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

Volker Grimm [a,b,*], Uta Berger [c]

[a] UFZ, Helmholtz Centre for Environmental Research—UFZ, Department of Ecological Modelling, Permoserstr. 15, 04318 Leipzig, Germany
[b] German Centre for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig, Deutscher Platz 5e, 04103 Leipzig, Germany
[c] Institute of Forest Growth and Computer Science, Technische Universität Dresden, PO 1117, 01735 Tharandt, Germany

ARTICLE INFO

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.

© 2016 Elsevier B.V. All rights reserved.

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

* Corresponding author at: Helmholtz Centre for Environmental Research—UFZ, Department of Ecological Modelling, Permoserstr. 15, 04318 Leipzig, Germany. Tel.: +49 341 235 1711.
E-mail address: volker.grimm@ufz.de (V. Grimm).

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

Table 1

Overview of model types and systems presented by the contributions of the special issue and the key elements, strategies, and features of next-generation ecological modelling they address. Some contributions also address issues of general understanding and resilience theory. The models used by Ayllón et al. (2016) and Stillman et al. (2016) use submodels of behaviour which were developed via pattern-oriented theory development (see Section 2.3).

Key elements			Title	System and methods	Model type(s)	Strategies & feautures	Reference[1]
			The effects of model and data complexity on predictions from species distributions models	• Plant or animal populations (generic) • Data vs. model complexity	• Correlative SDM	• Model analysis and parameterization	García-callejas and Araújo (2016)
			Same rainfall amount different vegetation - How environmental conditions and their interactions influence savanna dynamics	• Savanna • Vegetation • Soil • Hydrology	• Grid-based • Eco-hydrological	• Heterogeneous environment	Tietjen (2016)
			Evolutionary trends in fish schools in heterogeneous environments	• Fish schooling • Evolving behaviour from alternative submodels	• IBM • Grid-based	• First principles (energy budgets, foraging) • Adding evolution • Heterogeneous environments	Reuter et al. (2016)
			InSTREAM-Gen: Modelling eco-evolutionary dynamics of trout populations under anthropogenic environmental change	• River • Fish • Hydrodynamics • Habitat selection • Micro-evolution	• IBM • Grid-based • Quantitative genetics	• First principles (adaptive behaviour, energy budgets) • Standard submodels • Adding evolution • Resilience theory (persistence) • Heterogeneous environment	Ayllón et al. (2016)
			New predictions from old theory: Emergent effects of multiplestressors in a model of piscivorous fish	• River • Fish • Hydrodynamics • Habitat selection	• IBM • Grid-based	• First principles (adaptive behaviour, energy budgets) • Standard submodels • Resilience theory (response to multiple stressors) • Heterogenous environment	Belarde and Railsback (2016)
			Community dynamics under environmental change: how can next generation mechanistic models improve projections of species distributions?	• Plant or animal populations (generic) • Standardization	• Process-based SDM[2]	• First principles (local interactions, physiology) • Model analysis and parameterization	Singer et al. (2016)
			Merging trait-based and individual-based modelling: An animal functional type approach to explore the responses of birds to climatic and land use changes in semi-arid African savannas	• Savanna bird community • Animal functional types • Homeranges • Changes in habitat quality (vegetation composition)	• IBM[3] • Grid-based	• First principles (allometry) • Linking trait-based and individual-based modelling • Heterogeneous environment	Scherer et al. (2016)
			From sensing to emergent adaptations: modelling the proximate architecture for decision making	• Animals (generic) • Adaptive behaviour • Evolving submodels • Genetic algorithms	• IBM	• First principles (energy budgets, decision making) • Heterogeneous environments • Standard submodels	Eliassen et al. (2016)
			Integrating ecological insight derived from individual-based simulations and physiologically structured population models	• Animals (generic) • Population cycles Food chain	• Physiologically structured population models • IBM	• First principles (physiology, energy budgets) • Standard submodels	Nisbet et al. (2016)
			Predicting how many animals will be where: How to build, calibrate and evaluate individual-based models	• Animals (generic) • Energy budgets • Parameterization Approximate Bayesian Computing	• IBM • Grid-based	• First principles (energy budgets) • Standard submodels • Model parameterization	van der Vaart et al. (2016)
			Lessons learned from applying a gap model to complex forests and their carbon dynamics	• Tropical rain forests • Plant functional types • Carbon dynamics	• IBM • Trait-based • Grid-based Eco-physiological	• First principles (carbon fluxes) • Standard submodels (gap model)	Fischer et al. (2016)
			Deriving simple predictions from complex models to support environmental decision-making	• Shorebirds and wildfowls • Communication to decision makers • Decision support	• IBM	• First principles (energy budgets, foraging) • Heterogeneous environments • Resilience theory (thresholds)	Stillman et al. (2016)
			Machine learning meets individual-based modelling: self-organising feature maps for the analysis of below-ground competition among plants	• Plant populations (generic) • Inverse process identification	• IBM • SOM (self-organized feature maps)	• Standard submodels (field of neighbourhood) • Model analysis and parameterization	Peters et al. (2016)
			Divide and conquer: configuring submodels for valid and efficient analyses of complex simulation models	• Cascading design of simulation experiments (generic models) • Sheep-wolf-predation (as an example)	• IBM • Grid-based	• Standard submodels (testing)	Lorscheid and Meyer (2016)
			Robustness analysis: Deconstructing computational models forecological theory and applications	• Robustness analysis	• All computational models	• Resilience theory • Standard submodels (development)	Grimm and Berger (2016)
			Defining the next generation modelling of coastal ecotone dynamics in response to global change	• Coastal wetlands • Ecotones • Positive feedbacks	• Grid-based	• Heterogeneous environment • Resilience theory (ecotones)	Jiang et al. (2016)

Rotated left-margin labels (Key elements): Structural realism; Emergence; Predictions; General understanding; Emergence; Resilience; Resilience

[1] Sorted by the first name of the first author.
[2] SDM: species distribution model.
[3] IBM: individual-based model.

reflected via modelling light-dependent photosynthesis and carbon fixation. This architecture made FORMIND applicable to many different tropical forests (Fischer et al., 2016). Parameterization for new sites is challenging for this type of model, requiring stand inventories, light regime measurements, and manual calibration, but can be done in less than a year (A. Huth, *pers. communication*). Modern calibration techniques based on Approximate Bayesian Computing can make parameterization even more efficient (Hartig et al., 2011; Lehmann and Huth, 2015; van der Vaart et al., 2015, 2016).

To summarize: as prediction under new conditions has become a major task of ecological modelling, using first principles is a key element of next-generation ecological modelling whenever individuals and their behaviour are described explicitly. This does not mean that all behaviours have to emerge from first principles because this would make a model unmanageable (Railsback and Grimm, 2012). Models of the future need to be based on the right mix of emergent and imposed behaviours given the questions asked and the data and resources available for model development. The corresponding increase in model complexity could be offset by using standardized submodels (see below) as established and thoroughly tested units (Lorscheid and Meyer, 2016).

2.2. Heterogeneous and dynamic abiotic environments

Grid-based simulation models became popular once the personal computers made sufficient computing power generally available (e.g., Ermentrout and Edelstein-Keshet, 1993; Jeltsch and Wissel, 1994; Jeltsch and Moloney, 2002). In these models, plants are usually not represented as individuals, but via percent cover in a grid cell, or spatial unit, of a certain size (Jiang et al., 2016; Tietjen, 2016). To explicitly represent plants, the "zone-of-influence" approach (Weiner et al., 2001) was established about 15 years ago (e.g., Berger et al., 2008; Peters et al., 2016).

Still, in most of the early spatially explicit models, the interaction between dynamic heterogeneous habitats and the performance of individuals were ignored or represented only implicitly. Next-generation ecological models will have to do better than that because it is this interaction that ultimately determines what we observe in nature and need to understand. Taking into account first principles, rather than "demographic thinking", is the key for modelling this interaction. Several contributions to the special issue demonstrate this. For example, the highly dynamic nature of rivers led to the design of the model InSTREAM-Gen (Ayllón et al., 2016). The depth, flow velocity, temperature, turbidity, predation risk, and competition that trout are exposed to changes constantly. The even-more-dynamic habitat of rivers regulated for hydropower is represented by Belarde and Railsback (2016) as one of two stressors that individual pike minnow must adapt to; cumulative population effects of the stressors emerge from individual behaviour and interactions, including size-based predation as in the bass model of DeAngelis et al. (1980). Tietjen (2016) demonstrates that in vegetation models for regions where water is limited, as in savannas, physical factors affecting water availability, like soil texture and topography, cannot be ignored. The field of ecohydrology is based on this premise, and other fields might follow and focus more on those environmental factors that most limit the performance of individual plants.

Abiotic factors determine individual choices and performance, but what individuals actually do modifies abiotic conditions, affecting the biota in turn. This kind of ecological self-organization is especially prominent in forests and coral reefs, where organisms create the conditions under which they can live, but is present also in virtually all systems at all scales. Ecotones are a result of such interactions, where the response to abiotic conditions, e.g., water level and salinity at coasts, and internal feedback mechanisms

of salt-tolerant and intolerant species, becomes visible in abrupt boundaries between vegetation types (Jiang et al., 2016).

To summarize: including first principles in the models of individuals and their behaviour allows representation of interactions among individuals and their adaptive behaviour in a dynamic environment. Thereby, the same biotic models can be applied to a wide range of regions and environmental conditions. The generic part of next-generation models is thus implemented via the first principles underlying biotic and abiotic processes, while the contingent part emerges from the behaviour and performance of individuals in specific heterogeneous and dynamic environments.

2.3. Theory development: Linking behaviour and physiology to ecology

When ecologists have sought to identify general principles and theories beyond the level of the individual, they developed quite different conceptual frameworks and approaches for different aspects of ecological systems – populations, communities, ecosystems, landscapes – which in turn are diverse by themselves depending on whether the focus is on animals, plants, microbes, and terrestrial, freshwater, or marine systems.

So far, no generally accepted ecological theory has emerged from all these fields. This led Don DeAngelis and co-authors (Huston et al., 1988), and others before them (Łomnicki, 1978; Kaiser, 1979; Uchmański, 1985), to emphasize the fundamental role of individuals when it comes to understand and explain ecological systems. The promise of the individual-based approach was to "unify ecological theory" (Huston et al., 1988), but it took more than two decades before this potential started to unfold (Grimm, 1999). One reason for this lag was the legacy of "demographic thinking" mentioned above; another reason was that general theory was sought at levels beyond the individual. Such theory might still be developed but probably not without being rooted in theories that address the individual level (Evans et al., 2013a, 2013b).

Pattern-oriented theory development (Grimm et al., 2005; Grimm and Railsback, 2012; Railsback and Grimm, 2012) has been suggested as a way forward in this direction: consider an IBM that includes all (a)biotic factors and processes assumed to be essential as a virtual laboratory in which you test alternative models, or theories, of the behaviour of individuals. For testing, compare model output at different hierarchical levels to multiple patterns observed in reality and select the sub-model that performs best. A "theory" in this context is a model of individual behaviour that is good enough to realistically reproduce patterns at the population or community level. In this special issue, again the models of trout (Ayllón et al., 2016) and shorebirds (Stillman et al., 2016; see also Stillman et al., 2015) are the best examples.

Pattern-oriented theory development means to improve models, or theories, of individuals' behaviour and physiology by testing them in their heterogeneous and dynamic environment (Railsback and Grimm, 2012). This enlarges the potential of behavioural and physiological ecology, where theories are mostly tested at the level of individuals, which can limit their usefulness in population contexts (Railsback and Harvey, 2002, 2013). For example, Martin et al. (2013) implemented Dynamic Budget Theory (DEB; Kooijman, 2010) in an IBM of daphnia and found that, to reproduce observations at the population level, the assumption of an energy buffer was not needed. This led to a simplified version of DEB, DEB-KISS (Jager et al., 2013).

There is some controversy in the literature regarding the best way to model energy budgets (Kooijman, 2010; Sibly et al., 2013; van der Vaart et al., 2016) or metabolism (West et al., 1997), but few of these theories have yet been tested in the context of populations in heterogeneous environments. Such tests are critical, though, as demonstrated by Lin et al. (2013, 2014). They found that predictions

of metabolic scaling theory regarding biomass–density relationship in self-thinning stands of plants only hold if competition among individuals is mainly asymmetric and, hence, aboveground. If competition is mainly belowground and symmetric, interactions among individuals can no longer be ignored and metabolic scaling exponents cannot directly be extrapolated to populations or ecosystems.

Theory development also requires use of mathematical approaches in parallel to computational ones. For simple models, powerful analytical techniques and software tools exist to explore and understand system behaviour (Pagel et al., 2008); bifurcation analysis and the implementation of structured models are examples (De Roos et al., 1992). Nisbet et al. (2016) demonstrate how comparing and linking individual-based and physiologically structured population models can facilitate the analysis of cycles emerging in simple food chains.

Most experienced modellers certainly are developing theories of individual behaviour in the way outlined here, but rarely document the process. The experience with models for which theory development was explicit (Stillman et al., 2015) leads us to encourage a culture of documenting how certain submodels are developed and tested. A framework for this documentation is TRACE, a standard format for documenting model development and "evaludation" (Grimm et al., 2014; Augusiak et al., 2014). Instead of presenting models as "just working fine" (Grimm and Berger, 2016), theory development, and also robustness analysis (Grimm and Berger, 2016), should more often be addressed explicitly in next-generation ecological modelling.

2.4. Linking trait-based and individual-based modelling

Trait-based approaches have become very popular in community ecology and vegetation science (McGill et al., 2006; Litchman and Klausmeier, 2008; Suding et al., 2008). This popularity is partly due to the increasing number and volume of trait databases that allow correlation of habitat features with trait values (e.g., Kattge et al., 2011), and partly due to the recognition that, in community ecology, taxonomic units might be less relevant in explaining observed patterns than traits-based features (McGill et al., 2006). So far, though, the practice of trait-based approaches seems to be more correlative than mechanistic.

Two contributions to the special issue demonstrate the great promise of integrating trait-based and individual-based approaches via functional types. The design of FORMIND is based on plant functional types, which constitute certain trait combinations (Fischer et al., 2016). Scherer et al. (2016) use allometric relationships to define, for birds, a set of traits related to body mass, in particular home range size. Together with traits characterizing habitat requirements, they "pack" the home ranges of birds of several species into stylized landscapes with different proportions of habitats needed by the birds; they thereby predict how changes in landscape composition will affect different species. This approach was adopted from Buchmann et al. (2011), who used it for mammals. Currently this approach does not include species interactions or population dynamics, and model predictions still need to be tested.

Nevertheless, the trait-based examples suggest that next-generation ecological modelling will include community models that use the same generic approach for multiple species. The same idea was the basis of the forest gap models, e.g., JABOWA (Botkin et al., 1972) and FORMIND (Köhler and Huth, 1998; Fischer et al., 2016). A further example is the grassland model IBC-Grass (May et al., 2009; Körner et al., 2014; Weiss et al., 2014), in which plant functional types are assembled via permutations of a set of traits and interactions are modelled via the generic zone-of-influence approach (Peters et al., 2016). Community structure and composition are not defined by the modeller, but emerge, starting from ten

seedlings each from 81 plant functional types. A similar approach was used for marine fish communities (Giacomini et al., 2009; Giacomini et al., 2013), in a model with one generic type of size-based trophic interaction, similar to the early fish IBM of DeAngelis et al. (1980).

2.5. Adding microevolution

In ecological models, evolution has usually been ignored because it was believed to run on a different time scale. However, there is now clear evidence that microevolution, i.e. natural selection operating in every generation without necessarily leading to speciation, often cannot be ignored when explaining ecological phenomena (Hairston et al., 2005). In this special issue, microevolution is included in the trout model InSTREAM-Gen (Ayllón et al., 2016).

In IBMs, adding evolution, be it via approaches of population or quantitative genetics, is straightforward because the basic unit of evolution, the individual, is represented in IBMs anyway. This is well demonstrated by Reuter et al. (2016). The model describes a generic fish population where individual fish switch between solitary behaviour and schooling, depending on the foraging efficiency they achieve under a particular spatial and temporal food distribution. The model contributes to a better understanding of the interplay between the adaptation of individual behaviour and environmental settings. This understanding is possible because the energy budgets underlying swimming and reproduction are represented, demonstrating once again the power of models based on first principles.

The challenge, however, is to select the traits allowed to evolve, because making all traits evolvable is unfeasible, both technically and conceptually. Still, the field of eco-evolutionary dynamics is young (Pelletier et al., 2009) and the critical mass of models needed to identify trends and gaps has not yet been achieved. Nevertheless, whenever "evolutionary rescue" of populations can be relevant for their response to, e.g., climate change, next-generation models need to include the option of exploring microevolution (Frank et al., 2011; Piou and Prévost, 2012; Ayllón et al., 2016).

Microevolution can also be used to let adaptive behaviour traits in a model evolve via genetic algorithms. This approach has been used in cases where the modellers could not, or did not want to, come up with rules describing adaptive decisions because the factors and trade-offs affecting these decisions seemed too complicated (Strand et al., 2002). More recently, starting from "hedonic modelling" (Giske et al., 2003), emotions have been represented in such models as they seem to play a big role in how animals make decisions. In this special issue, Eliassen et al. (2016) focus on neurobiological and organismal states linked to emotions like hunger or fear. This approach is promising and might ultimately also lead to better "theories" of human decision-making than those currently used in most agent-based models (An, 2012).

2.6. Standardized submodels

Next-generation ecological models will increasingly have to be based on first principles and represent the heterogeneity and dynamics of abiotic factors. They will thus often be more complex than most models developed so far. In particular, when the role of biodiversity is to be explored, models inherently need to be complex and sometimes even include factors that are not essential in a baseline situation but might become essential under other conditions, thereby avoiding "false exclusions" (Topping et al., 2015).

It took pioneers in this kind of modelling years, sometimes more than a decade of person-years, to develop, parameterize, and test such models (Huth et al., 1998; Topping et al., 2003; Stillman et al., 2015), but in all these cases the huge initial investment paid off

extremely well, as the models then could be used and adopted for a wide range of similar systems and related questions.

Next-generation models will be easier to develop and test than those early "big models" because they can be based on standardized sub-models that use first principles and have been established as "theories" of certain behaviours. For example, the promise of DEB theory (Kooijman, 2010) is that exactly the same energy budget model can be used for all animal species, with only the parameters needing to be determined via fitting the model to growth and reproduction data of individuals. So far, this theory has not been tested very much in the population context (Martin et al., 2012, 2013), and further tests of this and similar theories (Sibly et al., 2013) are needed. There is good hope, though, that in the future we will be able to use standardized sub-models of energy budgets, physiology, and behaviour, which will facilitate model development, testing, and communication. Like today, when it is acceptable to just use established sub-models like Holling's functional responses if we have to describe the behaviour of predators, in the future we should be able to select from two or three established foraging or home range models that have different well-known properties and data requirements.

Perhaps even more important than standardized submodels of individuals are standard models of interactions, because ecology is about interacting, not isolated, individuals. In gap forest models like FORMIND, vertical competition for light is the standard approach (Botkin et al., 1972; Fischer et al., 2016). Grid-based models consider interactions among neighbouring cells (Jiang et al., 2016; Tietjen, 2016). In the zone-of-influence approach, interactions depend on the distance between and size of plants (May et al., 2009; Lin et al., 2013, 2014; Peters et al., 2016). For interactions among animals, the zone-of-influence can also work in models where modelling interactions includes sensing of the presence of competitors (Piou et al., 2007) or potential prey or predators (Schmitz, 2000), or sensing the rank of members in a social hierarchy (Hemelrijk, 1999). Trophic interactions can also be size-based, as often is the case for fish, with large fish eating smaller fish regardless of species (DeAngelis et al., 1980; DeAngelis and Gross, 1992; Shin and Cury, 2001; Giacomini et al., 2009, 2013; Belarde and Railsback, 2016).

To summarize: the coherence, effectiveness, and usefulness of future ecological models depend on the development and establishment of standardized submodels, which include theories of individual behaviour and standard representations of interactions among individuals. "Standardized" means that these submodels can be used for a wide range of species, systems, and environments; with only re-calibration or minor amendments. Particularly important are models of interactions: good new ideas for representing them in a generic way will have huge impact.

2.7. Resilience theory and multiple stressors

Grimm et al. (1999) suggest that IBMs, like probably any complex computational ecological model, should be used more often to address key questions asked also in classical theoretical ecology. In particular, stability properties (Grimm and Wissel, 1997) should be explored more often. They are central "currencies" in ecology because the questions of why ecological systems exist and how they cope with disturbances and change are the most fundamental questions of ecology. Moreover, virtually all of current and future ecology has to deal with the applied question of how ecological systems will respond to new conditions including global and regional changes. Is the capacity of a system large enough to keep it functioning more or less the same, or will it gradually or abruptly change its functioning and, in turn, the services it delivers to humans? Nevertheless, progress in this direction has been very slow, perhaps because computational modellers tend to be ignorant of or not caring about classical theory and its questions.

A good demonstration of how complex models based on first principles, well-tested theories, and a realistic representation of habitat heterogeneity and dynamics can be used to explore stability properties is the study by Belarde and Railsback (2016). They implemented two stressors, man-made flow fluctuations that affect food availability temperature, and an exotic competitor. In a factorial design with six levels per stressor, they compared fish survival over about four months at 28 different sites. They found multiplicative effects of the two stressors in about 70% of the 28×36 cases, and synergistic (stronger than multiplicative) in about 20%, and antagonistic (weaker than multiplicative) in 10%. They could explain these different responses in terms of habitat features that affected the fish and their interactions with exotic competitors in different ways. This study is a unique example of how general principles applied in complex environments can lead to very diverse responses at small scales, so that predicting the overall response depends on detailed knowledge about habitat features. Stillman and Goss-Custard (2010) reach the same level of detailed predictions with their shorebird models, which are also driven by abiotic factors (tides, topography, distribution of different prey species).

Ayllón et al. (2016) model brown trout populations at the edge of their geographic distribution. They then simulated the addition of two stressors: higher temperatures due to climate change, and reduced flows due to land-use change. They then explore whether the populations were able to persist with and without adaptation to new conditions via microevolution. They thus quantified, without explicitly referring to it, resilience, or buffer, mechanisms of small populations.

In contrast, Jiang et al. (2016) explicitly discuss the resilience of the position of the coastal ecotone between tree and grass-dominated vegetation to changes in environmental drivers. They show that both sharp environmental gradients and internal positive feedback mechanisms, where plants modify their environment in favour of themselves, can lead to sharp ecotonal boundaries. They conclude that the response to gradual global change can be quite diverse.

Next-generation ecological modelling has to address questions of stability properties, in particular resilience sensu Holling (1973), more often and more explicitly. Modellers should thus be aware of the basic concepts of resilience theory (Gunderson et al., 2009; Cumming, 2011) and of basic approaches and concepts of classical ecological modelling (Nisbet and Gurney, 1982; Wissel, 1989; DeAngelis, 1992; Nisbet et al., 2016).

2.8. Model analysis and parameterization

As mentioned before, next-generation ecological models will require a certain level of complexity to be useful. It took ecological modelling more than two decades to learn how to cope with this increasing complexity, but there are now many related approaches, as we outlined above: using first principles, developing standardized submodels of individuals and their interaction, addressing the same set of questions about stability properties.

Two more challenges are parameterization and model analysis. Ecological models can easily include tens, and sometimes even more, parameters. If all these had to be determined from scratch for every new model, ecological modelling would grind to a halt. However, standardized submodels can be parameterized separately, sometimes using observations and experiments on individuals. For example, the trout model used by Ayllón et al. (2016) uses many submodels that were parameterized prior to the development of the full model, for example the feeding and growth model. A thorough, separate, analysis of submodels can also reduce the range

of parameter values that need to be taken into account in global sensitivity analyses (Lorscheid and Meyer, 2016).

For the full model, established parameter-fitting methods exist and are straightforward to implement in ready-to-use software packages (Thiele et al., 2014). Ayllón et al. (2016) demonstrate the typical sequence: first, ranges for all parameters are specified. Then screening methods identify the most sensitive parameters and parameter interactions, which then can be calibrated using the existing data and patterns. Then, global analyses of the most important parameters, usually based on efficient sampling of parameter space, can quantify the relative importance of the processes that these parameters represent. To this end, usually thousands of simulations have to be run, which 10 or more years ago would have been prohibitive for models like in InSTREAM-Gen that take 30 min or more per run. However, nowadays most researchers have access to computing clusters so that simulations can be run on hundreds or thousands of CPUs (van der Vaart et al., 2016). Using such clusters will be essential for next-generation ecological modellers.

van der Vaart et al. (2016) and see also van der Vaart et al. (2015) introduce Approximate Bayesian Computing (ABC) as a promising, computing-intensive way of parameterizing complex models. The principles of this approach are based on using prior information about parameters in a more systematic way (Hartig et al., 2011). van der Vaart et al. (2016) demonstrate how ABC works in principle, using the most basic approach, rejection-ABC. However, rejection-ABC is not always very efficient and powerful. Better approaches are under development in this quickly developing field.

A further great promise of ABC was outlined by van der Vaart et al. (2016): if we compare model versions that include alternative submodels to a set of observed patterns to select the best submodel, we are essentially comparing apples to oranges when the submodels have different kinds and numbers of parameters. For statistical models, Akaike's information criterion is a way to account for the difference in complexity of the submodels, but such an accounting for dynamic models was not possible so far (but see Piou et al., 2009).

Rejection-ABC has the advantage that it automatically corrects for differences in model complexity if each model is run equally often (Beaumont, 2010). The more parameters a submodel has, the more sparsely the 'correct' parameter settings will be sampled. More complex models therefore can be selected as best only if the additional parameters indeed increase the overall model's explanatory power (van der Vaart et al., 2016).

A major challenge of complex models is to understand how their main results emerge. Often, this understanding depends on the experience of the modeller, who tested all kinds of alternative model assumptions and settings while developing and testing the model. For example, Belarde and Railsback (2016) and Jiang et al. (2016) explain their main findings very well by using narratives instead of formal analyses. Such narratives can actually be more convincing than complex statistical tests as they put the complex interactions within a model into a more simple and coherent framework. They can also help to communicate the output of complex models to decision makers, in particular when they are related to thresholds or tipping points where certain desired functions or aspects are lost (Stillman et al., 2016).

However, even a model's developer often does not have an intuitive understanding of how its results emerge. Moreover, not all narratives are convincing or robust. Therefore, Grimm and Berger (2016) suggest establishment of robustness analysis as an approach that complements sensitivity analysis. The basic idea is to take a model that reproduces certain desired patterns and therefore "looks fine" and try to destroy its ability to look fine. For very simple models, e.g., the breeding synchrony model of Jovani and Grimm (2008), this can mean replacing simplifying model assumptions with more complex ones, but for most next-generation models

this will mean replacing realistic model settings with simpler or unrealistic ones. For example, the environment can be made more homogeneous or static, or individual behaviour can be represented with simpler submodels. By doing this in a systematic, step-wise way, we can learn which features of our model are in fact essential for reproducing desired patterns. For example, local interactions that determine recruitment in forest gaps can be de-localized to see whether local interaction was important to describe (Rammig and Fahse, 2009; it was). In contrast, Elkin et al. (2012) found that which of three alternative growth models for individual trees was used made no difference at the landscape level but did at smaller scales, in particular in transition zones with changing species composition. Grimm and Berger (2016) argue that the routine exploration of scenarios and submodels that "cannot occur in nature" (Kaiser, 1979) will facilitate understanding complex models and theory development in general.

A further approach for understanding complex models is probably practiced by many modellers, but not communicated very often and therefore probably not done systematically: the separate analysis of submodels. Lorscheid and Meyer (2016) use an educational example to demonstrate how systematic and thorough analysis of submodels should be done (see also Lorscheid et al., 2012). Their recommendation corresponds to the plea for the development of tested and standardized submodels, or theories, outlined above.

Analysis and parameterization of complex models are perhaps the most important challenges of next-generation modelling, but, as many contributions to this special issue show, experience, skills, and techniques have accumulated over recent decades. These challenges should thus not stop us from developing and using the kind of models we actually need if we want to develop both general theory and practical solutions for environmental problems.

2.9. Linking species distribution models to mechanisms

Correlative modelling approaches that link species distribution with the abiotic environment have become so popular that currently the most-cited authors in ecology are the pioneers in this field. The fact that there are standard methods for developing species distribution models (SDM) and parameterizing them with relatively simple presence/absence observations is key to this success story. Criticism of classical, correlative SDM addresses the uncertainty of present ecological niches in changing environments. A simple increase of computational complexity, however, is not sufficient to increase the predictive performance, as shown by García-Callejas and Araújo (2016), who compare five different SDM approaches ranging from envelope methods to vector machines. In contrast, properties of distribution data are strong predictors of model success. This conclusion accounts, e.g., for data containing information about the attraction or inhibition of species in joint habitats (García-Callejas and Araújo, 2016). These signals of biotic interactions are considered by recent SDM approaches targeting mechanistic, process-based description including life histories, physiology, and intra- and interspecific interactions (Singer et al., 2016).

Nevertheless, higher reliability of these models can be only achieved if the newly included processes can be sufficiently parameterized. For this, Singer et al. (2016) propose a modelling protocol that includes (1) a knowledge-based pre-selection of the ecological processes to be included, (2) a combination of direct parameterization and pattern-oriented calibration, (3) a comprehensive test of the model's uncertainty, (4) a feedback loop between simulation experiments and empirical research, and (5) a standardized strategy of documenting the model and communicating the history of the model's tests to improve the transparency and reliability of predictions. Most elements of this protocol are also in other recommendations for good modelling practice (Schmolke et al., 2010;

Grimm et al., 2014), but by being specifically tailored to SDMs they could increase the power of SDM if applied as road map for trans-disciplinary research, as suggested by the authors.

3. Discussion

The features of next-generation ecological modelling discussed in the previous section are all related to the three main topics we chose as the basis for this special issue (Fig. 1). *Emergence* requires that we represent heterogeneous environments and use submodels of key behaviours of individuals (or small spatial units) that are based on first principles. Consequently, pattern-oriented theory development, submodel testing, and the establishment of standardized submodels are needed. If we do these steps well, the ability to make testable predictions emerges naturally, leading to *structural realism*, i.e. a higher chance that our models capture the key aspects of an ecological system's internal organization. We might sometimes need to add micro-evolution, and for community models we might need to use functional types in a trait-based approach instead of taxonomic units such as species. To cope with the increasing complexity of next-generation models, we have techniques for model analysis and parameterization, and ultimately we use those models to go beyond mere predictions and gain general insights about the buffer and recovery mechanisms underlying the resilience of ecological systems.

Ten out of the 16 contributions to the special issue present IBMs as examples. This prevalence of IBMs partly reflects our own background in individual-based modelling, but it also reflects the trend that individual-/agent-based modelling will play a key role in future ecological modelling. Certainly IBMs are not needed

for all systems and questions, as demonstrated nicely by Jiang et al. (2016) and Tietjen (2016), who use grid-based models where system behaviour emerges from the behaviour of small spatial cells. Correlative models will also continue playing an important role. García-Callejas and Araújo (2016) demonstrate the power of species distribution models that are well parameterized with data representing interactions among species.

However, to tackle questions of community ecology and biodiversity research, IBMs will have to play a larger role in the future. Modelling in these fields is still dominated by either correlative approaches or Lotka–Volterra type modelling. The latter is nice for demonstrating ideas and concepts, but has very limited potential for emergence and structural realism. Interestingly, the trait-based approach for community ecology that has been proposed as a new framework (McGill et al., 2006) could easily be implemented by next-generation individual-based modelling. McGill et al. (2006) suggest four themes which are linked by a more physiological approach: (1) Functional traits: they have already been successfully used in IBMs; (2) Environmental gradients: they are readily included in IBMs; (3) Interaction milieu: instead of pair-wise interaction between species, IBMs represent local interactions of individuals in their local environment, which can be highly variable in species, spatial configuration, and specific trait values; (4) Performance currency: instead of summary population-level metrics like the intrinsic rate of increase, which are virtually impossible to determine in reality, physiology-based metrics like energy intake or seed output are suggested. These themes correspond to the "first principle" feature outlined above. The framework of McGill et al. (2006) has been cited many times, but it seems not to have yet produced a major breakthrough in theoretical community ecology. We
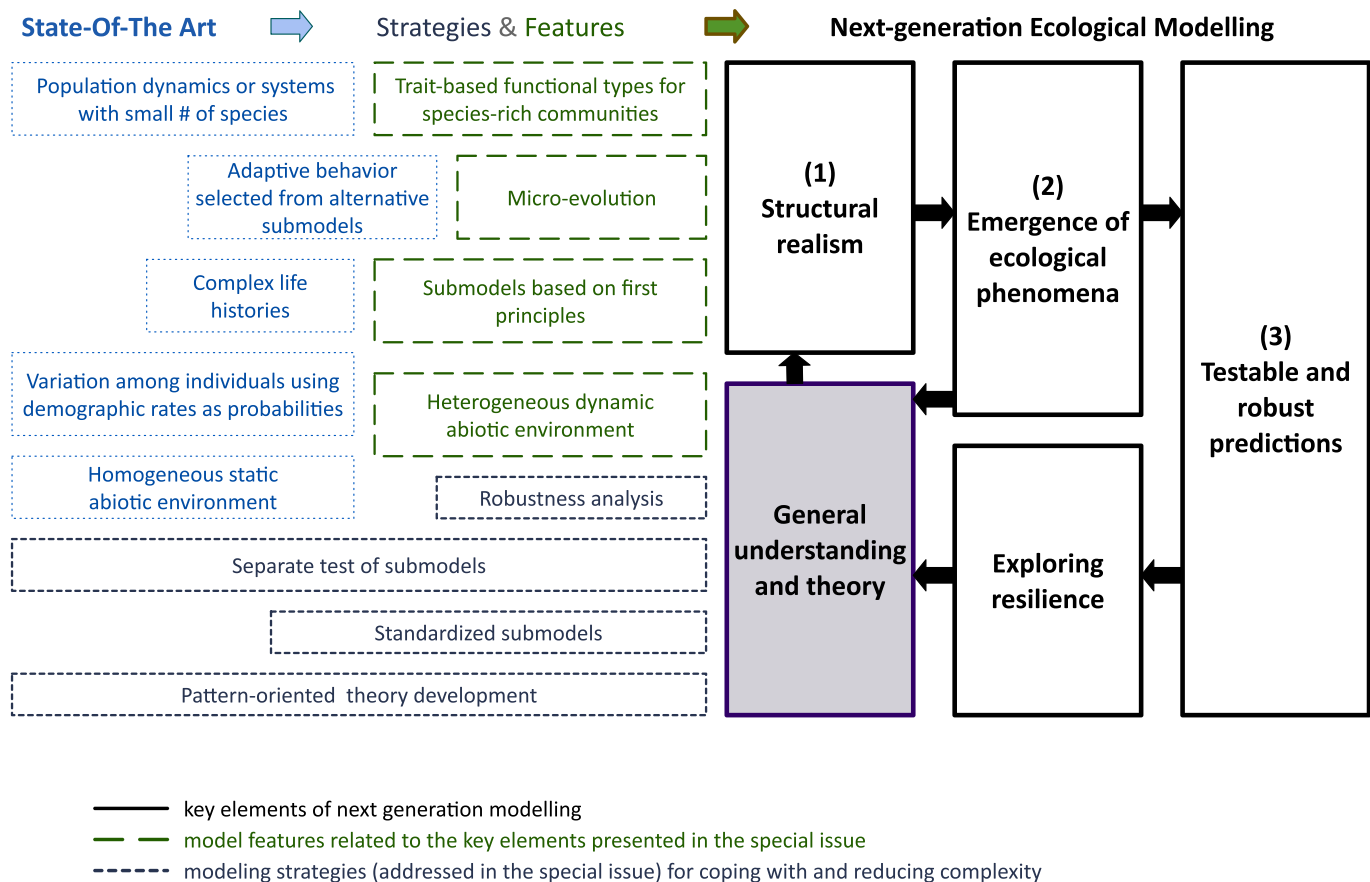

Fig. 1. Strategies and features next-generation ecological modelling, as presented and discussed in the contributions to the special issue. The key elements (1–3) are the basis for this special issue. For detailed discussions of each element, see text.

believe that next-generation modelling as outlined above is needed to put that framework into practice.

A challenge of trait-based approaches is that often trait values are taken more or less arbitrarily from their "permissible" range. Trait values are thereby turned into hidden parameters for model calibration (Scheiter et al., 2013), which can easily make a model structurally unrealistic. This can be prevented by using maximum likelihood estimation of parameter values (Scheiter et al., 2013), or by considering intraspecific trait variation. Moreover, letting community composition emerge from a pool of possible functional types can help avoid the imposition of trait values and combinations (see, e.g., May et al., 2009).

Another challenge for future ecological modelling is to integrate the different modelling approaches that dominate biodiversity and ecosystem research (Loreau, 2010). When modelling biodiversity, focus usually is on composition and structure and thus on organisms. When modelling ecosystems, focus usually is on functions and hence on the flow and pools of nutrients and energy between and in different compartments. To unify ecological theory, structure and function need to be represented at the same time. Both Mokany et al. (2016) and Scheiter et al. (2013) make several important suggestions to achieve this unification but do not arrive at the same conclusion we are drawing from this special issue: to unify ecological theory, next-generation individual-based or grid-based models as outlined above will be needed. Individual-organisms are the building blocks of ecological phenomena, they are the only ecological unit to which first principles from physics, chemistry and evolutionary can be linked, and they can include state variables that represent both structural and functional traits. A good example is the forest model FORMIND which has been used to address both questions related to biodiversity, for example of bird communities inhabiting a forest, and function, for example the effect of forest fragmentation on standing carbon stocks (Fischer et al., 2016).

The most important challenge of next-generation modelling is to devise general theory and understanding. How certain dynamics emerge in complex models can be hard to understand, leading to the stereotype they are "as hard to understand as nature". This stereotype is, like many others, completely wrong. Even complex models are much simpler than reality and, most importantly, can be manipulated in all aspects and completely observed—both of which are certainly impossible in nature. Still, we need more in-depth model analyses. Global sensitivity analysis is one important approach, but we argue that robustness analysis is an essential complementary approach (Grimm and Berger, 2016).

In general, the analysis of next-generation models should address the big questions of ecology regarding: stability properties, including resilience, and their underlying mechanisms; the role of biodiversity; and how ecosystem services can be ensured for future generations. Though it might seem that we just advocate making models even more complex, our ultimate aim is simplicity: general concepts and theories that support a more comprehensive understanding of ecological systems so that they can be managed and used in more sustainable ways. We believe, though, that ecological modelling and theory first need to embrace, not ignore, complexity. The roadmap for the future has been characterized by Topping et al. (2015) by using the Latin proverb "Per aspera ad astra"—through the hardships of complex modelling to the stars of predictive general theory.

Acknowledgments

References

An, L., 2012. Modeling human decisions in coupled human and natural systems: review of agent-based models. Ecol. Modell. 229, 25–36.

Augusiak, J., Van den Brink, P.J., Grimm, V., 2014. Merging validation and evaluation of ecological models to 'evaluation': a review of terminology and a practical approach. Ecol. Modell. 280, 117–128.

Ayllón, D., Railsback, S.F., Vincenzi, S., Groeneveld, J., Almodóvar, A., Grimm, V., 2016. InSTREAM-Gen: modelling eco-evolutionary dynamics of trout populations under anthropogenic environmental change. Ecol. Modell. 326, 36–53.

Beaumont, M.A., 2010. Approximate Bayesian computation in evolution and ecology. Annu. Rev. Ecol. Evol. Syst. 41, 379–406.

Belarde, T.A., Railsback, S.F., 2016. New predictions from old theory: emergent effects of multiple stressors in a model of piscivorous fish. Ecol. Modell. 326, 54–62.

Berger, U., Piou, C., Schiffers, K., Grimm, V., 2008. Competition among plants: concepts, individual-based modelling approaches, and a proposal for a future research strategy. Perspect. Plant Ecol. Evol. Syst. 9, 121–135.

Botkin, D.B., Janak, J.F., Wallis, J.R., 1972. Some ecological consequences of a computer model of forest growth. J. Ecol. 60, 849–872.

Buchmann, C.M., Schurr, F.M., Nathan, R., Jeltsch, F., 2011. An allometric model of home range formation explains the structuring of animal communities exploiting heterogeneous resources. Oikos 120, 106–118.

Breckling, B., Reuter, H., 1996. The use of individual based models to study the interaction of different levels of organization in ecological systems. Senck. Marit. 27, 195–206.

Cumming, G.S., 2011. Spatial Resilience in Social-Ecological Systems. Springer, London.

De Marchi, S., Page, S.E., 2014. Agent-based models. Annu. Rev. Polit. Sci. 17, 1–20.

De Roos, A.M., Diekmann, O., Metz, J.A.J., 1992. Studying the dynamics of structured population models: a versatile technique and its application to Daphnia. Am. Nat. 139, 123–147.

DeAngelis, D.L., Cox, D.K., Coutant, C.C., 1980. Cannibalism and size dispersal in young-of-the-year largemouth bass: experiment and model. Ecol. Modell. 8, 133–148.

DeAngelis, D.L., 1992. Dynamics of Nutrient Cycling and Food Webs. Chapman and Hall, New York, NY.

DeAngelis, D.L., Gross, L.J., 1992. Individual-based Models and Approaches in Ecology: Populations, Communities and Ecosystems. Chapman Hall, New York, NY.

Eliassen, S., Andersen, B.S., Jørgensen, C., Giske, J., 2016. From sensing to emergent adaptations: modelling the proximate architecture for decision-making. Ecol. Modell. 326, 90–100.

Elkin, C., Reineking, B., Bigler, C., Bugmann, H., 2012. Do small-grain processes matter for landscape scale questions? Sensitivity of a forest landscape model to the formulation of tree growth rate. Landscape Ecol. 27, 697–711.

Ermentrout, G.B., Edelstein-Keshet, L., 1993. Cellular automata approaches to biological modeling. J. Theor. Biol. 160, 97–133.

Evans, M.R., Bithell, M., Cornell, S., Dall, S.R.X., Diaz, S., Emmott, S., Ernande, B., Grimm, V., Hodgson, D.J., Lewis, S.L., Mace, G.M., Morecroft, M., Moustakas, A., Murphy, E., Newbold, T., Petchey, O., Smith, M., Travis, J.M.J., Benton, T.G., 2013a. Predictive systems ecology. Proc. R. Soc. London, Ser. B: Biol. 280, 1452.

Evans, M.R., Grimm, V., Johst, K., Knuuttila, T., de Langhe, R., Lessells, C.M., Merz, M., O'Malley, M.A., Orzack, S.H., Weisberg, M., Wilkinson, D.J., Wolkenhauer, O., Benton, T.G., 2013b. Do simple models lead to generality in ecology? Trends Ecol. Evol. 28, 578–583.

Fischer, R., Bohn, F., Dantas de Paula, M., Dislich, C., Groeneveld, J., Gutiérrez, A.G., Kazmierczak, M., Knapp, N., Lehmann, S., Paulick, S., Pütz, S., Roedig, E., Taubert, F., Köhler, P., Huth, A., 2016. Lessons learned from applying a gap model to complex forests and their carbon dynamics. Ecol. Modell. 326, 124–133.

Frank, B.M., Piccolo, J.J., Baret, P.V., 2011. A review of ecological models for brown trout: towards a new demogenetic model. Ecol. Freshwater Fish 20, 167–198.

Gallien, L., Münkemüller, T., Albert, C.H., Boulangeat, I., Thuiller, W., 2010. Predicting potential distributions of invasive species: where to go from here? Diversity Distributions 16, 331–342.

García-Callejas, D., Araújo, M.B., 2016. The effects of model and data complexity on predictions from species distributions models. Ecol. Modell. 326, 4–12.

Giacomini, H.C., De Marco, P., Petrere, M., 2009. Exploring community assembly through an individual-based model for trophic interactions. Ecol. Modell. 220, 23–39.

Giacomini, H.C., DeAngelis, D.L., Trexler, J.C., Petrere, M., 2013. Trait contributions to fish community assembly emerge from trophic interactions in an individual-based model. Ecol. Modell. 251, 32–43.

Giske, J., Mangel, M., Jakobsen, P., Huse, G., Wilcox, C., Strand, E., 2003. Explicit trade-off rules in proximate adaptive agents. Evol. Ecol. Res. 5, 835–865.

Grimm, V., Wissel, C., 1997. Babel, or the ecological stability discussions: an inventory and analysis of terminology and a guide for avoiding confusion. Oecologia 109, 323–334.

Grimm, V., 1999. Ten years of individual-based modelling in ecology: what have we learned and what could we learn in the future? Ecol. Modell. 115, 129–148.

Grimm, V., Wyszomirski, T., Aikman, D., Uchmański, J., 1999. Individual-based modelling and ecological theory: synthesis of a workshop. Ecol. Modell. 115, 275–282.

Grimm, V., Revilla, E., Berger, U., Jeltsch, F., Mooij, W.M., Railsback, S.F., Thulke, H.-H., Weiner, J., Wiegand, T., DeAngelis, D.L., 2005. Pattern-oriented modeling of agent-based complex systems: lessons from ecology. Science 310, 987–991.

Grimm, V., Railsback, S.F., 2012. Pattern-oriented modelling: a 'multi-scope' for predictive systems ecology. Philos. Trans. R. Soc. London, Ser. B 367, 298–310.

Grimm, V., Augusiak, J., Focks, A., Frank, B.M., Gabsi, F., Johnston, A.S.A., Liu, C., Martin, B.T., Meli, M., Radchuk, V., Thorbek, P., Railsback, S.F., 2014. Towards better modelling and decision support: documenting model development, testing, and analysis using TRACE. Ecol. Modell. 280, 129–139.

Grimm, V., Berger, U., 2016. Robustness analysis: deconstructing computational models for ecological theory and applications. Ecol. Modell. 326, 162–167.

Gunderson, L.H., Allen, C.R., Holling, C.S., 2009. Foundations of Ecological Resilience. Island Press, Washington.

Hairston, N.G., Ellner, S.P., Geber, M.A., Yoshida, T., Fox, J.A., 2005. Rapid evolution and the convergence of ecological and evolutionary time. Ecol. Lett. 8, 1114–1127.

Hartig, F., Calabrese, J.M., Reineking, B., Wiegand, T., Huth, A., 2011. Statistical inference for stochastic simulation models–theory and application. Ecol. Lett. 14, 816–827.

Hastings, A., 2011. Introduction to the Simon Levin 70th birthday special issue of theoretical ecology. Theor. Ecol. 4, 111.

Hemelrijk, C.K., 1999. An individual-orientated model of the emergence of despotic and egalitarian societies. Proc. R. Soc. London, Ser. B: Biol. 266, 361–369.

Holling, C.S., 1973. Resilience and stability of ecological systems. Annu. Rev. Ecol. Evol. Syst. 4, 1–23.

Hogeweg, P., Hesper, B., 1990. Individual-oriented modelling in ecology. Math. Comput. Modell. 13, 83–90.

Huth, A., Ditzer, T., Bossel, H., 1998. The Rain Forest Growth Model FORMIX3-Model Description and Analysis of Forest Growth and Logging Scenarios for the Deramakot Forest Reserve (Malaysia). Erich Goltze Publishers, Göttingen.

Huston, M., DeAngelis, D., Post, W., 1988. New computer models unify ecological theory. BioScience 38, 682–691.

Jager, T., Martin, B.T., Zimmer, E.I., 2013. DEBkiss or the quest for the simplest generic model of animal life history. J. Theor. Biol. 328, 9–18.

Jeltsch, F., Wissel, C., 1994. Modelling dieback phenomena in natural forests. Ecol. Modell. 75, 111–121.

Jeltsch, F., Moloney, K.A., 2002. Spatially explicit vegetation models: what have we learned? Prog. Bot. 63, 326–343.

Jiang, J., DeAngelis, D.L., Teh, S.-Y., Krauss, K.W., Wang, H., Li, H., Smith III, T.J., Koh, H.-L., 2016. Defining the next-generation modeling of coastal ecotone dynamics in response to global change. Ecol. Modell. 326, 168–176.

Jovani, R., Grimm, V., 2008. Breeding synchrony in colonial birds: from local stress to global harmony. Proc. R. Soc. London, Ser. B: Biol. 275, 1557–1564.

Kaiser, H., 1979. The dynamics of populations as result of the properties of individual animals. Fortschritte der Zoologie 25, 109–136.

Kattge, J., Díaz, S., Lavorel, S., Prentice, I.C., Leadley, P., Bönisch, G., Garnier, E., Westoby, M., Reich, P.B., Wright, I.J., Cornelissen, J.H.C., Violle, C., Harrison, S.P., Bodegom, B.M.V., Reichstein, M., Enquist, B.J., Soudzilovskaia, N.A., Ackerly, D.D., Anand, M., Atkin, O., Bahn, M., Baker, T.R., Baldocchi, D., Bekker, R., Blanco, C.C., Blonder, B., Bond, W.J., Bradstock, R., Bunker, D.E., Casanoves, F., Cavender-Bares, J., Chambers, J.Q., Chapin, F.S., Chave, J., Coomes, D., Cornwell, W.K., Craine, J.M., Dobrin, B.H., Duarte, L., Durka, W., Elser, J., Esser, G., Estiarte, M., Fagan, W.F., Fang, J., Fernández-Méndez, F., Fidelis, A., Finegan, B., Flores, O., Ford, H., Frank, D., Freschet, G.T., Fyllas, N.M., Gallagher, R.V., Green, W.A., Gutierrez, A.G., Hickler, T., Higgins, S., Hodgson, J.G., Jalili, A., Jansen, S., Joly, C., Kerkhoff, A.J., Kirkup, D., Kitajima, K., Laughlin, D., Lee, T.D., Leishman, M., Lens, F., Lenz, T., Lewis, S.L., Lloyd, J., Llusià, J., Louault, F., Ma, S., Mahecha, M.D., Manning, P., Massad, T., Medlyn, B., Messier, J., Moles, A.T., Müller, S.C., Nadrowski, K., Naeem, S., Niinemets, Ü., Nöllert, S., Nüske, A., Ogaya, R., Oleksyn, J., Onipchenko, V.G., Onoda, Y., Ordoñez, J., Overbeck, G., Ozinga, W.A., Paula, S., Pausas, J.G., Peñuelas, J., Phillips, O.L., Pillar, V., Poorter, H., Poorter, L., Poschlod, P., Prinzing, A., Prolux, R., Rammig, A., Reinsch, S., Reu, B., Sack, L., Salgado-Negret, B., Sardans, J., Shiodera, S., Shipley, B., Siefert, A., Sosinski, E., Soussana, J.-F., Swaine, E., Swenson, N., Thompson, K., Thornton, P., Waldram, M., Weiher, E., White, M., White, S., Wright, S.J., Yguel, B., Zaehle, S., Zanne, A.E., Wirth, C., 2011. TRY—a global database of plant traits. Global Change Biol. 17, 2905–2935.

Köhler, P., Huth, A., 1998. The effects of tree species grouping in tropical rainforest modelling: simulations with the individual-based model FORMIND. Ecol. Modell. 109, 301–321.

Körner, K., Pfestorf, H., May, F., Jeltsch, F., 2014. Modelling the effect of belowground herbivory on grassland diversity. Ecol. Modell. 273, 79–85.

Kooijman, S.A.L.M., 2010. Dynamic Energy Budget Theory for Metabolic Organisation. Cambridge University Press, Cambridge.

Lehmann, S., Huth, A., 2015. Fast calibration of a dynamic vegetation model with minimum observation data. Ecol. Modell. 301, 98–105.

Litchman, E., Klausmeier, C.A., 2008. Trait-based community ecology of phytoplankton. Annu. Rev. Ecol. Evol. Syst. 39, 615–639.

Lin, Y., Berger, U., Grimm, V., Huth, F., Weiner, J., 2013. Plant interactions alter the predictions of metabolic scaling theory. PLoS ONE 8, e57612, http://dx.doi.org/10.1371/journal.pone.0057612.

Lin, Y., Huth, F., Berger, U., Grimm, V., 2014. The role of belowground competition and plastic biomass allocation in altering plant mass–density relationships. Oikos 123, 248–256.

Łomnicki, A., 1978. Individual differences between animals and the natural regulation of their numbers. J. Anim. Ecol. 47, 461–475.

Loreau, M., 2010. Linking biodiversity and ecosystems: towards a unifying ecological theory. Philos. Trans. R. Soc. London, Ser. B 365, 49–60.

Lorscheid, I., Heine, B.O., Meyer, M., 2012. Opening the 'black box' of simulations: increased transparency and effective communication through the systematic design of experiments. Comput. Math. Organ. Theor. 18, 22–62.

Lorscheid, I., Meyer, M., 2016. Divide and conquer: configuring submodels for valid and efficient analyses of complex simulation models. Ecol. Modell. 326, 152–161.

Martin, B.T., Zimmer, E.I., Grimm, V., Jager, T., 2012. Dynamic Energy Budget theory meets individual-based modelling: a generic and accessible implementation. Method. Ecol. Evol. 3, 445–449.

Martin, B.T., Jager, T., Nisbet, R.M., Preuss, T.G., Grimm, V., 2013. Predicting population dynamics from the properties of individuals: a cross-level test of Dynamic Energy Budget theory. Am. Nat. 181, 506–519.

May, F., Grimm, V., Jeltsch, F., 2009. Reversed effects of grazing on plant diversity: the role of below-ground competition and size symmetry. Oikos 118, 1830–1843.

May, R.M., McLean, A. (Eds.), 2007. Theoretical Ecology: Principles and Applications. Oxford University Press, Oxford.

McGill, B.J., Enquist, B.J., Weiher, E., Westoby, M., 2006. Rebuilding community ecology from functional traits. Trends Ecol. Evol. 21, 178–185.

Mistro, D.C., Rodrigues, L.A.D., Brazil, A.S., 2005. Special issue on theoretical ecology and mathematical modelling: problems and methods. Ecol. Modell. 188, 499–500.

Millennium Ecosystem Assessment, 2003. Ecosystems and Human Well-being. Island Press, Washington.

Mokany, K., Ferrier, S., Connolly, S.R., Dunstan, P.K., Fulton, E.A., Harfoot, M.B., Harwood, T.D., Richardson, A.J., Roxburgh, S.H., Scharlemann, J.P.W., Tittensor, D.P., Westcott, D.A., Wintle, B.A., 2016. Integrating modelling of biodiversity composition and ecosystem function. Oikos 125 (1), 10–19, http://dx.doi.org/10.1111/oik.02792.

Morozov, A., 2013. Mathematical modelling in theoretical ecology: introduction to the special issue. Math. Modell. Nat. Phenom. 8, 1–4.

Nisbet, R.M., Gurney, W., 1982. Modelling Fluctuating Populations. Wiley, Chichester.

Nisbet, R.M., Martin, B.T., de Roos, A.M., 2016. Integrating ecological insight derived from individual-based simulations and physiologically structured population models. Ecol. Modell. 326, 101–112.

Pagel, J., Fritzsch, K., Biedermann, R., Schröder, B., 2008. Annual plants under cyclic disturbance regime: better understanding through model aggregation. Ecol. Appl. 18, 2000–2015.

Pelletier, F., Garant, D., Hendry, A.P., 2009. Eco-evolutionary dynamics. Philos. Trans. R. Soc. London, Ser. B 364, 1483–1489.

Peters, R., Lin, Y., Berger, U., 2016. Machine learning meets individual-based modelling: self-organising feature maps for the analysis of below-ground competition among plants. Ecol. Modell. 326, 142–151.

Piou, C., Berger, U., Hildenbrandt, H., Grimm, V., Diele, K., D'Lima, C., 2007. Simulating cryptic movements of a mangrove crab: recovery phenomena after small scale fishery. Ecol. Modell. 205, 110–122.

Piou, C., Berger, U., Grimm, V., 2009. Proposing an information criterion for individual-based models developed in a pattern-oriented modelling framework. Ecol. Modell. 220, 1957–1967.

Piou, C., Prévost, E., 2012. A demo-genetic individual-based model for Atlantic salmon populations: model structure, parameterization and sensitivity. Ecol. Modell. 231, 37–52.

Railsback, S.F., 2001. Concepts from complex adaptive systems as a framework for individual-based modelling. Ecol. Modell. 139, 47–62.

Railsback, S.F., Harvey, B.C., 2002. Analysis of habitat-selection rules using an individual-based model. Ecology 83, 1817–1830.

Railsback, S.F., Grimm, V., 2012. Agent-Based and Individual-Based Modeling: A Practical Introduction. Princeton University Press, Princeton, NJ.

Railsback, S.F., Harvey, B.C., 2013. Trait-mediated trophic interactions: is foraging theory keeping up? Trends Ecol. Evol. 28, 119–125.

Rammig, A., Fahse, L., 2009. Simulating forest succession after blowdown events: the crucial role of space for a realistic management. Ecol. Modell. 220, 3555–3564.

Reuter, H., Kruse, M., Rovellini, A., Breckling, B., 2016. Evolutionary trends in fish schools in heterogeneous environments. Ecol. Modell. 326, 23–35.

Roughgarden, J., 2012. Individual Based Models in Ecology: An Evaluation, or How Not to Ruin a Good Thing. Paper presented at the Philosophy of Science Association Biennial Meeting San Diego, California, ⟨http://philsci-archive.pitt.edu/9434/1/RoughgardenPSA2012IBMLecture.pdf⟩.

Scheiter, S., Langan, L., Higgins, S.I., 2013. Next-generation dynamic global vegetation models: learning from community ecology. New Phytol. 198, 957–969.

Scherer, C., Jeltsch, F., Grimm, V., Blaum, N., 2016. Merging trait-based and individual-based modelling: an animal functional type approach to explore the responses of birds to climatic and land use changes in semi-arid African savannas. Ecol. Modell. 326, 75–89.

Schmitz, O.J., 2000. Combining field experiments and individual-based modeling to identify the dynamically relevant organizational scale in a field system. Oikos 89, 471–484.

Shin, Y.J., Cury, P., 2001. Exploring fish community dynamics through size-dependent trophic interactions using a spatialized individual-based model. Aquat. Living Res. 14, 65–80.

Sibly, R.M., Grimm, V., Martin, B.T., Johnston, A.S., Kułakowska, K., Topping, C.J., Calow, P., Nabe-Nielsen, J., Thorbek, P., DeAngelis, D.L., 2013. Representing the acquisition and use of energy by individuals in agent-based models of animal populations. Method. Ecol. Evol. 4, 151–161.

Stillman, R.A., Goss-Custard, J.D., 2010. Individual-based ecology of coastal birds. Biol. Rev. 85, 413–434.

Stillman, R.A., Railsback, S.F., Giske, J., Berger, U., Grimm, V., 2015. Making predictions in a changing world: the benefits of individual-based ecology. BioScience 65, 140–150.

Stillman, R.A., Wood, K.A., Goss-Custard, J.D., 2016. Deriving simple predictions from complex models to support environmental decision-making. Ecol. Modell. 326, 134–141.

Strand, E., Huse, G., Giske, J., 2002. Artificial evolution of life history and behavior. Am. Nat. 159, 624–644.

Suding, K.N., Lavorel, S., Chapin, F.S., Cornelissen, J.H.C., Díaz, S., Garnier, E., Goldberg, D., Hooper, D.U., Jackson, S.T., Navas, M.L., 2008. Scaling environmental change through the community-level: a trait-based response-and-effect framework for plants. Global Change Biol. 14, 1125–1140.

Scheffer, M., Beets, J., 1994. Ecological models and the pitfalls of causality. Hydrobiologia 275/276, 115–124.

Schmolke, A., Thorbek, P., DeAngelis, D.L., Grimm, V., 2010. Ecological models supporting environmental decision making: a strategy for the future. Trends Ecol. Evol. 25, 479–486.

Singer, A., Johst, K., Banith, T., Fowler, M.S., Groeneveld, J., Gutiérrez, A.G., Hartig, F., Krug, R.M., Liess, M., Matlack, G., Meyer, K.M., Pe'er, G., Radchuk, V., Voinopul-Sassu, A.-J., Travis, J.M., 2016. Community dynamics under environmental change: how can next-generation mechanistic models improve projections of species distributions? Ecol. Modell. 326, 63–74.

Thiele, J.C., Kurth, W., Grimm, V., 2014. Facilitating parameter estimation and sensitivity analysis of agent-based models: a cookbook using NetLogo and 'R'. J. Artif. Soc. Soc. Simul. 17 (3), 11, http://jasss.soc.surrey.ac.uk/15/3/8.html.

Tietjen, B., 2016. Same rainfall amount different vegetation—how environmental conditions and their interactions influence savanna dynamics. Ecol. Modell. 326, 13–22.

Topping, C.J., Hansen, T.S., Jensen, T.S., Jepsen, J.U., Nikolajsen, F., Odderskær, P., 2003. ALMaSS, an agent-based model for animals in temperate European landscapes. Ecol. Modell. 167, 65–82.

Topping, C.J., Alrøe, H.F., Farrell, K.N., Grimm, V., 2015. Per aspera ad astra: through complex population modeling to predictive theory. Am. Nat. 186, 669–674.

Uchmański, J., 1985. Differentiation and frequency distributions of body weights in plants and animals. Philos. Trans. R. Soc. London, Ser. B 310, 1–75.

van der Vaart, E., Beaumont, M.A., Johnston, A.S., Sibly, R.M., 2015. Calibration and evaluation of individual-based models using Approximate Bayesian Computation. Ecol. Modell. 312, 182–190.

van der Vaart, E., Johnston, A.S., Sibly, R.M., 2016. Predicting how many animals will be where: how to build, calibrate and evaluate individual-based models. Ecol. Modell. 326, 113–123.

Vincenot, C.E., Giannino, F., Rietkerk, M., Moriya, K., Mazzoleni, S., 2011. Theoretical considerations on the combined use of system dynamics and individual-based modeling in ecology. Ecol. Modell. 222, 210–218.

Weiner, J., Stoll, P., Muller-Landau, H., Jasentuliyana, A., 2001. The effects of density, spatial pattern, and competitive symmetry on size variation in simulated plant populations. Am. Nat. 158, 438–450.

Weiss, L., Pfestorf, H., May, F., Körner, K., Boch, S., Fischer, M., Müller, J., Prati, D., Socher, S.A., Jeltsch, F., 2014. Grazing response patterns indicate isolation of semi-natural European grasslands. Oikos 123, 599–612.

West, G.B., Brown, J.H., Enquist, B.J., 1997. A general model for the origin of allometric scaling laws in biology. Science 276, 122–126.

Wissel, C., 1989. Theoretische Ökologie: Eine Einführung. Springer, Heidelberg.

Wolff, W.F., 1994. An individual-oriented model of a wading bird nesting colony. Ecol. Modell. 72, 75–114.