectures also protect soils against erosion and other forms of land degradation (Stokes et al., 2009). Due to their inherent multifunctional nature, root architectures are difficult to understand intuitively. Thus, models are of utmost importance to analyse the complexity of root architectures and their functions.

Root architectures result from the organised expansion of a multitude of apical meristems (root tips), which develop in a series of elongation and initiation events. Current models use computer simulations to mimic these processes. The geometry of roots and their arrangement within the root system are assembled iteratively from a set of virtual apical meristems, whose activities are simulated independently from each other (Pagès et al., 2004; Wu et al., 2007; Lucas et al., 2011). Root architectural models can, in turn, be used to make predictions on water and nutrient uptake by coupling growth to physical models (Ge et al., 2000; Doussan et al., 2006; Zhang et al., 2007; Wiegers et al., 2009).

Unfortunately, for root architectural models it has proved to be difficult to define their parameters and assign them values (Tsegaye et al., 1995). They also require sophisticated algorithms, in order to be coupled to soil models (Draye et al., 2010; Leitner et al., 2010). Simplified approaches, such as root density models, could be used to overcome these shortcomings. Density-based models aggregate root properties into root distribution functions. Changes with time of density distribution functions can then be modelled empirically, for example using sliding exponential

* Corresponding author. Tel.: +44 1382 568521; fax: +44 8449 285429.
E-mail address: lionel.dupuy@hutton.ac.uk (L.X. Dupuy).

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profiles (Gerwitz and Page, 1974; King et al., 2003) or mechanistically using partial differential (Acock and Pachepsky, 1996; Bastian et al., 2008). In the latter case, analytical methods can provide simple growth functions (de Willigen et al., 2002; Schnepf et al., 2008). Approximated numerical solutions can also be obtained to analyse more complex systems (Reddy and Pachepsky, 2001). However, density-based models were seldom used to model ensembles of interacting plants. One remaining challenge is to limit the number of unknowns in numerical simulations, so that solutions can be obtained by standard desktop computers.

This paper presents a density-based approach to model ensembles of root systems in the field. The root system is defined as a deformable domain and density distribution functions are used to model the distribution of roots within this domain. We expanded the system of differential equations introduced in a previous work (Dupuy et al., 2010), which proposed an Eulerian solver, and developed a Lagrangian approach to solve equations on 3D deformable grids. The performance of our solver was compared to results obtained in a two-dimensional setting, where the conservation equation could be solved analytically. Finally, a simple case of crop–weed competition was studied to illustrate applications to field-based crop processes.

2. Materials and methods

2.1. A density-based framework to model root systems dynamics

In this paper, the dynamic structure of the root system is represented as a combination of density distribution functions, following the principles proposed in a previous work (Dupuy et al., 2010). First, root tip density (ρ_a) indicates regions where growth occurs. Secondly, root length density (ρ_l) is defined as the total root length per unit soil volume. Root length density is required, for example, to predict water and nutrient uptake from the soil (King et al., 2003). Finally, branching density (ρ_b), defined as the number of connections per unit soil volume, models the topology of root connections. Root density distribution functions are defined on domains that include both: (i) spatial coordinates (x,y,z) of roots in soil (Fig. 1A) and (ii) their direction of growth (Fig. 1B), which is defined in a local spherical coordinate system, more specifically gravitropic angle α and plagiotropic angle β (see Fig. 1). A root and its growth direction are therefore characterised by a point $\mathbf{m}$ in a 5-dimensional space $\mathbf{m}=(x,y,z,\alpha,\beta)\in E,\ E\subset\mathbb{R}^5$ (Fig. 1C). In this setting, a root density distribution function is a mapping $\rho : E\mapsto\mathbb{R}$ such that $\int_\Omega\int_V \rho dV\, d\Omega$ represents the total quantity of roots contained in volume V and whose growth direction

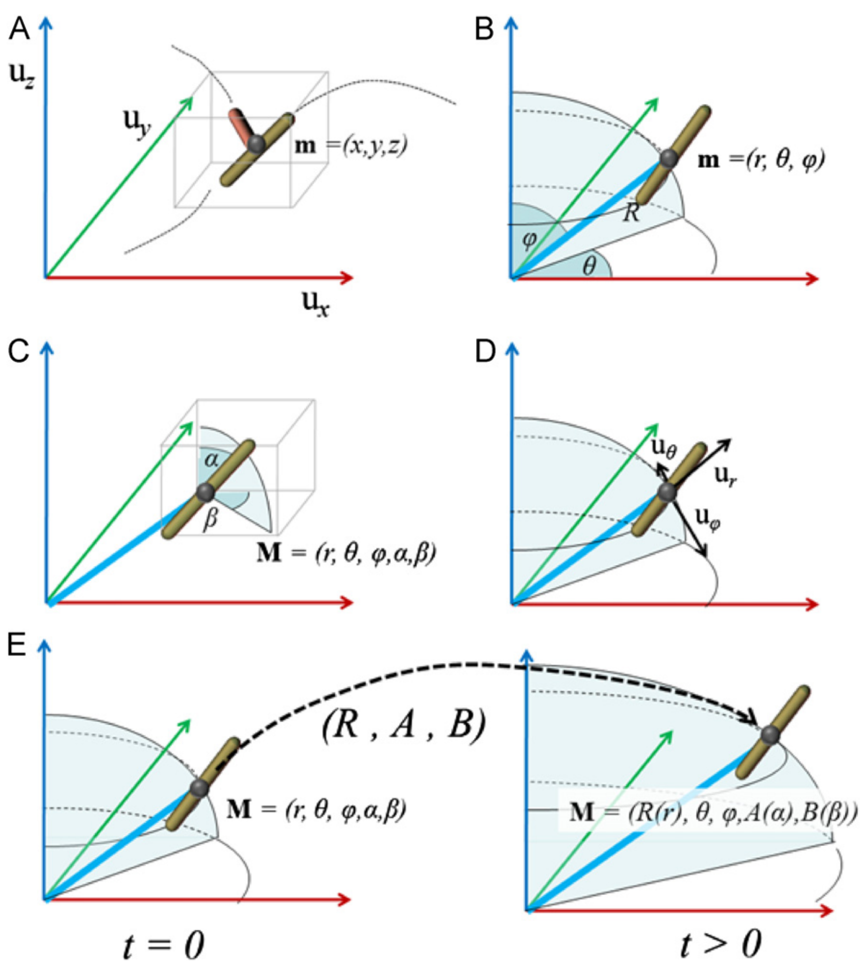

Fig. 1. Describing root systems with density distribution functions. (A) Root systems are characterised locally at point $\mathbf{M}=(x,y,z)$, by root densities (*e.g.* number of root tips or total length of root per unit volume, here depicted by brown cylinders). (B) Root coordinates can also be expressed in a spherical coordinate system, so that the position of roots $\mathbf{M}$ is defined by a radius and azimuth and zenith angles: $\mathbf{M}=(r,\theta,\varphi)$. (C) Root orientation must complement root position, so that the expansion of the root system can be predicted. The coordinate system is therefore expanded to record the direction of roots. Root direction in the spherical coordinate system is defined by inclination and azimuth angles (α,β). (D) A spherical coordinate system defines a local basis $(\mathbf{u_r},\mathbf{u_\theta},\mathbf{u_\varphi})$, and hence allows the modelling of deformations of the root domain. (E) In a Lagrangian setting, material coordinates of a reference state is defined at $t=0$, so that $\mathbf{M}=(r,\theta,\varphi,\alpha,\beta)$. The deformed state, which results from the growth of the root system, is then expressed as a function of the reference state $\mathbf{M}=(R(r),\theta,\varphi,A(\alpha),B(\beta))$. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)