Ecological Modelling 326 (2016) 177–187

Contents lists available at ScienceDirect

Ecological Modelling

journal homepage: www.elsevier.com/locate/ecolmodel

Structural realism, emergence, and predictions in next-generation ecological modelling: Synthesis from a special issue

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ARTICLE INFO

Article history:
Available online 2 February 2016

Emergence
First principles
Grid-based models
Individual-based models
Parameterization
Pattern-oriented theory development
Prediction
Resilience
Robustness analysis
Standardized submodels
Structural realism
Theory
Trait-based

ABSTRACT

The two main challenges of ecological modelling are to yield more general understanding and theory and to provide testable and robust predictions. To achieve this, emergence, structural realism, and prediction have to become key elements of designing models. In the special issue "Next-generation ecological modelling", which is dedicated to Donald DeAngelis on the occasion of his 70th birthday, 16 contributions present and discuss main features of next-generation ecological modelling. One key feature is to base the description of individuals' behaviour and interactions on first principles rooted in energetic or evolutionary theory. To cope with increasing model complexity, standardization, separate testing of alternative submodels against multiple output patterns, and documenting these tests will be required. Including micro-evolution is essential to capture organisms' response to changing conditions. Functional types may be used instead of species for representing communities. Model analysis will be challenging, but robustness analysis, which tries to break models' explanations, can help to tell signals from noise and identify general mechanisms underlying the internal organization of ecological systems. Ultimately, next-generation modelling should aim at developing general theory to better understand stability properties and mechanisms. This understanding then can provide the basis for restoring, maintaining, or strengthening the resilience of ecosystems and supporting sustainable management of natural resources.

1. Introduction

Developing ecological theory is not an academic exercise. In a world facing unprecedented rates of change in climate, land use, and global interactions, understanding the functioning of ecological systems and forecasting their responses have become critical for ensuring ecosystem services (Millennium Ecosystem Assessment, 2003). We need reliable general concepts and theories that can guide the sustainable use of natural resources. The attempt to devise such theories exclusively via simple strategic modelling, which ignores complexity and imposes system behaviour, did not lead to usable results (Evans et al., 2013a). Likewise, early attempts to embrace complexity in systems simulation models in the 1960s failed (Scheffer and Beets, 1994). The last two decades, however, have seen major advances in developing predictive models that take into account spatial relationships, variability of habitats and resources, individual behaviour, physiology, bioenergetics, and stoichiometry, and that cover multiple levels of organization and scales from local subpopulations via communities to the globe (e.g., Gallien et al., 2010; Evans et al., 2013a; Grimm and Railsback, 2012; Scheiter et al., 2013; De Marchi and Page, 2014; Stillman et al., 2015).

It thus seems that ecological modelling is currently reaching the "next level" towards predictive and re-usable theory that can support environmental decision-making (Evans et al., 2013b), but different sub-disciplines developed their approaches along different pathways. The latter limits coherence and effectiveness in ecological modelling and theory development. We believe that ecological modelling has matured to the point where the following three essential elements of next-generation modelling can be identified: (1) *Structural Realism*, (2) *Emergence* and (3) *Predictions*. For the special issue we invited contributions addressing concepts, modelling approaches, or theories related to these elements.

We considered these elements particularly essential because: (1) Models have to simplify, which requires some tweaking of model structure and parameters (Grimm and Berger, 2016). To

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http://dx.doi.org/10.1016/j.ecolmodel.2016.01.001

what degree, then, does the model capture the organization of the real system, and to which of its details should we pay attention to understand its functioning? We need indicators of *structural realism* and a new culture of communicating them. (2) Imposing empirically observed parameters and functional relationships limits the scope of a model to the conditions under which these parameters and relationships were observed. To allow models to make robust predictions for changing conditions, key processes and behaviours should emerge from lower-level processes, for example from physiological traits, fitness seeking behaviours, or feedbacks between organisms and their abiotic environment. That way we link two or more hierarchical levels of ecosystems and demonstrate the interconnections between mechanisms, structures and overall constraints. In our view, *emergence* is no "hocus-pocus" (Roughgarden, 2012) but a practical and essential aspect of model design. (3) Model outputs are often referred to as *predictions*, even if they result from heavy calibration. A clearer conceptual distinction of calibration, extrapolation, forecasting, and prediction is needed. The latter denotes responses to new conditions, for which no previous data exist. Key questions are: what should ecologists try to predict, and how can we assess the quality of model predictions?

Below we will first distil, from the 16 contributions to this special issue, common and therefore probably essential features of next-generation modelling. We will then discuss how we can cope with the additional complexity that comes with these features. We cannot offer the one and only royal road to ecological modelling of the next decade or more, because the diversity of ecology will continue to exist, often calling for tailored solutions in specific cases. We hope, though, to present general design concepts for modelling and strategies for theory development, which guide future ecologists to start always, independent of their unique system, by asking the same structured sets of questions and to select tools and approaches from a common pool.

With the 16 articles presented here, we of course do not claim to have captured all elements of future ecological modelling and theory. In particular, we did not include, with one exception, analytically formulated models. These models will keep playing an important role in theory development; and we also fully acknowledge their importance for describing essential features of all computational models we are focusing on (e.g., Vincenot et al., 2011; Sibly et al., 2013; Martin et al., 2013; van der Vaart et al., 2016). However, their methodology, mostly based on calculus or matrix algebra, is established and recent trends in applying this methodology are covered well elsewhere (e.g., Mistro et al., 2005; May and McLean, 2007; Hastings, 2011; Morozov, 2013).

2. Essential features of next-generation ecological modelling

Table 1 provides an overview of the contributions to this special issue, including the system and processes addressed, model type used, and specific elements of next-generation ecological modelling discussed. All of these elements are related to the three features of structural realism, emergence, and prediction that we consider essential for next-generation ecological modelling. In the following, we briefly sketch these elements and refer to the contributions to this special issue in which they were addressed; all references in this section to publications from 2016 are from the special issue.

2.1. First principles

A characteristic of classical theoretical ecology is the use of demographic, or vital, rates (e.g., mortality and fecundity) to describe population dynamics depending on age, size, or developmental stage of the organisms. This "demographic thinking" was also adopted in early IBMs, often with demographic rates interpreted as probabilities. For example, mortality was implemented as the probability that an organism does not survive a certain period of time. If data on mortality exist and if the model is used for environmental settings similar to those under which those data were collected, this approach works well with IBMs but is conceptually quite similar to structured models (cf. Nisbet et al., 2016). However, usually we strive to apply models to a wide range of conditions and nowadays also to conditions for which no data exist because they represent new scenarios.

In such situations, modelling key elements of an individual's life cycle from lower hierarchical levels is more appropriate, e.g., modelling mortality as emerging from individual behaviours such as selecting certain habitats and interacting with their biotic and abiotic environment. Vital rates are thereby deduced from "first principles" which translate the current condition of an organism and its environment to behaviours and, eventually, vital rates. These first principles are taken from (1) physics, chemistry, and physiology (Fischer et al., 2016; van der Vaart et al., 2016), or (2) evolutionary theory (Ayllón et al., 2016; Belarde and Railsback, 2016; Eliassen et al., 2016; Stillman et al., 2015, 2016).

It took individual-based modellers, despite the efforts of some pioneers (Kaiser, 1979; Hogeweg and Hesper, 1990; Wolff, 1994; Breckling and Reuter, 1996; Railsback, 2001), more than three decades to overcome the imprinting of "demographic thinking" of classical theory and to accept that more complexity in representing individuals is needed to make IBMs more flexible and predictive. Several contributions to the special issue reflect this trend. In Ayllón et al. (2016), daily habitat selection is based on maximizing a fitness measure which takes into account both growth and mortality risk over a certain future time span. Individuals estimate how they would perform if they chose a certain option assuming that present conditions would remain the same over the next 90 days. This decision, however, is updated every day and leads to realistic behaviours as shown by Railsback and Harvey (2002, 2013).

Four studies focus on the consideration of the energy budget of organisms and foraging decisions for modelling the fate of populations and communities facing changing environmental conditions (Belarde and Railsback, 2016; van der Vaart et al., 2016; Stillman et al., 2016; Eliassen et al., 2016). van der Vaart et al. (2016) present an axiomatic framework for modelling energy budgets (see also Sibly et al., 2013) and thus contribute to the various existing frameworks (e.g., Kooijman, 2010; Martin et al., 2012) which all have different pros and cons that ultimately need to be tested at the population level (Martin et al., 2013; see also the section "Theory development" below).

In contrast to animal ecology where the consideration of energy budgets and adaptive foraging decisions is still on the rise, in plant ecology and vegetation science using first principles has a long tradition and even an established name: "process-based modelling". In the context of "dynamic global vegetation models" (DGVM; Scheiter et al., 2013), this means considering, e.g., photosynthesis, physiology, CO_2 exchange via stomata, etc. This development can be explained by the early focus of vegetation science on predicting the response to changing temperature, precipitation regimes, and CO_2 concentrations in the atmosphere (e.g., Tietjen, 2016). However, process-based vegetation models often address the global scale and are thus too coarse-grained to get the interaction between species right.

Therefore, the approach taken in the forest simulator FORMIND (Huth et al., 1998; Köhler and Huth, 1998; Fischer et al., 2016) is promising and revealing: it is a combination of process-based and individual-based modelling. Interactions between individuals are described, as in the widely used forest gap models (Botkin et al., 1972), via vertical competition for light. First principles are