Trees (2012) 26:1679–1682
DOI 10.1007/s00468-012-0778-4

EDITORIAL

Special topic: integrating modelling and experimentation

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Published online: 4 October 2012

A tendency prevails in plant science that experimentalists while striving for empirical evidence, and modellers as anchored in theoretical grounds, pursue research in separate scientific worlds each, i.e. hardly focus on joint conceptual interfaces in establishing new knowledge. Such a lack of interaction is a crucial impediment in promoting theory on plant and plant systems performance and, hence, persistence. One must bear in mind that theory building is one component within an interacting "magic tripod" of knowledge establishment (Lüttge and Hütt 2009; Lüttge 2013), with the other two "legs" representing empirical research versus abstraction and integration through numeric modelling. Quantitative, process-based and cause-effect related, i.e. mechanistic modelling is of relevance here. The deficit of interaction between experimenting and modelling astonishes, as intrinsically these two scientific domains are coupled in mutualistic ways. The interaction produces beneficial outcome to both of them, quite similar to ecological mutualism as occurring between evolutionarily associated organisms. Experiments provide databases for the algorithmic anchoring of modelling, with the algorithms reaching, to some extent at least, beyond ranges of observation. By this, models become hypotheses to be tested against further empirical evidence. Falsification in turn initiates the next generation of empirical investigations. A "spiral" is promoted which—by further tightening experiment and model development to each other during each turn–is able to consolidate knowledge and theory building. Moreover, verification can be conclusive, if occurring repeatedly under various simulation scenarios (Gayler et al. 2013), as this enhances the reliability of the chain of underlying hypotheses which make up any numeric research model (Priesack et al. 2013). Such models possess the strength of being non-destructive in unveiling evidence, and of supporting the detection of hidden mechanistic relationships or even clarification of seemingly conflicting observations (Gayler et al. 2013), in particular, if factorial scenarios are too complex for experimental assessment. Pre-requisites for such "analytical mutualism" with experimentation are model features that explore and integrate key processes in system functioning across spatio-temporal scales while being dynamic in response to environment and striving for optimization between predictive robustness and coverage of factorial complexity.

One variant of modelling are statistical approaches, in particular, if the scope is to be widened towards assessing the degree of universality of empirical findings. The challenge here is to arrive at respective conclusions if the empirical evidence originates from manifold and contrasting observational scenarios, perhaps even elaborated in the absence of over-arching research concepts. The ultimate outcome of statistical modelling is the identification of such variables, which most distinctly respond to same driving factors under different scenarios. The crucial feature of such approaches is that they can advance beyond the current fashion of asking for hypotheses with all their inherent speculations as a basis for performing and presenting scientific research. *Model-hypotheses* based on algorithms in feedback with experimentation can replace *speculation-hypotheses*. With the statistical modelling in

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the absence of preset hypotheses, information is "learned" from the database about data which are most indicative of the entire dataset (zu Castell et al. 2013). In such ways, the empirical research with its increasingly available huge databases is directed to mechanisms, which are most decisive for the understanding of biological universality.

The need for integrative modelling in close coupling with empirical research has increased, as in parallel the demand for an extended view on "systems biology" has been recognized (Lüttge 2012). Such a view reaches beyond the diverse molecular "omics" concepts, acknowledging the organismic interaction networks in resource flux and information signalling, both plant-internally and at the multi-organismic genotype and species scales of ecosystems (cf. Sandermann and Matyssek 2004). Accordingly, integration is needed, borne by science theory, across experimentation and modelling, with the latter being based on numeric and bio-statistical approaches, as the envisaged dimension of integration is not accomplishable solely through experimental research.

The demand for fostering scientific interaction between experimentalists and modellers within the scope pointed out above raised the motivation of this Special Topic. The topic was inspired also by an almost concurrently published volume of the Springer book series "*Ecological Studies*" (Vol. 220, Matyssek et al. 2013), conceptually pursuing the outlined rationale on the issue of resource flux within and between plants at the system level under the theme of "Growth and Defence in Plants—Resource Allocation at Multiple Scales". The wide scope of the book examining generic principles of allocation in herbaceous and woody plants is focused by this Special Topic on forest trees and ecosystems under scenarios of climate change and air pollution. On such grounds, this Special Topic originates from the EU-funded COST Action FP0903 "*Climate Change and Forest Mitigation and Adaptation in a Polluted Environment*" (MAFor; "http://www.cost-fp0903.ipp.cnr.it"), with the major aims to foster understanding of the ecological state and potential of forests in view of the action title, and in particular, of reconciling related process-oriented research, long-term monitoring and modelling activities. Within such focus, the rationale of unifying experimentation and modelling is accentuated as follows (cf. Matyssek et al. 2012):

1. Emphasis on long-term integration, climatically and edaphically from local to continental dimensions, and long-range transport phenomena of air pollutants within research concepts that orient at the dynamic and multi-factorial nature of environmental scenarios, without neglecting episodic and extreme events;
2. Clarification of variation (i.e. plasticity) in forest tree and ecosystem response to present and presumed future scenarios (i.e. over a wide range of spatio-temporal scales; Mohren et al. 1992, Matyssek et al. 2013) as being linked to biogeochemical processes;
3. Enhancement of robustness in risk assessment through promoting phytotoxically oriented dose–response relationships without neglecting mechanistic grounding of stress avoidance and tolerance (cf. Matyssek et al. 2007, 2008).
4. Derivation of proxies of complex functional interrelationships (Sandermann and Matyssek 2004) allowing integration in model structures and scenario simulations.

In this Special Topic, four publications are gathered that pursue the focused rationale each as outlined above in presenting intrinsic links between empirical research and modelling.

The sequence is opened by Krause et al. (2012) about long-term tracing of catchment ^{15}N additions in a mountainous spruce forest, unifying measurements and model simulations. The latter are yielding long-term projections about the fate of ecosystem-level N accumulation. A substantial role of understory vegetation is recognized in controlling the transfer of deposited N into soil pools, while this additional N uptake resulted in minor effects on ecosystem-level carbon sequestration.

The following two contributions fathom capacities of combining experimentation and modelling in the context of ozone (O_3) risk assessment. By Wieser et al. (2012) this is demonstrated in adult forest trees by use of branch cuvettes for gas exchange analysis. Exploring aspects of branch-level carbon autonomy, cuvette measurements may serve as crown-level surrogates within the scope of defined methodological pre-cautions to consolidate O_3 uptake algorithms and dose–response functions in modelling tree sensitivity. Grünhage et al. (2012) demonstrate advancement of O_3 flux-based risk assessment in adult beech forests by validating the flux-effect prediction of a *soil–vegetation–atmosphere transfer* (SVAT)-type model through a database which was acquired during the 8-year free-air O_3 canopy exposure experiment (Karnosky et al. 2007) conducted at Kranzberg Forest/Germany (Matyssek et al. 2010). Modelled phytotoxic O_3 doses and potential losses in biomass formation were nearly consistent with the outcome using site-unspecific parameterisation, although the analysis indicated high O_3 risk under ambient air. Under experimentally enhanced O_3 exposure, underestimation of the O_3 risk was reflected in comparisons of measured versus modelled ranges of growth limitation.

In the fourth contribution, zu Castell and Ernst (2012) return to address the progress in developing new principles of modelling which are needed for new views on systems biology as alluded to above. In addition to the numeric modelling approaches of the three preceding publications, authors focus on statistical concepts, raising the question of how to analytically cope with the complexity in experimental data at the genome, proteome and metabolome level in relation to whole-tree and ecosystem performance. Conclusions from complexity theory are recalled in view of current approaches in the field of bioinformatics and the demands of extended systems biology. On such grounds, derivation of analytical methodologies is highlighted, capable of coping with the challenge posed by evidential complexity.

Similar to the need for fostering complementarities between empirical research and modelling, empirical databases need to be diversified through innovative experimentation in order to enhance modelling precision (Calfapietra et al. 2009; Matyssek et al. 2012, 2013). To such ends, research projects must be designed from the very beginning as one functional and integrated unity that makes intense interaction between experimentalists and modellers a pre-requisite for accomplishing joint project aims. Hence, more than presenting hypotheses with speculations narrowing the outlook during actual performance of research, a permanent communication on both experimental design and model development is mandatory. This is essential for complying with mutual needs of empirical and modelling work for developing the wide understanding of biological systems as complex as trees and forests and for achieving substantial synergism in knowledge. Merging of the two research domains is a must in view of the global and interrelated impacts of air pollution and climate change on forest ecosystems—so we wish this Special Topic to give impetus to meeting this demand.

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