Proceedings of the 7th International Conference on Functional-Structural Plant Models, Saariselkä, Finland, 9 - 14 June 2013. Eds. Risto Sievänen, Eero Nikinmaa, Christophe Godin, Anna Lintunen & Pekka Nygren. http://www.metla.fi/fspm2013/proceedings. ISBN 978-951-651-408-9.

Integrating multiple scale dynamics: Application to *Fagus sylvatica* under ozone exposure

Yongzhi Ong*, Katarína Smoleňová, Michael Henke and **Winfried Kurth**
Department of Ecoinformatics, Biometrics and Forest Growth, Georg-August University of Göttingen, Büsgenweg 4, 37077 Göttingen, Germany
**correspondence:* yong@gwdg.de

Highlights: An integrated dynamic model of ozone concentration trends, stand dynamics, radiation interception, structural growth, functional systems and molecular pathways is constructed for beech trees. The model composes incomparable spatial decompositions and functional processes in a single graph-based framework. Extensions to the programming language XL for multi-scale rule-based modeling are applied in order to gain insights into the challenges that scale integration poses on language formalisms.

Keywords: XL language, GroIMP platform, multi-scale, up-scaling, down-scaling, *Fagus sylvatica*, ozone

INTRODUCTION

European beech (*Fagus sylvatica*) is one of the most important tree species in central Europe (Scalfi et al. 2004). Models and observations indicate increasing concentrations of tropospheric ozone in Europe since 1996 (Denby et al. 2010). The trends, however, are not consistent throughout Europe. A general north to south gradient in accumulated ozone exposure over a threshold of 40 parts per billion (AOT40) can be seen. Tropospheric ozone triggers oxidative stress responses in the enzymes of the Shikimate pathway (Betz et al. 2009) as well as in protein levels related to the Calvin cycle (Kerner et al. 2011) in beech trees. These responses lead to structural (e.g. leaf lesions) and functional (e.g. photosynthetic capacity) depreciations.

In previous studies, relationships between the environment (in terms of radiation, precipitation and temperature) and trees or stands have been represented in functional-structural models (Sinoquet and Le Roux 2000) mostly at a single spatial and temporal scale level. At the scale of stands, models have been created for the dynamics of competition and dispersion (Kurth et al. 2012). Within the scale of individual trees, structural topology has been decomposed into various scales of representation (Godin and Caraglio 1998), whereas functional models have been re-arranged into multiple aspects (Cieslak et al. 2011). Carbon partitioning and morphological plasticity in beech trees were addressed by a model in Letort et al. (2008). At an even finer scale, studies at the transcript and protein levels of trees have been conducted (Abril et al. 2011). In this study, the dynamics expressed by selected models from different scales are integrated and implemented using the programming language XL with extensions for multi-scale modeling (Ong 2012). The objectives are to gain insights into the non-linear causalities experienced by ozone-exposed beech trees and to address practical challenges and performance issues posed by scale integration.

MODEL DESCRIPTION AND SIMULATION

A partially ordered set, a so-called structure of scales (Fig. 1) is used to represent the inter-scale relationships. The coarsest scale consists of geographical data, light sources and climatic conditions. The second scale describes a stand and includes positional information of trees. A rule-based stand structure model works at this scale. Individual beech trees with aggregated information also reside here. The stand scale is refined into two incomparable scales: the growth unit scale and the crown scale. The crown scale contains collective information of tree crowns and crown layers. The layers contain unique vertical height sections that divide the tree crown one-dimensionally. The crown scale is further refined into an internode scale. The internode scale is adjointly a refinement of the growth unit scale. The crown scale also refines to the metabolic network scale. For reasons of efficiency, we simulate the ozone modulated metabolisms not for each entity in the internode scale separately, but collectively for plant organs in a layer. The model segregates spatial scales but uses a single temporal scale.

A type graph is specified after the structure of scales. The type graph consists of nodes representing the modules (in the sense of the language XL (Kniemeyer 2008)), i.e. the types of objects of each scale in the structure of scales and the allowed relationships between them. More specifically, a unique directed edge type representing a ”refinement” relationship is adopted to relate modules from coarser scales to finer scales. Graph matching and re-writing rules depend on these relationships during intepretation.

The annual mean AOT40 values (in µg m^{-3}.h) of selected locations ranging between northern Europe and southern Europe from the computation results of Denby et al. (2010) are used to initiate separate plots at the environment scale (Fig. 2). Annual sunlight exposure hours and changes to AOT40 are computed in individual plots using rules during simulation.

An irregular and dynamic forest stand structure in the bounded environment is simulated with crown radius dynamics under competition similar to that proposed by Kurth et al. (2012). However, the stand structure model is modified such that individual trees are represented using only singular nodes. The individual trees are further refined into their complete topological structures and crown structures (Fig. 2).

The structural growth of individual beech trees at two scales is simulated. The finer internode scale consists of buds, leaves and internodes while the coarser scale consists of annual growth units (Godin and Caraglio 1998). Photon tracing technique (Hemmerling et al. 2008) is employed to determine the photon flux for each leaf. For each tree, the photon flux per crown layer is computed as the mean photon flux of leaves in the layer. As sun leaves are less responsive to oxidative stress as compared to shade leaves (Olbrich et al. 2010), metabolic processes in crown layers are modulated using the layer's photon flux. Photosynthetic output for each leaf is computed as a result of photon flux on the leaf and a factor of the metabolic state at its residing crown layer and plot node. A transport system based on the implementation by Hemmerling et al. (2008) allows basi-petal transport with allocation and export of carbon assimilates from leaves to organs (buds and internodes). The exported carbon assimilate is redistributed in the tree structure from a common pool using a weighted system (Kang and de Reffye 2007). Secondary growth is modeled based on a pre-allocated percentage for maintenance respiration as well as organ volume (Strobel 2004). The radii of internodes at the base of buds are used to determine the number of primordial leaves formed in the buds (Cochard et al. 2005). Thereafter, the type of growth units (long or short) and number of internodes are determined based on the number of primordial leaves in the buds.

The crown layers are connected to the metabolic network instance via a refinement relationship. The Shikimate pathway is modeled using a multi-scale graph-based representation similar to the implementation in Ong and Kurth (2012) and based on Maus et al. (2011). Four of the seven enzymes in the pathway are induced in response to ozone concentrations (Betz et al. 2009) in the connected macro-scale.

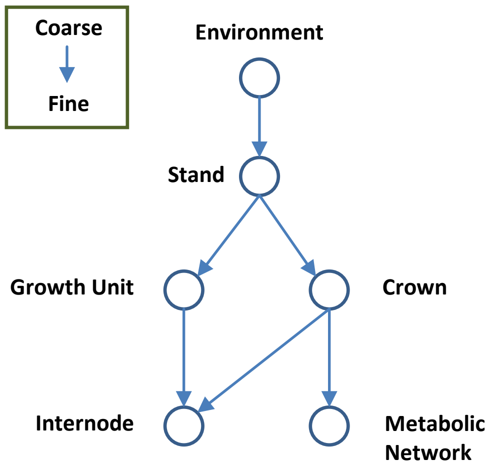

Fig. 1. Structure of scales depicting inter-scale relationships. The circles are abstract representations of the scales in the model.

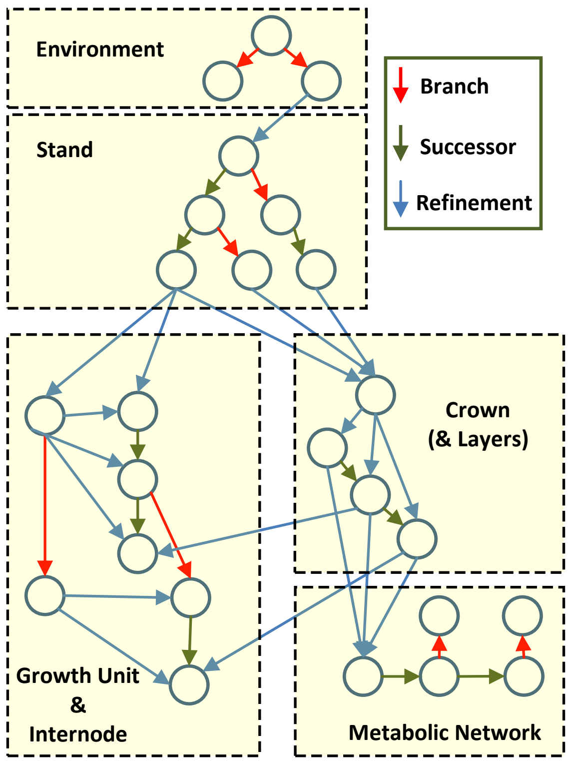

Fig. 2. Illustration of the dynamic graph model. Dotted boxes correspond to scales in the structure of scales. Individual circular nodes are instances of entities. Only important edge connections are shown.

RESULTS AND DISCUSSION

The multi-scale graph model and XL language extensions have enabled scale integration ranging from environmental and stand dynamics to beech functional-structural and metabolic processes. The basic data structure of our model is a directed graph, which is subject to restrictions given by a partially ordered set. This very general model backbone allows to represent scales in a coherent way which are incompatible in terms of refinement (e.g., topology: growth units versus geometry: crown layers). In its current version, our model serves as a proof-of-concept prototype and is not yet validated against field data.

The use of refinement edges between scales mandates customized graph traversal patterns in addition to classical turtle interpretation for graphical interpretation. Such traversal patterns are specified using rules in XL. The model size is computationally demanding and instantiation techniques (Smoleňová et al. 2012) to allow partially-unique trees are potentially useful in this aspect. Lastly, real-time level-of-detail visualization suitable for such increasingly large multi-scaled models is required for interactivity.

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