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MuSCA: a multi-scale source-sink carbon allocation model to explore carbon allocation in plants. An application on static apple-tree structures.

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Running title: MuSCA multi-scale carbon allocation model

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1 ABSTRACT

2 **Background and aims**

3 Carbon allocation in plants is usually represented at a topological scale, specific to each model.
4 This makes the results obtained by different models, and the impact of their scales of
5 representation, difficult to compare. In this study, we developed a Multi Scale Carbon
6 Allocation model (MuSCA) that allows using different, user-defined, topological scales
7 of a plant, and assessing the impact of each spatial scale on simulated results and
8 computation time.

9 **Methods**

10 Model multi-scale consistency and behavior were tested on three realistic apple tree structures.
11 Carbon allocation was computed at five scales, spanning from the metamer (the finest
12 scale, used as a reference) up to 1st order branches, and for different values of a sap
13 friction coefficient. Fruit dry mass increments were compared across spatial scales and
14 with field data.

15 **Key Results**

16 The model was able to represent effects of competition for carbon assimilates on fruit growth.
17 Intermediate friction parameter values provided results that best fitted field data. Fruit
18 growth simulated at the metamer scale differed from about 1% at growth unit scale up
19 to 60% at first order branch and fruiting unit scales. Generally, the coarser the spatial
20 scale the more predicted fruit growth diverged from the reference. Coherence in fruit
21 growth across scales was also differentially impacted, depending on the tree structure
22 considered. Decreasing the topological resolution reduced computation time by up to
23 four orders of magnitude.

24 **Conclusions**

25 MuSCA revealed that the topological scale has a major influence on the simulation of carbon
26 allocation. This suggests that the scale should be a factor which is carefully evaluated
27 when using a carbon allocation model, or when comparing results produced by different
28 models. Finally, with MuSCA, trades-off between computation time and prediction
29 accuracy can be evaluated by changing topological scales.

30 **Keywords:** MuSCA, multi scale, carbon allocation, plant growth, tree growth, functional-structural
31 plant modeling, FSPM, multiscale tree graph, source, sink, apple, plant architecture

1 INTRODUCTION

2 Carbon allocation is the process by which carbon assimilated by leaves, or stored in the form
3 of carbohydrates, is transferred, via the conductive vessels (or phloem tissue) to other plant parts,
4 where it is used primarily for respiration and growth. It is generally accepted that the phloem sap
5 moves as a consequence of osmotically generated pressure gradient, as described by the Münch
6 theory (Münch 1930). Gradients are generated by the differences in the concentrations of carbon
7 (C) assimilates between C-sources (mainly leaves, where C-assimilates are loaded into the phloem)
8 and sinks (where C-assimilates are unloaded from the phloem). The Münch theory has been refined
9 over time (e.g. with the introduction of the leakage-retrieval mechanism (Thorpe *et al.* 2005) and
10 complementary hypotheses have been proposed to explain the lack of fit with experimental
11 evidences (e.g. sieve tubes decomposed in shorter, overlapping components, at the edge of which
12 solutes are transported at the expense of internal energy) (De Schepper *et al.* 2013). The underlying
13 principles, however, are still considered as valid. As such, the C-allocation process is thought to
14 depend primarily on the amount and distribution of the available C-supplies, on demands along the
15 plant structure and on the possibility of C-supplies to flow via the phloem (Ryan and Asao 2014). In
16 models of small plants, however, the simplifying assumption that distance has no effect on C-
17 availability or phloem osmotic potential (known as the ‘common assimilate pool’) can be made
18 (Heuvelink 1995; Guo *et al.* 2006; Luquet *et al.* 2006; De Swaef *et al.* 2003).

19 When plant topology increases in complexity, the modeling approaches to C-allocation
20 present in the literature can be organized in four, partly overlapping, categories (Thornley and
21 Johnson 1990; Lacoïnte 2000; Le Roux *et al.* 2001; Génard *et al.* 2008): models based on empirical
22 relationships between plant parts and/or the environment; teleonomic models representing the plant
23 as moving towards an a priori defined specific state; source–sink driven models, in which different
24 plant components are supposed to attract C-assimilates with different strengths and lastly transport
25 resistance and biochemical models, which represent phloem transport as starting from osmotic
26 gradients and biochemical conversions. The most mechanistic models, which represent osmotic
27 flows as starting from osmotic gradients, imply complex formalizations and highly detailed plant
28 descriptions and therefore received relatively limited attention (Bancal 2002). The modest
29 mathematical complexity of source sink models has led to them becoming the focus of a much
30 larger number of studies. In all cases the representation of C-allocation on large tree structures
31 described at high resolution remains computationally intractable (Balandier *et al.* 2000; Bancal
32 2002).

33 Each model represents the plant structures, and the process of carbon allocation, at a specific
34 scale. The choice of scale may be driven by management or research needs, by the computation

1 time needed for the simulations and by the resolution at which the calibration and testing data was
2 obtained. Such scales range from the individual metamer (M) (Allen *et al.* 2005) to collections of
3 metamers that, grouped according to criteria such as their age, position or organ type (Kang *et al.*
4 2008), constitute larger portions of a tree structure, such as branches, main axis or even whole plant
5 compartments (Lakso and Johnson 1990; Kang *et al.* 2008).

6 By way of example, the L-PEACH model (Grossman and DeJong 1994; Allen *et al.* 2005) is
7 a reference for completeness of the described processes and represents tree growth over multiple
8 years. This uses a transport resistance analogy to mimic C-transport at the M scale (internode, leaf,
9 fruit). The SIMWAL model represents the growth of a young walnut tree across several years. This
10 is organized in axes, which are divided into growth units (GU, the scale of C-allocation),
11 themselves composed of internodes and nodes (Balandier *et al.* 2000). A GU is an organisation
12 level typical of plants with rhythmic growth. It corresponds to a portion of axis developed without
13 interruption during an elongation period, and can be visually identified as bounded by two zones of
14 scales that had protected the apical meristem in the bud during resting period. The QualiTree model
15 represents growth and quality of fruits on a peach tree structure, at the fruiting unit (FU) scale,
16 during a single growth season (Lescourret *et al.* 2011, Pallas *et al.* 2016). A FU includes the set of
17 shoots born from a common section of one year old wood. In this model all the different types of
18 organs in a FU are considered similar with respect to assimilates exchange, which depends on their
19 respective distances only.

20 The computation of C-allocation by a model is affected by both the formalism used to
21 describe the physiological processes and the discretization of the plant. Because of this, identifying
22 what causes differences in results produced by different models can be difficult.

23 The present work proposes a new, source-sink, **Multi-Scale Carbon Allocation** model
24 (named MuSCA), whose aim is to allow for a flexible definition of topological plant scales
25 concomitant with the simulation of carbon allocation. The model relies on the use of Multi-scale
26 Tree Graph (MTG) (Godin and Caraglio 1998), a formalism inspired by the observation of the
27 multi-scale organization of plant structures (Barthélémy 1991; Barthélémy and Caraglio 2007;
28 Balduzzi *et al.* 2017). MTG allows for the topological description of a plant at multiple, nested,
29 spatial scales on the same graph. In addition to the connections and boundaries of the described
30 topological scales, intensive (e.g. organ type) or extensive (e.g. geometrical features) properties can
31 be assigned to the individual plant component at any scale. MTG has been previously used in plant
32 architecture analyses (Costes *et al.* 2003), in radiation interception (Da Silva, Han, and Costes
33 2014), as well as to simulate physiological processes (Fournier *et al.* 2010; Ndour *et al.* 2017;

1 Barillot *et al.* 2018) or model plant-pathosystems (Garin *et al.* 2014, 2018; Robert *et al.* 2018)
2 (albeit by using a single scale at a time).

3 In this paper, we provide an overview of the MuSCA model, define its scope and inputs,
4 present the formalisms used to compute C-allocation and to move across scales. The model is
5 calibrated for the apple tree (*Malus x domestica Borkh.*), Fuji cultivar, for C-demands. It is linked to
6 a radiative model for the estimation of C-assimilates by leaves. The model is then applied on three
7 contrasted apple tree structures and for different values of an empirical sap friction parameter, and
8 the effects of competition for C-assimilates on fruit growth are analyzed. Field observations are
9 then compared to the fruit growth distribution simulated on one tree structure to retain the sap
10 friction parameter values that might best represent sap flow dynamics. The ability of the multi-scale
11 formalism to produce similar results across scales and the influence of the scale of representation on
12 the simulated carbon allocation are analysed. Finally, the trade-off between computational
13 efficiency and accuracy are discussed, also in respect to the possible interactions between specific
14 tree structure and the topological scale used.

15 MATERIALS AND METHODS

16 Model Description

17 *Overview*

18 MuSCA is a generic, functional structural plant model (FSPM) (Vos *et al.* 2010)
19 representing the carbon allocation and organ growth of a plant at different, user-defined, spatial
20 scales, while taking into account competition and distances between carbon sinks and supplies
21 present on the plant (Fig.1). The model has a modular architecture and each module is generalized
22 so that only a few of them are specific to a given cultivar or species (Table 1, Table 2). The model
23 is integrated in the open-source OpenAlea environment (Pradal *et al.* 2008, 2015) and implemented
24 in the Python language. The model reuses existing OpenAlea components, such as the MTG
25 dynamic data-structure (Godin and Caraglio 1998; <https://github.com/openalea/mtg>), used to
26 represent the multiscale topology of plant structures, the PlantGL library (Pradal *et al.* 2009) used to
27 represent the 3D geometry, and the RATP radiative model (Sinoquet *et al.* 2001). The MuSCA
28 model simulates biomass accumulation over a single vegetative season.

29 *Input plant structures and creation of new scales*

1 The input plant structures of MuSCA are MTGs where individual plant components are
 2 characterized by qualitative or quantitative information. Qualitative information refers to the organ
 3 type or the type of connection between vertex and parent (i.e. branching or succession).
 4 Quantitative information may include parameters such as the geometry or age of a plant component.
 5 This information can be used to create criteria defining the membership of individual plant
 6 components to larger groups of adjacent plant components.

7 *Movement of carbon*

8 The movement of the available carbon (F_{ij}), from a C-supply (i) to a C-sink (j), is
 9 represented as a function of the C-available in the supply (ACP_i), the sink C-demand ($Demand_j$) (eq.
 10 1a), and is inversely related to the distance ($dist$) between source and sink and to a sap friction
 11 parameter (h) (eq. 1b), along the plant topology. The h factor is an empirical friction parameter,
 12 proposed in previous source-sink carbon allocation models (Balandier *et al.* 2000; Lescourret *et al.*
 13 2011). Larger values of this parameter amplify the effects of distance resulting in relatively large
 14 amounts of C allocated next to the source, while a value of zero implies no effect of distance. This
 15 equation is inspired by a previously defined equation (SIMWAL model, Balandier *et al.* 2000).

$$17 F_{ij} = \frac{Demand_j * f(dist_{ij}, h) * ACP_i}{\sum_{k=1}^n Demand_k * f(dist_{ik}, h)} \quad (\text{eq. 1a})$$

$$18 f(dist_{ij}, h) = \frac{1}{(1 + dist_{ik})^h} \quad (\text{eq. 1b})$$

19
 20 If in excess, the C-allocated to a plant component will just fulfill its C-demand, while the
 21 excess will be stored in a reserve pool for this compartment and be considered as a supply provided
 22 by that component on the following time-step (Balandier *et al.* 2000). However, since simulations
 23 in this study lasted for only one day, this phenomena never occurred.

24 The carbon allocated to a topological element is eventually divided among the different
 25 organs that constitute it (at the metamer scale: fruit, leaf, internode), proportionally to their
 26 individual carbon demand.

27 *Calculation of distances*

28 A representation of the C-allocation process coherent at multiple topological scales requires
 29 the definition of an equation for the calculation of distances, independent of the scale of
 30 representation.

1 Modeling C-allocation is computationally demanding as, in a source-sink formulation, it
 2 requires to compute the distance between all pairs of carbon sinks and sources in the tree. In a
 3 MTG, sources and sinks are represented by vertices in a tree graph. The complexity of computing
 4 the distance between all pairs is quadratic, i.e. requires around n^2 operations, for a tree of n
 5 vertices. We thus designed an algorithm, based on the multi-scale organization of plants, which
 6 allows to reduce the number of operations by reducing the number of independent plant vertices
 7 that must be compared.

8 Each MTG vertex (i) is characterized, among other properties, by three dimensional
 9 coordinates (basal and top), the possibility to have a parent (named $i-1$), and one or multiple sons
 10 (the vertex i is the son of its parent). In a MTG, a vertex at a coarser scale (I , called complex) is
 11 composed of one or more vertices at the finer scale (called components of I), as in the case of a
 12 shoot composed of several internodes.

13 The distance ($dist_{i,j}$) among two vertices (i, j) in a MTG depends on the sequence of vertices
 14 that connect i and j (called topological path). It corresponds to the sum of i) the semi-lengths of the
 15 extremities i and j , and ii) the length of the topological path between the bases of i and j (eq. 2a, 2b
 16 Fig.2). The semi-length of an element at different scales is computed as the distance between its
 17 base and barycenter.

18 In order to assess the length of this path, it is necessary to identify the Greatest Common
 19 Ancestor (GCA) of vertices i and j (Fig.2). Given the two paths connecting the tree root to i and j ,
 20 the Greatest Common Ancestor of vertex i and vertex j , $GCA(i,j)$, is identified as the vertex that is
 21 contained in both paths and that is the closest to i and j . The topological path between i and j is the
 22 union of the vertices between i and $GCA(i,j)$ and the path between j and $GCA(i,j)$ with $GCA(i,j)$
 23 (Fig.2). The length of the path ($dist_{i,j}$) is computed as the sum of the length of each of its internal
 24 elements plus the semi-lengths of its extremities, minus twice the length of the GCA (Fig.2, eq.2a).
 25 In addition, the distance between the basis of the first two elements of the path, that are directly
 26 inserted in the $GCA(i,j)$ and are not connected with each other, is added (eq.2a). This is the case at
 27 corser scale when different ramifications are connected to the trunk at different location. When the
 28 GCA is either i or j , the length is just the sum of the length of all its internal elements plus the semi-
 29 length of its extremities (eq.2b).

30

$$31 \quad dist_{i,j} = semilength_i + dist_{i,GCA} + dist_{j,GCA} + semilength_j - 2length(GCA) +$$

$$32 \quad dist(base_{son(CGA)i}, base_{son(CGA)j}) \quad (\text{eq. 2a})$$

33

34 where $son(GCA)i$ (resp. j) is the first descendant in the path($i, GCA(i,j)$) (resp. j).

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if GCA is i or j,

$$dist_{i,j} = dist_{i-1,j-1} + semilength_i + semilength_j \quad (\text{eq. 2b})$$

The calculation of the spatial coordinates of the basis and barycenters depends on the scale (Fig.2B). At M scale, the basal coordinates of a vertex correspond to the top coordinates of its *parent* vertex (eq. 3a). For the basal vertex of the MTG, the only without a parent, coordinates are stored in the complex of the same vertex. Barycenter coordinates are obtained as the mean of its top and base coordinates (eq. 3b).

At coarser scales, the basal coordinates of a vertex I are the basal coordinates of its first component at the metamer scale i.e. the one whose parent does not belong to I (eq. 3c). These basal coordinates are inherited from top coordinates of its parent (see eq. 3a).

Regarding the coordinates of the barycentre of a coarse scale vertex, these are calculated as the mean of the coordinates of the barycenters of its components, weighted by their individual lengths (as in eq. 3d for the x coordinate).

At metamer scale:

$$base_i = top_{parent(i)} \quad (\text{eq. 3a})$$

$$barycenter_{x,i} = \frac{top_{x,i} + base_x}{2} \quad (\text{eq. 3b})$$

At coarse scales:

$\forall i \in I \mid parent(i) \text{ not } \subseteq I:$

$$base_I = top_{parent(i)} \quad (\text{eq. 3c})$$

$$barycenter_{x,I} = \frac{\sum barycenter_{x,i} * length_i}{\sum length_i} \quad (\text{eq. 3d})$$

Up- and down- scaling

In MuSCA, some of the plant properties available at one scale are used to provide a description of the same properties at a coarser (up-scaling) or finer (down-scaling) scale. This is done in simulations running at coarse scales, prior and after the calculation of carbon flows, respectively by calling up- and down- scaling functions (except for the initial calculation of biomasses, see part From geometry to biomass). The up-scaling of properties such as biomass, carbon supplies and demands of plant parts is simply done by summing up the property values

1 stored in all the vertices that are contained within the topological boundaries of the coarser scale
2 component. Conversely, down-scaling the same properties from a coarse scale component to its
3 constituting elements requires some assumptions. In particular, when the carbon allocated to a
4 coarse scale component is down-scaled, it is assigned proportionally to the relative carbon demands
5 of its constituent elements.

6 Application to realistic tree structures: the case of apple (*Malus x domestica Borkh*)

7 In order to assess the ability of the model to simulate similar growths across multiple scales, to
8 represent competition for C-assimilates and the effect of the scale on computation time, we applied
9 MuSCA on different tree structures of apple trees, represented at multiple topological scales). These
10 were MTGs of three apple trees simulated by the MAppleT architectural model (Costes *et al.* 2008).
11 MAppleT combines markovian models for the simulation of growth unit succession and branching
12 with a biomechanical model for axis bending. Along growth units, individual leaf area was
13 simulated based on a logistic function and assuming different final values of leaf areas for the
14 preformed (7 leaves) and neoformed parts of the GU (Da Silva *et al.*, 2014a). This model was
15 previously calibrated on Fuji cultivar (Costes *et al.*, 2008) and so that it could be used to generate
16 one four year old ‘Fuji’ tree that was used in this study. Moreover, two other trees were simulated
17 by initiating simulations using two different sequences of lateral types along the trunk observed on
18 trees originated from a bi-parental population, as previously proposed by Da Silva *et al.* (2014b).
19 These two trees were selected within the population in order to test our C allocation model on trees
20 displaying contrasted architectures. Simulations were run for each individual tree on a single day, so
21 that the direct effect of changing the topological scale could be analyzed while excluding possible
22 retroactions and cumulative effects (such as the re-use of C delivered in excess to a plant
23 component). A partly cloudy day of late June (day of the year = 182) was chosen to drive
24 photosynthesis. This allowed on the one hand C-limiting conditions to occur (the use of very sunny
25 days resulted in C-allocation generally satisfying the whole fruit C-demand), and on the other hand
26 to represent trees in which shoot elongation, and thus the creation of new internodes, ended. Initial
27 fruit dry weight was set to be identical for all fruits and equal to 8 g (Reyes *et al.* 2016).

28 For the application of the carbon allocation model on tree structures, we developed a few
29 modules containing some species specific parameters and allometric relationships (Table 1, Table
30 2). These were needed, firstly to convert the geometric descriptions of the trees contained in the
31 MTGs into values of biomass (Supplementary Information: Input tree structures), and then to
32 estimate the values of carbon demands for dry matter accumulation (see Source and Sink strengths).

33 *Source and Sink strengths*

1 In MuSCA, the amount of C-assimilates available from photosynthesis in individual leaves
2 is estimated with a radiative model: RATP: (Sinoquet *et al.* 2001) integrated within the OpenAlea
3 platform and running on MTG structures (see also Supplementary Information: Inputs of the
4 MuSCA model). In RATP the tree structure is first discretized into voxels of user-defined size. The
5 voxel specific mean leaf area density (turbid medium assumption) is calculated based on the plant
6 3D representation in space. This is then used to compute the direct and diffused PAR and NIR light
7 intercepted in each voxel, and its related photosynthesis, every 30 minutes, across the whole day.
8 The C-assimilation estimated per leaf unit surface is first associated to each leaf and integrated over
9 the whole day, and then converted into dry matter uptake per leaf per day. In this study, a previous
10 calibration of RATP for the apple trees, Fuji cultivar (Massonnet *et al.* 2006), was used.

11 Sink strengths were calculated as the sum of the carbon demands for dry matter
12 accumulation into the plant structure and the carbon lost by respiration (Table 2). The first term was
13 assumed to follow maximum potential relative growth rates. Maximum potential growth curves
14 were obtained by fitting thermal-time-dependent gompertz functions to organ-type-specific
15 maximum dry weights (Grossman and DeJong 1995) of proleptic and epicormic shoots, and fruits
16 of apple Fuji trees growing in conditions where competition for carbohydrates was minimized
17 (Reyes *et al.* 2016). Their normalized derivatives (Hunt 1982; Grossman and DeJong 1995)
18 represent the seasonal patterns of organ type specific activities (or maximum potential relative
19 growth rates). Regarding the old wood, the slope of a linear relationship fitted through the logarithm
20 of the relative growth rate of the old wood biomass vs growing degree days (GDD) obtained by
21 Reyes et al. (2016) was used. Values of sink activities of the current days were then used, together
22 with the organ dry weight and the Growing Degree Days (GDD), to estimate the C-demand for dry
23 matter accumulation ($DMDemand_j$) of the same day (eq.4) (Marcelis 1996) at the metamer scale.

$$24 \\ 25 \quad DM\ Demand_j = sink\ dry\ weight * sink\ activity(GDD)_{organtype} * GDD_{day} \text{ (eq.4)}$$

26
27 Respiration was split into maintenance and growth components as proposed by Lescourret et
28 al. (2011) and Pallas et al. (2016). The maintenance components was modeled as proportional to dry
29 mass, a Q10 law, and a maintenance respiration parameter. Growth respiration was considered as
30 proportional to the growth respiration coefficient and to the sum of the carbon demanded for
31 maintenance respiration and for the dry matter increase. Parameter values provided by Pallas et al.,
32 2016 were used.

33 *Definition of topological scales*

1 Five biologically relevant scales of representation of trees were used. Two of them are
2 commonly used in MTG (metamer and growth unit) and three are newly defined (trunk, branches
3 and shoots; 1st order branch and inter-branches; fruiting unit) (Fig.3). New scales were defined by
4 setting criteria for the identification of edges, along the plant topology, among which all elements
5 could be considered as belonging to the same group. The finest scale considered was the metamer
6 (M) (or phytomer) that is composed of a node and its leaf(ves) and axillary bud(s) plus the
7 subtending internode. This scale was considered as a reference for the representation of carbon
8 allocation in this study. The second scale corresponds to the GU (Barthélémy 1991). The third scale
9 corresponded to the discretization of the tree in main trunk, first order branches originating from it
10 and the leafy shoots (Trunk, Branches and Shoots, TBS). The fourth scale corresponded to first
11 order branches originating from the main trunk, but without considering the individual shoots
12 separately (BR1). The fifth scale corresponded to the FU. In all scales, the root was considered as a
13 compartment in itself.

14 *Simulation of fruit growth*

15 We run simulations for the three apple tree structures represented at the five topological scales
16 defined above. In order to identify a biologically sensible value of the friction parameter (h), this
17 was varied across a range of almost two orders of magnitude (0.5-16).

18 We tested the model ability to simulate competition for the available C among tree organs at M
19 scale. This was done by analysing the growth of individual fruits in relation to both the fruit load
20 and the carbon assimilated in the surrounding of the analysed fruit. In particular, a neighborhood of
21 the analyzed fruit is defined as the set of metamers for which the geometrical distance between their
22 barycenter and the barycenter of the metamer containing the fruit is lower than a given threshold.
23 Considered a growing fruit, the ratio between the amount of C-assimilated and the number of fruits
24 present in its neighborhood represents a comfort index with respect to the availability of C for fruit
25 growth and the occurrence of competition with other fruits. As such, the correlation between this
26 ratio and the simulated growth of individual fruits belonging to the same neighborhood illustrates
27 whether fruit growth is affected by the competition for C-assimilates occurring within the area
28 around the analysed fruit. Based on these considerations, the values of C-assimilated and the
29 number of other fruits in the surrounding of individual fruits present on each tree was calculated for
30 neighborhoods of incremental radii (radii of 5, 15, 25, 35, 45, 55, 65, 75, 95, 115, 135 cm) and for
31 different friction parameters. Then, a correlation between the ratio (C-assimilated/number of fruits)
32 and the simulated growth of individual fruits belonging to the same neighborhood was calculated
33 for each radius and friction parameter value. Significance of the correlations was then adjusted for

1 multiple comparisons with the Bonferroni correction (i.e. dividing the significance level of the test,
2 $p\text{-value} = 0.05$, by the number of correlations for which significance was tested: eleven distances).

3 Biological relevance was also tested by comparing the simulated growth on the Fuji tree
4 structure and harvested fruit size distribution on field trees of the same age (four years old) and
5 cultivar. Based on the assumption that fruit weight obtained in early growth stages is correlated to
6 the fruit weight at harvest (Stanley *et al.* 2000), we compared the distributions of the normalized
7 values of the carbon allocated in our simulations with fruit weight measured at harvest (Costes,
8 unpublished data). Similarity among distributions was also assessed in terms of Root Mean Squared
9 Error (RMSE) between distribution counts. Based on these results, a narrower range of friction
10 parameter values was identified as more biologically relevant and used in further analysis.

11 The coherence of simulations across scales was tested by correlating the fruit growth obtained at
12 each coarse scale with the one at M scale, used as a reference. Results obtained for equal friction
13 parameter and same tree structure were considered together. For each coarse scale component, the
14 average of the fruit growth obtained at M scale within the boundaries of the coarse scale component
15 was computed. As such, a one-to-one comparison was possible between mean growth at M and
16 other (coarser) scales. Deviations between M and the other scales were assessed visually on
17 correlation plots, and by means of the coefficient of variation of the root mean squared error (CV
18 RMSE).

19 The effect of using different topological scales on the number of plant components and on
20 simulation time was also analyzed. All simulations were run on a computer equipped with an Intel
21 i7-6700HQ 2.59 Ghz CPU, 8Gb RAM; OS: Windows 10 Home, 64bit.

22 RESULTS

23 Testing physiological assumptions

24 Relative growth rate (RGR) of shoots in the Fuji tree structure at M scale increased with the
25 values of the friction parameter while, for fruits and old wood, it increased for h values from 0.25 to
26 respectively 4 and 2, and then decreased until a value of 16 (Table 3). In other terms, the higher the
27 values of the friction parameter the higher was the growth occurring close to the C-source. RGRs of
28 old wood and shoots were comprised between normal growth observed in the field and maximum
29 potential growth data used for calibration of sink demands (between $5.3 \cdot 10^{-3}$ and $3.1 \cdot 10^{-2}$ mg/g for
30 the old wood, between 0.4 and 1.2 mg/g for shoots; Reyes *et al.* 2016). Conversely, fruit growth
31 was between 35% and 51% lower in respect to the fruit growth observed in the normal field
32 conditions (1.9 and 2.8 mg/g for fruits).

1 Simulation results at M scale show the impact of the friction parameter (h) in determining
2 the area around an individual fruit within which this competes for C-assimilates with other fruits
3 (Fig.4A, B). As shown by the significant correlations among fruit growth and comfort index (ratio
4 between C-assimilated and number of fruits), the neighborhood within which fruit growth is
5 affected by competition for C is relatively large (>0.9 m) for small values of the friction parameter
6 (0.5 - 4). This means that the within-tree variability in fruit growth is mostly related to C-sources
7 located far from it. In other terms, a large part of the tree structure affects the growth of each
8 individual fruit. Conversely, for high friction parameter values (8, 16), fruit growth is affected
9 mainly by the C provided by close leaves and possibly the competition with neighboring fruits
10 (neighborhood < 0.9 m) (Fig.4B).

11 The normalized fruit dry weight simulated on the four-year old Fuji tree was compared to
12 that of fruits measured at harvest in a two similar trees, in order to evaluate what range of the
13 friction parameter best fit the observed fruit size distribution (Fig.4C). The lowest RMSE values
14 were obtained with h parameter values between 4 and 16. High values, however, produced skewed
15 distributions with variability larger than the one obtained in the field ($h = 16$). Conversely, for low h
16 values (0.5, 1) distributions had a consistently lower variability than in the field. Similar variability
17 and low RMSE values were obtained with the friction parameter values of four and eight.

18 C-allocation at multiple scales

19 Changing the scale of representation of the tree from M to coarser scales sharply decreased
20 the number of represented topological components of the tree structures. Trees at GU, TBS, BR1
21 and FU scales contained respectively about 12.7%, 8.6%, 1.6%, and 1.2% the elements they had at
22 M scale (Table 4).

23 Changing topological scale had also a significant impact on fruit growth. In order to ease the
24 interpretation, and based on the above fitted values, only results for the best friction parameter
25 values ($2 \leq h \leq 8$) are presented. Fruit growth at GU and TBS scales was more correlated to
26 results at M scale than at coarser scales (BR1, FU) (Fig.5). Generally, in simulations at coarse
27 scales, fruit growth predictions was lower in respect to the M scale. For instance, when running the
28 simulations at FU scale, differences in mean fruit dry weight compared to those obtained at M scale
29 (used in the PEACH model, Allen *et al.* 2005) went up to 60% in terms of coefficient of variation of
30 the RMSE (Fig.6B).

31 As expected, multiple fruits belonging to the same coarse scale component had the same
32 growth (size of spheres on Fig.3). This was due to the facts that that all fruits at the beginning of the
33 simulation had identical weight and that the carbon allocated to a coarse scale component is
34 proportionally divided according to individual metamer carbon demand. As a consequence, the

1 higher the resolution in representing the plant structure (Metamer > Growth Unit > TBS > 1st order
2 Branching \approx Fruiting Unit), the higher number of different fruit growth achieved (Fig.5). Globally,
3 the lower the friction parameter the lower the range of fruit growth variability, in all the tree
4 structures and at all topological scales (Fig.4C, Fig.5D). The corollary of these observations is high
5 values of the friction parameters result in a relatively wide range of fruit growth at all scales, but
6 with lower within-tree variability when moving from a M to a coarse scale.

7 Simplification of the tree structures and computation efficiency

8 Computation time was found as a third order polynomial function of the number of
9 components in the plant (Supplementary Information - Fig.1). The reduction in the number of
10 represented plant components, obtained by changing scale from M to FU (down to 0.8%) in the
11 presented simulations, resulted in a gain in computation time of up to four orders of magnitude
12 (down to 0.2%) (Table 4).

13 The reduction in computation time associated with the use of coarser scales (Table 4)
14 corresponded to an increased discrepancy (in terms of the Coefficient of Variation of the Root
15 Mean Squared Error: CV RMSE) in the results obtained between M and other scales (Fig.6B). Error
16 varied from values next to zero at low friction parameters at GU scale, to values up to sixty percent
17 for higher frictions and BR1 or GU scales, and was generally higher for higher friction parameter
18 values. There were however minor exceptions to this general behavior, with low friction parameter
19 values occasionally providing slightly higher discrepancies than higher values (e.g. for $h = 4$ at
20 BR1 scale in the Ap-05 and Ap-10 tree structure, in respect to $h = 8$).

21 DISCUSSION

22 Multi-scale coherence, impact on predictions and computation time

23 To our knowledge, MuSCA is the first C-allocation model that allows simulating C-
24 allocation at multiple topological scales within a plant representation. Simulation results revealed
25 that the model was able to produce results which are highly correlated with the M scale, especially
26 when running at GU scale (Fig.5). As a rule of thumb, the deviation between predictions obtained at
27 M and other scales increased when up-scaling and for increasing friction parameter values (Fig.5,
28 Fig.6).

29 Differences in C allocated to fruits at M and other scales are due to two factors. Firstly, after
30 allocation, the C received by the different plant parts belonging to a component is no longer
31 influenced by their individual positions. As such, the model represents the effects of distances
32 among the components at the coarse scale selected for the simulation, but not among its constituting

1 elements at the finer scale. Second, while the top and basal coordinates of a coarse scale component
2 are inherited from the finer scale components present at its extremities, the coordinates of its
3 barycentre are not. Indeed these are computed as the mean of the coordinates of its components,
4 weighted by their individual lengths. When distances and C-flows are calculated, this generates
5 deviations in respect to the M scale

6 The deviations between M and other scales were also affected by the specific plant structure
7 (Fig.5). This is likely related to the non-linearity of the simulated process and its relation to the
8 different discretization of the plant. In trees, the different contribution in respect to the available C
9 of annual organs (leaves and fruits) and the presence of the moderate C-sink of woody organs may
10 create contrasting patches in terms of C-supplies and C-sinks (Fig.4). When the tree is discretized at
11 different scales, the distances between patches of sources and sinks and their constituting elements
12 are modified. By changing discretization, the set of distances to which the non-linear function (eq.
13 1) is applied to compute C flows also changes, implying sharp differences in C-allocation. Changes
14 are thus related to the geometry of the tree structure as well as to the specific friction parameter, as
15 they determine the spatial domain and the impact of the C-allocation rule. In this regard, further
16 research would be required to explore the impact of commonly applied equations for C-allocation
17 (e.g. eq. 1, equations in Balandier *et al.* 2000; Lescourret *et al.* 2011) on tree architectures
18 contrasting in terms of distributions of sinks and supplies in relation to their discretization.

19 Changing topological scale also had a strong impact on the computation time. This is an
20 important limiting factor for the simulation of carbon allocation in complex tree structures, and
21 consequently simulations of tree growth at high spatial detail tends to be limited to relatively young
22 plants (Balandier *et al.* 2000; Pallas *et al.* 2016). Computation time in MuSCA closely
23 approximates a third order polynomial function of the number of represented plant components
24 (Supplementary Information - Fig.1), suggesting the need to reduce plant complexity to simulate
25 plant growth with this type of source-sink model. In this study, the GU scale was able to reproduce
26 values and fruit growth distributions almost identical to M, while saving computation time (Fig.5,
27 Fig.6). It is possible that the optimal scale of representation may be influenced by tree size. Because
28 of the exponential increase in tree topological complexity with tree age, relatively small variations
29 in C-dynamics in early growth stages may have important consequences for the development of the
30 tree structure at later stages. We propose the hypothesis that intermediate scales comprised between
31 M and GU may further decrease the deviations in respect to M scale. We further suggest that a
32 mixed use of high and relatively low topological resolutions, respectively for young and older trees,
33 may optimize prediction accuracy while still allowing for simulations on mature trees.

1 Testing physiological assumptions

2 The formalization used in MuSCA to calculate C-allocation (eq. 1a) (Balandier *et al.* 2000)
3 represented the impact of C-availability and competition among sinks, such as the fruits (Fig.4) on
4 fruit growth variability.

5 RGRs at compartment level was lower range of field observations. This is due to the choice
6 for simulations of a partly cloudy day, in which C-assimilation could limit growth, resulting in
7 enhanced competition for C (whereas simulations in very sunny days resulted in higher growth and
8 reduced fruit growth variability, data not shown).

9 In MuSCA, the considered friction parameter (h , eq. 1) is empirical and does not correspond
10 to a clear biological process. As in previous studies, this parameter has been estimated by trial and
11 error (Balandier *et al.* 2000). Nonetheless, the comparison between the simulated and harvested
12 normalized fruit growth distribution suggests that h values should be between four and eight
13 (Fig.4C). This suggests that neither a common assimilate pool (Heuvelink 1995) of carbon nor a
14 shoot or branch autonomy (Sprugel *et al.* 1991) was adequate for accounting for assimilate
15 partitioning within a fruit tree as observed in previous experimental studies (Walcroft *et al.* 2004;
16 Volpe *et al.* 2008). Moreover, fluxes from parts of trees with high carbon supply to parts with a low
17 one have already been used for modeling the within-tree variation in fruit size in peach and apple
18 trees (Lescourret *et al.* 2011; Pallas *et al.*, 2016). Nevertheless, it has also been observed that the
19 level of shoot or branch autonomy can vary depending on the phenological date with a higher
20 branch autonomy during summer period compared to winter (Lacointe *et al.* 2004). Further
21 simulations and analyses with MuSCA performed by dynamically tuning the friction parameter
22 values could help testing such behaviors.

23 Advantages of flexible C-allocation at multiple-scales

24 By making a dynamic use of MTG (Godin and Caraglio 1998) the presented model allows
25 us modifying the type of “individual entities” considered in source-sink exchanges within a plant
26 structure on the fly. This is also made possible by formalisms which are equally applicable at all
27 scales (Fig.2, eq. 2, 3) and inherit, from fine to coarse scales, the spatial (coordinates of scale
28 boundaries) and extensive (C-demands and supplies, Up- and down- scaling) properties necessary
29 for the calculation of C-flows.

30 The flexibility related to the multi-scale features of the model provides several opportunities.
31 While the topological scale typically represented in a plant models mirrors the interests of a
32 particular group of model users, changing the scale of representation makes the model of practical
33 interest for multiple objectives. As showed in this study, the model can be used to assess the
34 implications of using specific scales. From our results, in most cases and for trees of this size, the

1 GU scale would be a robust alternative to M, while allowing much faster simulations. Comparisons
2 of results among C-allocation models could be facilitated by adapting the scale of representation.
3 For instance, the individual fruit growth simulated at the FU scale can be compared with results
4 obtained by QualiTree (Lescourret *et al.* 2011).

5 In this study, MuSCA was applied on MTGs issued from the MAppleT architectural model
6 (Costes *et al.* 2008). However, MTGs coming from other sources, such as the several models
7 present in the OpenAlea environment, could also be used, given their compliance with certain
8 prerequisites. Also, the detail in the description of the plant could be less detailed since, technically,
9 a representation at metamer resolution is not strictly necessary. Indeed, in order to run MuSCA, the
10 plant description should simply allow for the identification of the organ types (via the presence of
11 leaves and fruits), their geometrical sizes (length and radiuses) and their topological connections
12 (succession, branching). This makes the model applicable on tree structures acquired in the field by
13 methods such as the Terrestrial Laser Scanner (TLS), followed by topological reconstruction of the
14 plant (Raumonen *et al.* 2013; Boudon *et al.* 2014; Reyes 2016). In addition, field data collected at
15 various topological scales might still be suitable for model testing. Indeed, by using the up- and
16 down-scaling, results simulated at any spatial scale can be brought to the scale at which the data for
17 validation are available.

18 Model limitations and further developments

19 MuSCA still neglects to represent some important physiological implication of the
20 distribution of sinks along the plant topology. In particular, the influence of individual sinks present
21 in the path between sources and sinks on the C-flow is not fully described, as in models based on an
22 electric analogy and the L-system formalisms (Allen *et al.* 2005; Cieslak *et al.* 2011). Indeed, two
23 identical C-sinks (D1, D2) present at the same distance from a source (S) will receive from this
24 source an identical amount of C, no matter if along the path between S and D1 there are stronger or
25 more abundant C-sinks than along the path between S and D2. Nevertheless, simple models as our
26 have the advantage to require the calibration of one parameter only compared to these previous
27 approaches.

28 It is important to remember that like other carbon allocation models applicable to large plant
29 structures, MuSCA makes use of an empirical parameter (the friction parameter). In this study we
30 identified a range of possibly sound parameter values, but more appropriate ones could be
31 experimentally estimated from measurements of the sap flow through marked isotopic carbon
32 (Hansen 1967), as well as measurements of fruit growth in simple tree structures with modified fruit
33 loads.

1 The MuSCA model could be further refined by using the MTG properties to increase the
2 computational efficiency without losing prediction accuracy. For instance, when running at coarse
3 scale, the direction of origin of C-assimilates might be used to account for distance also within the
4 boundaries of the coarse scale component.

5 The creation of new metamers should be included in order to allow for the simulation of
6 plant growth during elongation and growth periods (on not-fixed structures). In addition, given the
7 influence of pruning on the distribution and emergence of carbon sinks, the implementation of a
8 module describing reactions to this management practice (e.g. DeJong *et al.* 2012) would
9 significantly extend the applicability of the model to a broader range of real cases. Further, a more
10 detailed description of the root would be the starting point to investigate water and nutrient
11 limitations at the soil interface.

12 Regarding the use of MuSCA in the larger context, its generality can ease its adaptation to
13 different species. In addition, the modular implementation of MuSCA in the OpenAlea environment
14 facilitates the integration with other, previously developed, models, as it was the case for the
15 connection with the MAppleT (Costes *et al.* 2008) and the RATP models (Da Silva, Han, and
16 Costes 2014).

17 CONCLUSIONS

18 In this study we presented MuSCA, to our knowledge the first C-allocation model allowing
19 to simulate C-allocation at multiple topological scales of representation of the plant. The presented
20 model provides topologically-based methods to re-interpret/simplify the topological scale at which
21 the process of carbon allocation is simulated. The simulations revealed a major impact of the
22 topological scale, used to discretize C-sources and sinks, on the predicted C-allocation, even when
23 other C-allocation rules (equation for C-allocation and friction parameter) were kept constant. The
24 model can be used to identify which degree of simplification is acceptable for the representation of
25 plant structures without compromising the accuracy in the computation of carbon allocation. It can
26 be used on large plants, being aware of the trades-off in terms of computation time and prediction
27 accuracy. In addition, the flexible representation of the plant topology facilitates matching the needs
28 of different users, while using the same model. For instance, a relatively coarse scale (e.g. branch)
29 could be more suited for a farmer interested in fruit thinning, than a fine one (e.g. metamer) that
30 could be the target of a modeler interested in investigating the local drivers of individual fruit size
31 variability.

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1 Fig.1: Conceptual workflow of the model: (A) General framework for the application of the model; (B) the
2 core of MuSCA. (A): A multi-scale tree graph representing a plant structure at a given developmental stage
3 is provided. This is used, together with the Growing Degree Days (GDD), allometric relationships and plant
4 geometric information to compute initial volumes and biomasses of plant components at metamer (M) scale.
5 Carbon demands are estimated at metamer scale by making use of species specific seasonal sink activities,
6 biomasses and GDD at the current time step. The position of individual leaves on the plant structure is used
7 by the radiative model RATP to compute light interception and, together with meteorological conditions, the
8 individual leaf photosynthesis. (B): The workflow follows different paths depending on the selected scale:
9 M scale (solid lines) and coarser scales (dashed lines). The scale at which the plant is represented determines
10 up- and down-scaling processes. In case a coarse scale is chosen, carbon demands and supplies are up-scaled.
11 Carbon allocation is then computed among the plant components at the chosen scale. After allocation, if the
12 selected scale was a coarse one, the carbon allocated to each component is divided among its constituent
13 elements. Biomass of individual elements is eventually updated prior to moving to the next time-step. MTG:
14 Multi-scale Tree Graph. In *italics* are the steps containing species specific parameters.

15 Fig.2: Workflow and graphical representation of the calculation of distances. (A) Workflow for the
16 calculation of the distance between two vertices i, j : top coordinates of vertices are used to compute
17 coordinates of basis and barycenters for the whole topology. Given two vertices i, j , their distance is
18 calculated in three steps: the Greatest Common Ancestor (GCA) of i, j is identified; an iterative process sums
19 the length of the vertices connecting GCA to i and j ; the semi-lengths of i and j are also summed. (B)
20 Graphical representation of the: calculation of coordinates of basis and barycenters at (above) metamer (M)
21 scale. The base of a vertex corresponds to the top of its parent; coordinates of the barycentre of a vertex are
22 calculated from the ones of its top and base. (Middle) the base of a coarse scale vertex (capital I) corresponds
23 to the base of its first component (lowercase i), which is inherited from the top of its parent at M scale
24 (lowercase i-1); coordinates of the barycenter of a coarse scale vertex are obtained as the mean of the
25 coordinates of its own components at M scale, weighted by their lengths. (Below) calculation of the semi-
26 length of a vertex, identification of GCA and computation of distances along a path connecting two vertices
27 i, j . Data used as input of calculations are indicated by red rhombi and are connected by arrow to the
28 respective output represented by green crosses.

29 Fig.3: Simulation of carbon allocation and fruit growth on a tree structure represented at different spatial
30 scales during one day. Upper panels: tree parts represented with the same color belong to the same scale, i.e.
31 trees with an higher number of colors are made of a higher number of components. The number of
32 components at each scale is indicated in the corresponding low left corner. Lower panels: the volume of the
33 represented spheres is proportional to the normalized increment in fruit dry weight within the tree.
34 Simulations were run with a friction parameter equal to eight.

35 Fig.4: Physiological responses in simulations at M scale, in respect to different tree structures and friction
36 parameters (h). A: Three dimensional representation of the tree structures with fruit growth (obtained with h
37 parameter equal to 8). B: correlation between individual fruit growth and the ratio between carbon
38 assimilated and number of fruits evaluated in neighborhoods of increasing radiuses. C: Distributions of the
39 normalized simulated fruit growth (red, coloured bars) superposed with the normalized fruit dry weight
40 measured at harvest (black, empty bars), in the 4 years old simulated and observed Fuji trees for different
41 friction parameters. The Root Mean Squared Error (RMSE) between distribution counts for different friction
42 parameters is provided. The upper parts of the histograms for $h < 2$ are cut off in order to allow better
43 visualization of results on the vertical axis.

44 Fig.5: Mean daily fruit dry weight increment and its distribution (in Fuji apple cultivar) depending on the
45 topological scales (from left to right), tree structure (from top to bottom) and friction parameters h (symbols).
46 Correlation between carbon allocated to fruits per day at the selected coarse scale (y axes) vs carbon
47 allocated to fruits per day at M scale and averaged for all metamers belonging to a same component at
48 coarser scale (x axis) in A: Fuji, B: Ap-05, C: Ap-10. D: Fruit growth distribution in the Fuji tree structure
49 (dashed for $h=2$, dotted for $h=4$, solid for $h=8$).

1 Fig.6: Trade-off between computation time and prediction error. The logarithm of the computation time and
2 the Coefficient of Variation of the Root Mean Squared Error (CV RMSE) between fruit growth at different
3 topological scales in respect to the M scale, on three tree structures and for different friction parameters (h).
4 A: Fuji, B: AP-05, C: AP-10.

5 Supplementary Information - Fig.1: Computation time in respect to the number of represented structure
6 components.

7

1 Table 1: Model parameters and equation for estimation of biomasses.

| Parameter | Description | Value/range | Unit |
|----------------------|---|-------------|-------------------|
| dry_mass_to_C_mass | Ratio to convert carbon assimilated into biomass uptake | 2.105263158 | - |
| wood_density | Old wood density | 700 | Kg/m ³ |
| spec_leaf_surface | Per unit surface leaf dry mass | 0.08 | Kg/m ² |
| dry_to_fresh_DWratio | Ratio to convert apple fruit fresh to dry weight | 0.15 | - |
| shoot_to_root_growth | Vegetative shoot to root biomass ratio | 4.5 | - |

Generalized linear model to estimate shoot biomass (g) from length (cm) and thermal time (°C)

$$\text{Dry weight} = \exp (a + b * \log(\text{length}) + c * \text{GDD} + d * \text{length} + e * \log(\text{length} * \text{GDD}))$$

| | |
|---|--------------|
| a | -3.073409537 |
| b | 0.706724497 |
| c | 5.78E-05 |
| d | 0.020013707 |
| e | 9.81E-05 |

2

3

4 Table 2: Model parameters and equations for the estimation of carbon demand for dry matter
5 increase

| Parameter | Description | Value/range | Unit |
|----------------|--|---------------------------|---------------------------------------|
| trunk_activity | Sink activity for old wood | 0.000031 | g * g ⁻¹ * C ⁻¹ |
| leaf_activity | Range of values for leaf activity (from Look Up Table) | 0 to 1.9*10 ⁻³ | g * g ⁻¹ * C ⁻¹ |

Gompertz equation for fruits and shoots

$$\text{Dry weight} = a * \exp(b * \exp(c * \text{GDD}))$$

Normalized derivative

Relative Growth Rate =

$$(a * b * c * \exp(b * (\exp(c * \text{GDD}))) + c * \text{GDD}) / (a * \exp(b * \exp(c * \text{GDD})))$$

| Parameters | Fruit | Proleptic shoot |
|------------|----------|-----------------|
| A | 63.703 | 2.406 |
| B | -4.896 | -2.84 |
| C | -0.00104 | -0.00165 |

GDD: Growing degree days after bloom, after cutoff of base temperature of 4.5 °C.

6

7 Table 3: Relative growth rate at metamer scale for different friction parameter values (h) on the Fuji apple
8 cultivar. Figures are reported with five decimals in order to see RGR differences when using different h
9 values.

| h | Relative growth rate (mg g ⁻¹ dd ⁻¹) | | |
|------|---|-------|-------|
| | Old wood | Shoot | Fruit |
| 0.25 | 0.016 | 0.50 | 1.19 |
| 0.5 | 0.016 | 0.50 | 1.20 |
| 1 | 0.018 | 0.50 | 1.20 |
| 2 | 0.019 | 0.51 | 1.22 |
| 4 | 0.018 | 0.54 | 1.23 |
| 8 | 0.015 | 0.63 | 1.17 |
| 16 | 0.009 | 0.63 | 0.93 |

1

2

3 Table 4: Number of components included in tree structures at different scales.

| Tree structure | Scale | Number of components | % | Computation time (min) | % |
|----------------|-------|----------------------|------|------------------------|-------|
| Fuji | M | 3355 | 100 | 175.6 | 100.0 |
| | GU | 521 | 15.5 | 1.0 | 0.6 |
| | TBS | 320 | 9.5 | 0.6 | 0.4 |
| | BR1 | 29 | 0.9 | 0.4 | 0.2 |
| | FU | 67 | 2 | 0.4 | 0.2 |
| Ap-05 | M | 4579 | 100 | 313.8 | 100.0 |
| | GU | 535 | 11.7 | 1.5 | 0.5 |
| | TBS | 402 | 8.8 | 1.1 | 0.4 |
| | BR1 | 115 | 2.5 | 0.7 | 0.2 |
| | FU | 36 | 0.8 | 0.7 | 0.2 |
| Ap-10 | M | 4083 | 100 | 246.4 | 100.0 |
| | GU | 449 | 11 | 1.1 | 0.4 |
| | TBS | 302 | 7.4 | 0.8 | 0.3 |
| | BR1 | 59 | 1.4 | 0.6 | 0.2 |
| | FU | 36 | 0.9 | 0.6 | 0.2 |

4

Supplementary Information

Supplementary Information: Inputs of the MuSCA model.

| Variable | Description | Unit |
|---|---|-------------------|
| <i>Multi-scale Tree Graph description of a plant (.mtg)</i> | | |
| | Coordinates of the centre of the top of a plant | |
| <i>XX, YY, ZZ</i> | component | m |
| <i>radius</i> | tree component apical radius | m |
| <i>leaf_area</i> | leaf area surface | m ² |
| <i>fruit</i> | fresh fruit biomass | Kg |
| <i>observation</i> | organ type: trunk, other types | - |
| Topologica | | - |
| l connector | “>” for succession; “+” for branching | |
| Scale | | |
| boundary | “/” for boundary across scales | |
| <i>Meteorological file for the RATP model (.mto)</i> | | |
| day | day of the year | day |
| hour | index of the current semi-hour from midnight | 30 min |
| PARglob | global incident Photosynthetically Active Radiation | W m ⁻² |
| PARdif | diffused Photosynthetically Active Radiation | W m ⁻² |
| NIRglob | global incident Near Infrared Radiation | W m ⁻² |
| NIRdif | diffused Near Infrared Radiation | W m ⁻² |
| Ratmos | Total incoming radiation | W m ⁻² |
| Tsol | mean soil temperature | °C |
| Tair | mean air temperature | °C |
| Eair | H2O partial pressure | Pa |
| CO2air | CO2 partial pressure | Pa |
| Wind | wind speed above tree | m s ⁻¹ |

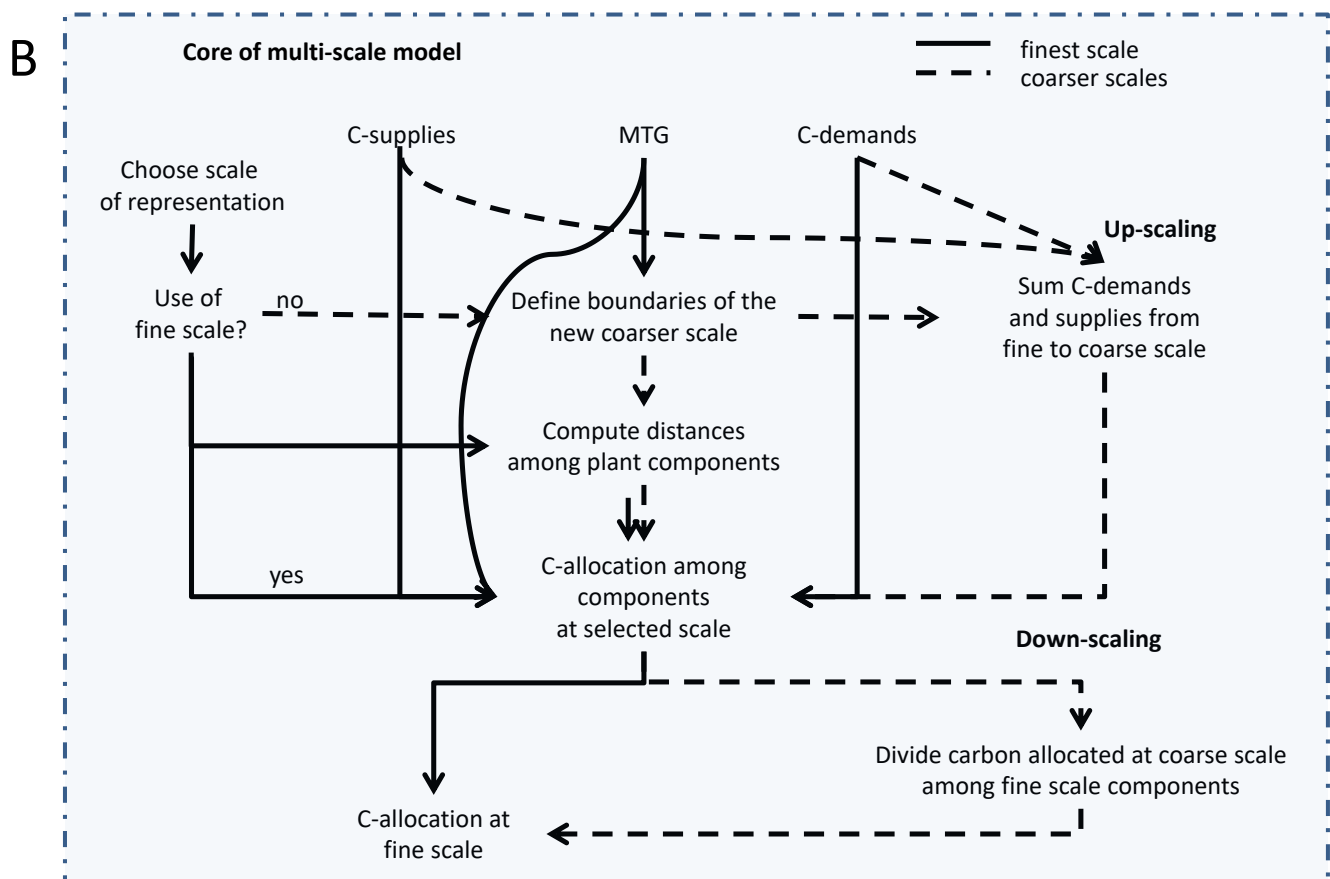
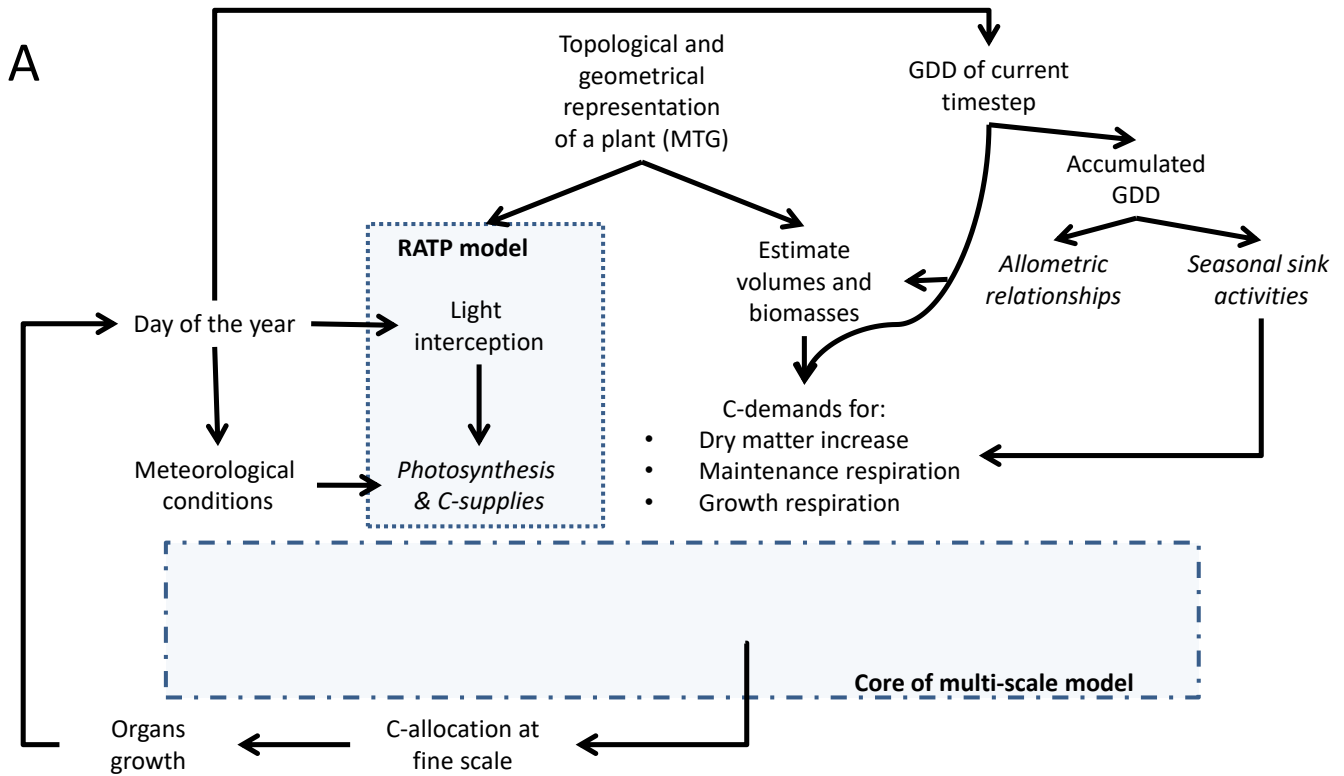
Supplementary Information: Input tree structures

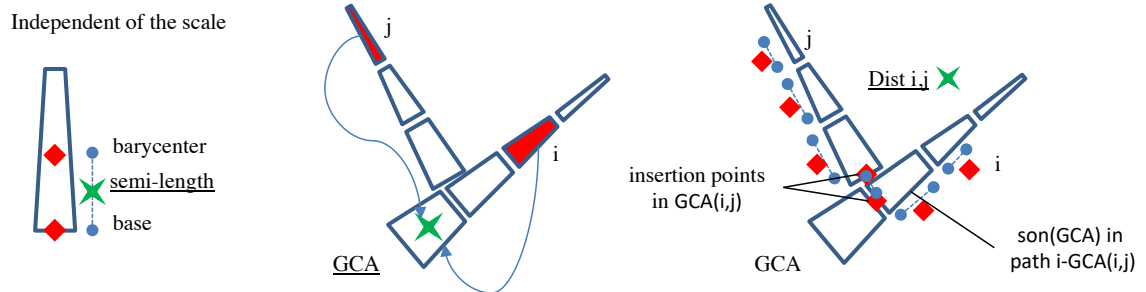
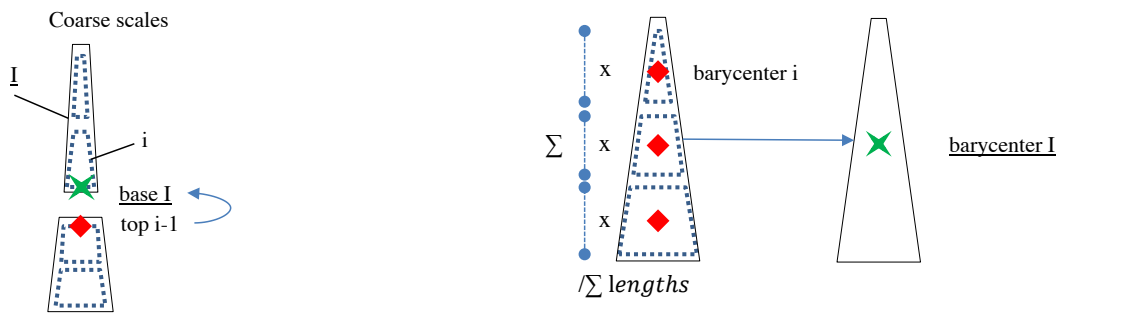
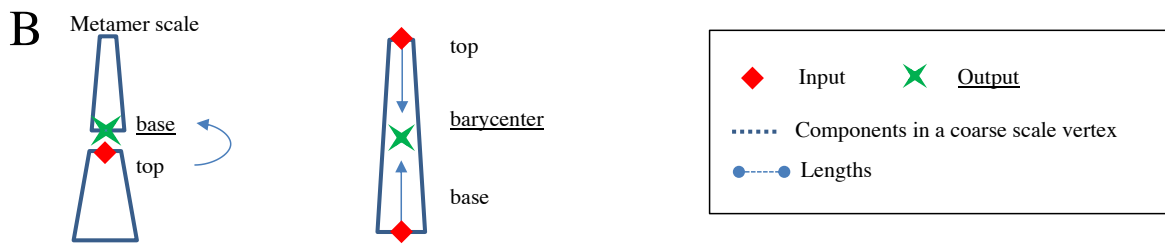
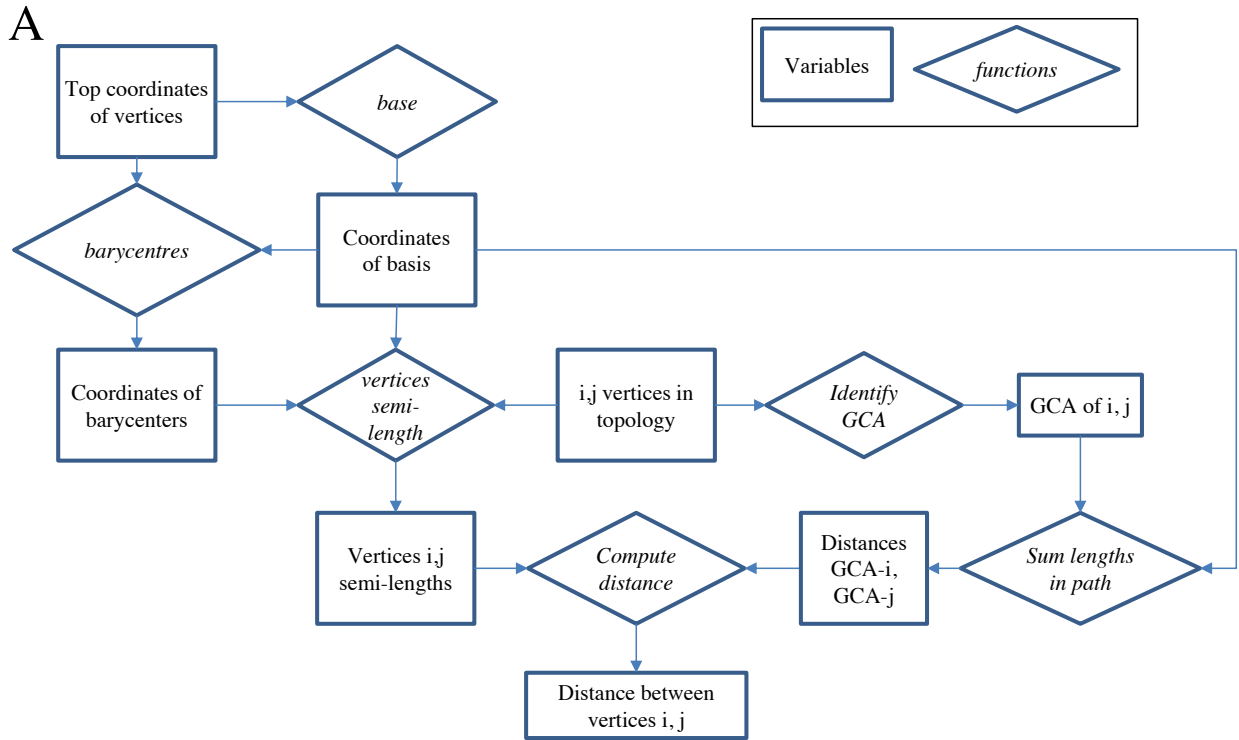
In the current application, input tree structures were MTGs produced by the MAppleT model (Costes *et al.* 2008). MAppleT includes (i) Markov models for simulating annual shoot branching and successive growth across years, (ii) a biomechanical model simulating the change in branch form over time, and (iii) a modified pipe-model to estimate axis radial growth. The leaf area and internode length depend on their rank along the shoot (Da Silva, Han, and Costes 2014). The MTGs output produced by MappleT are apple trees structures at a certain stage of development (given date of the year), represented at two scales, the growth unit and metamer. Metamer attributes are its apical and basal 3D coordinates, stem diameter, leaf area and fruit weight (if present).

1 At the beginning of the simulation, the model uses the geometrical description of the plant
2 and some species specific parameters (Reyes *et al.* 2016, in-field observations) to estimate the
3 initial dry weight of each plant component at the metamer scale (see Supplementary Information:
4 Inputs of the MuSCA model). In particular: dry weight of old wood and vegetative internodes are
5 computed as functions of their geometrical description (lengths and radiuses), and of a constant
6 (wood density) or a function of thermal time, respectively; fruits dry weight is calculated from fresh
7 weight and a constant (dry to fresh fruit dry weight ratio); leaf dry weight is calculated from surface
8 and a constant (per unit surface leaf dry mass) (Table 1). Dry mass of individual internodes is
9 calculated as follows: volumes of internodes are first computed as truncated cones, summed up to
10 provide the volume of individual shoots and stored at a “current year shoot” coarse scale. The
11 length of current year shoots is then obtained by summing the lengths of their internodes, and used
12 to estimate shoot biomass by means of a thermal-time dependent allometric relationship (Table 1)
13 (Reyes *et al.* 2016). Finally, the dry biomass of individual internodes is calculated as their
14 individual volumetric fraction in the shoot to which they belong, multiplied by the shoot dry
15 biomass.

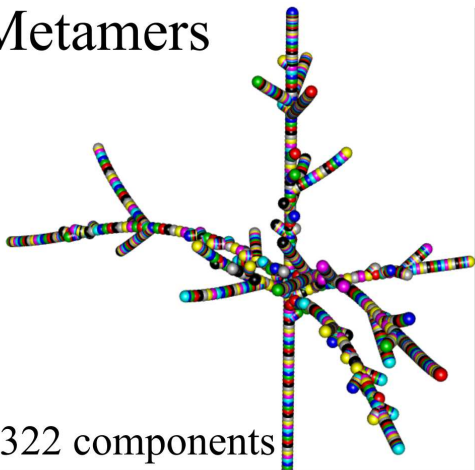
16 Regarding the root, a rough representation of this compartment was added to the plant. A
17 root mass, defined as proportional to the total mass of the current year shoots, is added to the root
18 metamer following the shoot/root functional balance assumption (Davidson 1969; Grechi *et al.*
19 2007). The length of the roots is represented as equal to half the average distance between the soil
20 and the vegetative shoots. The root basal coordinates are thus defined equal to the tree basal
21 coordinates, except for the vertical (z axis) component, to which the calculated distance is
22 subtracted (downward translation).

23



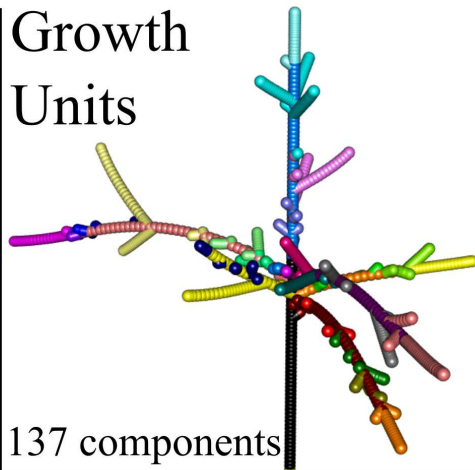


Metamers



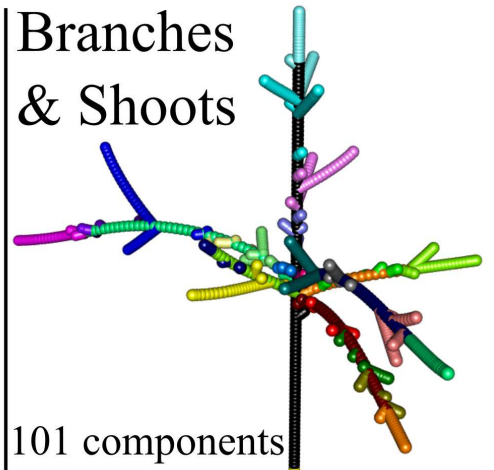
1322 components

Growth Units

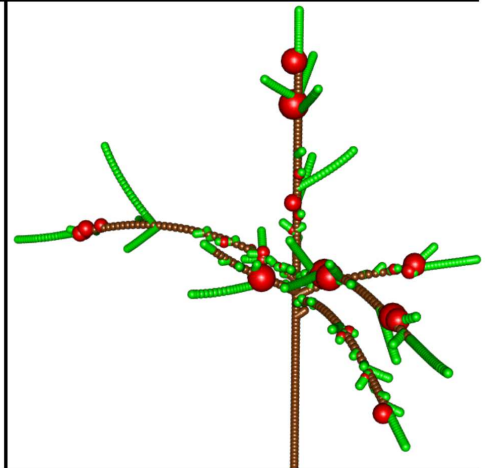
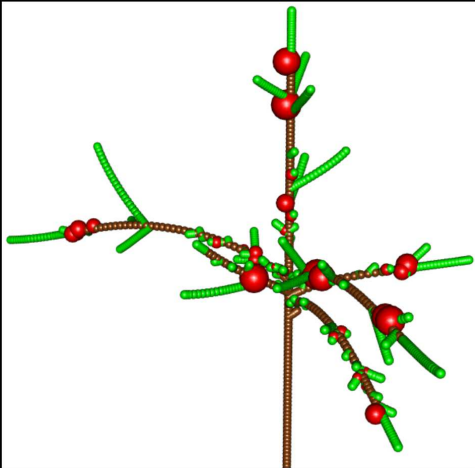
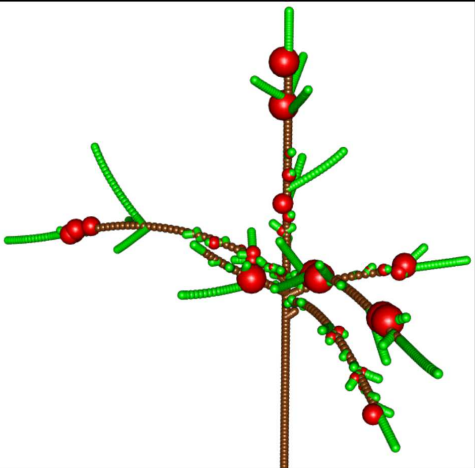


137 components

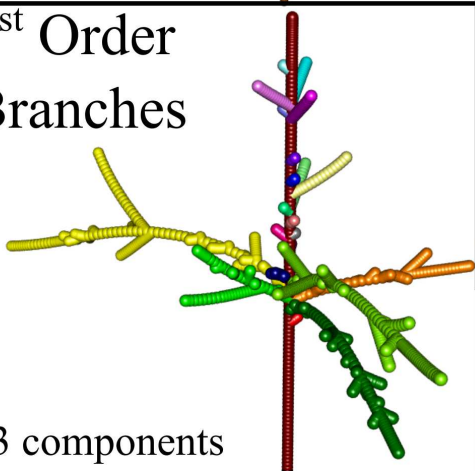
Branches & Shoots



101 components

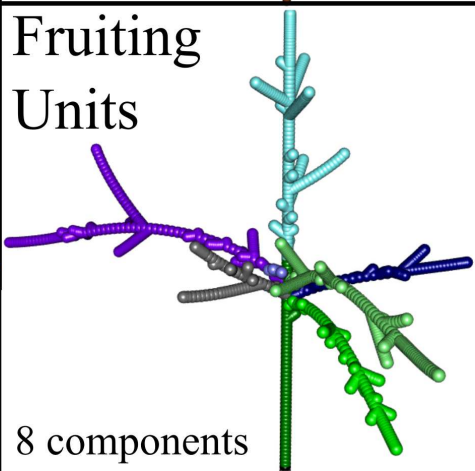


1st Order Branches

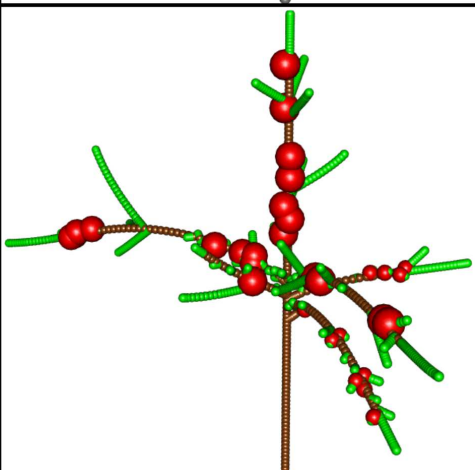
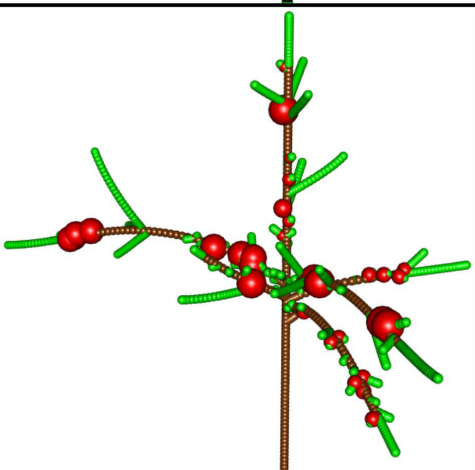


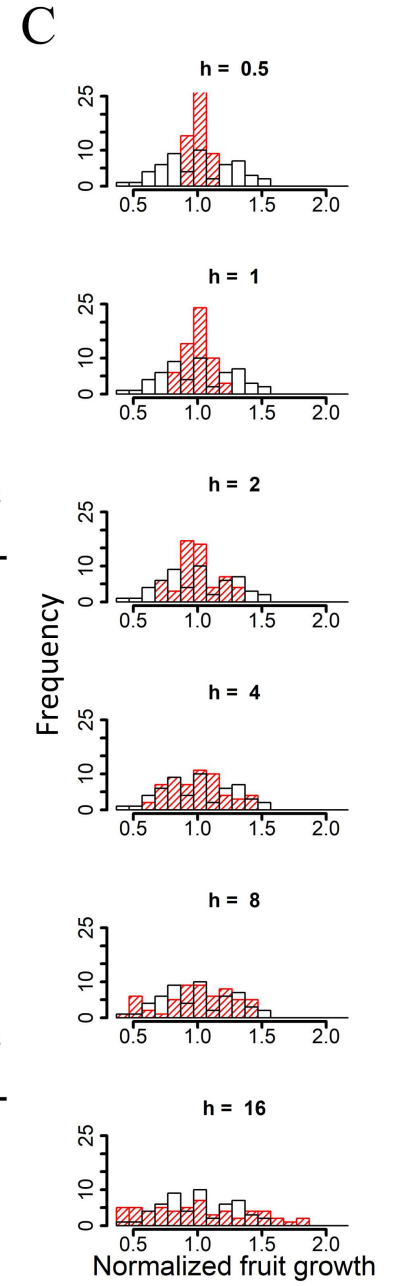
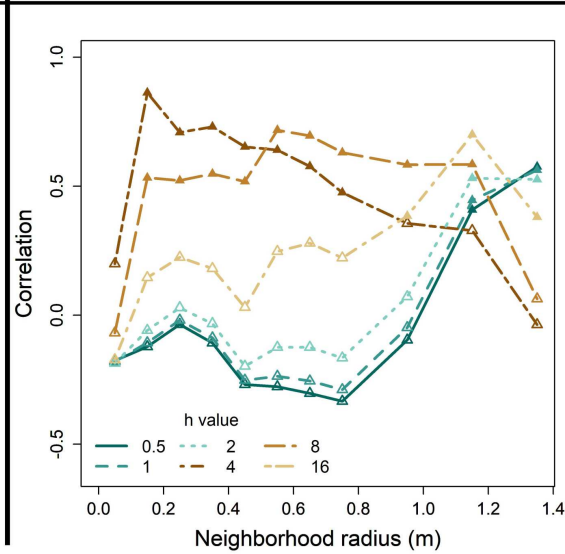
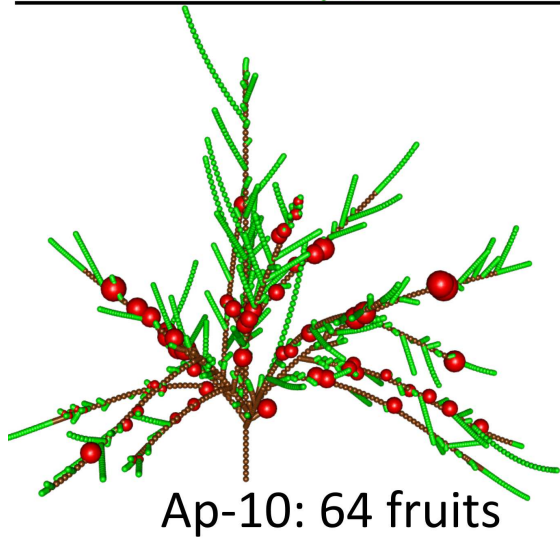
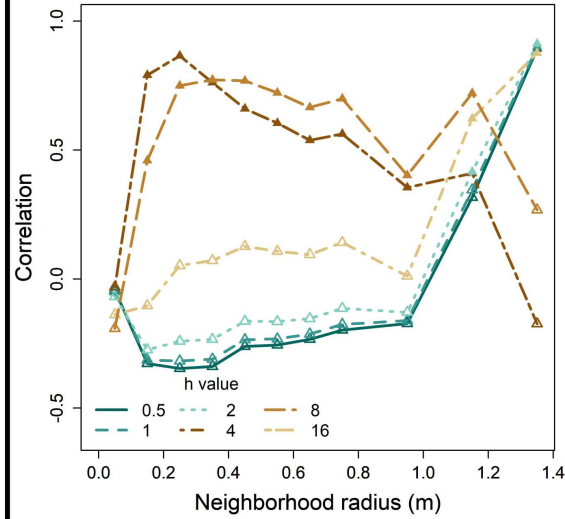
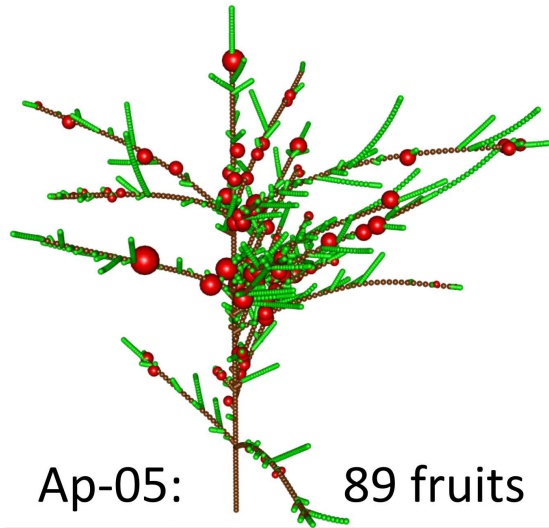
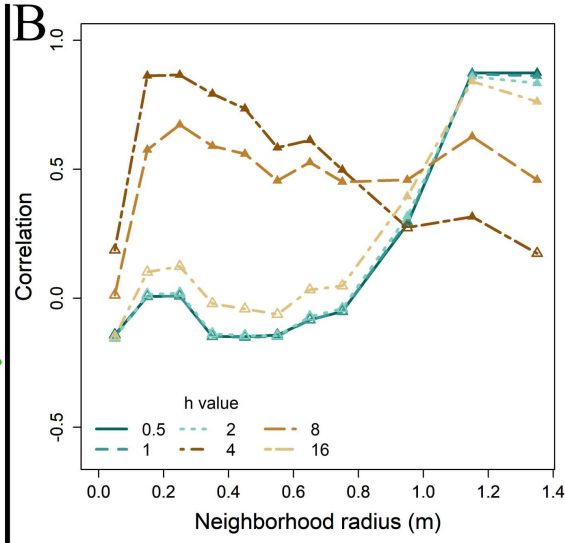
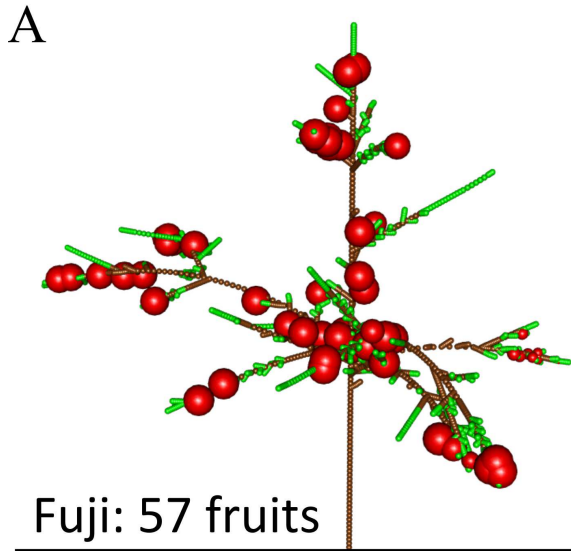
43 components

Fruiting Units



8 components





| friction | |
|---------------|------|
| parameter (h) | RMSE |
| 0.5 | 7.3 |
| 1 | 5.2 |
| 2 | 4.0 |
| 4 | 2.4 |
| 8 | 2.7 |
| 16 | 2.5 |

